CONFERENCE PROGRAM

Additional front matter information will be available with the Program Overview Booklet distributed at the conference.

This program was created on April 21, 2025 and is subject to change (e.g. presenter changes, oral presentation alternates, and more). The intention of this static document is as a resource for those who prefer not to use the Online Planner or Mobile App. The Online Planner and Mobile App will be "the" up-to-date source for detailed program information.

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PROGRAM OVERVIEW

SATURDAY, MAY 31 , 2025

9:00 am - 5:00 pm **Short Courses - ADV. REG IS REQUIRED. Course registration closes May 23.**

SUNDAY, JUNE 1, 2025

9:00 am - 5:00 pm **Short Courses - ADV. REG IS REQUIRED. Course registration closes May 23.**

9:00 am - 8:00 pm **Check-in and badge printing**

5:00 - 6:30 pm **Tutorial Lectures, Hall AB**

- 5:00 pm - Lisa Jones (UC San Diego): Hydroxyl Radical Protein Footprinting for Studying Higher Order Structure
- 5:45 pm - Shane Tichy (Agilent Technologies): Creating Tomorrow: The Art & Science of New Product Introductions (NPI)

6:45 - 7:45 pm **Opening Session, Carlito Lebrilla, presiding, Hall AB**
Opening Plenary Lecture: Selena Ahmed (PTFI): The Periodic Table of Food Initiative (PTFI): Mapping Food Quality of the Planet's Edible Biodiversity

7:45 - 9:00 pm **Welcome Reception, Exhibit-Poster Hall**

MONDAY, JUNE 2, 2025

7:30 am - 5:00 pm **Check-in and badge printing**

7:00 - 8:15 am **Corporate Member Breakfast Seminars, Convention Center AND Hilton Baltimore**

8:30 - 10:30 am **Oral Sessions (eight parallel sessions)**

- MOA am: Quantitative Proteomics: Instrumentation and Applications, Hall AB
- MOB am: Plants and Natural Products, Room 307-308
- MOC am: Instrumentation: Detection of High-Mass Analytes, Room 309-310
- MOD am: Metabolomics and Lipidomics: New Technologies and Applications, Room 314-317
- MOE am: Drug Discovery and Development: Qualitative and Quantitative, Ballroom II
- MOF am: Biomarkers: Quantitative Analysis, Ballroom I
- MOG am: GC-MS Instrumentations Instrumentation and Application, Ballroom III
- MOH am: Challenges in MS Analysis of Complex Mixtures, Ballroom IV

10:30 am - 2:30 pm **Poster Session, Exhibits, Lunch Break**
All posters present 10:30 am - 12:00 pm & 1:00 - 2:30 pm.

12:00 pm **Deadline to purchase Closing Event Ticket.** Ticket sales close Monday June 2 at 12pm NOON or when tickets sell out. There is a capacity limit for this event, buy your ticket NOW if you wish to join us at the National Aquarium.

12:00 - 1:00 pm **Networking Session in the Poster-Exhibit Hall**
Celebrating Women Mass Spectrometrists

2:30 - 4:30 pm **Oral Sessions (eight parallel sessions)**

- MOA pm: Biomarkers: Qualitative Analysis, Hall AB
- MOB pm: Stable Isotope Labeling Applications, Room 307-308
- MOC pm: Industry: Trace Analysis, Quality Control, and Automation, Room 309-310
- MOD pm: Fundamentals: Ionization Methods, Room 314-317
- MOE pm: Artificial Intelligence in MS in Instrumentation and Applications, Ballroom II
- MOF pm: Lipidomics: New MS Technologies and Applications, Ballroom I
- MOG pm: Instrumentation: New Hybrid and Multimodal Approaches, Ballroom III
- MOH pm: Biotherapeutics: Characterizations and Quantitation, Ballroom IV

4:45 - 5:30 pm **Plenary Session, Joseph A. Loo presiding**
Presentation of Al Yergey MS Scientist Awards and Award Lecture by Jack Henion for John B. Fenn Distinguished Contribution in Mass Spectrometry Award

MONDAY, JUNE 2, 2025, *continued*

5:45 - 7:00 pm **Evening Workshops** (hosted by ASMS Interest Groups or Independent organizers)

- 01 Career Paths for Mass Spectrometrists: A Speed Networking Workshop (Career Development Interest Group), Room 307-308
- 02 Real time Mass Spectrometry in Proteomics and Beyond (Independent), Room 309-310
- 03 Chemoproteomics: The Next Frontier for Drug Development (and more) (Independent), Room 314-317
- 04 Benchmarking Datasets for Untargeted Metabolomics and Exposomics and Compound Identification (Metabolomics Interest Group), Ballroom II
- 05 Top-Down Proteomics: Software and Data Analysis Strategies for Getting the Most Out of Your Data (Top-Down Proteomics Interest Group), Ballroom I
- 06 Latest Developments in Open Data Standards Practices in Proteomics (Independent), Ballroom III
- 07 Towards Guidelines for DIA Reporting Criteria (DIA Interest Group), Ballroom IV
- 08 MS Outreach: Knowledge Share and Instrumentation Donations (Developing World Outreach Interest Group), Room 336
- 09 Taste to Targets: Food, Flavor and Fragrance Workshop (Flavor Fragrance & Foodstuff Interest Group), Room 339-340
- 10 Nitrosamine Analysis in Pharmaceutics: Evolving Challenges and Emerging Solutions (Pharmaceuticals Interest Group), Room 341-342
- 11 Mass Spectrometry in Quality Control for Complex Biotherapeutics Modalities (Biotherapeutics Interest Group), Room 343-344
- 12 Photoionization MS: Where It Excels, Where It Falls Short, and How It Complements Other Methods (Photoionization MS Interest Group), Room 345-346
- 13 Undergraduate Research: Strategies for Success (Undergraduate Research in MS Interest Group), Room 347-348
- 14 Environmental Applications: You Are What You Eat and Breathe (Environmental Applications Interest Group), Room 349-350

8:00 - 11:00 pm **Corporate Member Hospitality Suites, Hilton Baltimore**

TUESDAY, JUNE 3, 2025

7:30 am - 5:00 pm **Check-in and badge printing**

7:00 - 8:15 am **Corporate Member Breakfast Seminars, Convention Center AND Baltimore Hilton**

8:30 - 10:30 am **Oral Sessions (eight parallel sessions)**

- TOA am: Biotherapeutics: Proteins, Antibodies, and Antibody Drug Conjugates, Hall AB
- TOB am: Instrumentation: Innovative Separation Approaches Coupled to MS, Room
- 307-308
- TOC am: Environmental: Innovative Approaches and Instrumentation, Room 309-310
- TOD am: Lipodomics: Targeted and Untargeted, Room 314-317
- TOE am: Informatics: Innovations, Ballroom II
- TOF am: Imaging: Pharmaceuticals, Metabolites, Lipids, and Glycans, Ballroom I
- TOG am: Forensics, Innovations and Applications, Ballroom III
- TOH am: Fundamentals: Unconventional Approaches in MS, Ballroom IV

10:30 am - 2:30 pm **Poster Session, Exhibits, Lunch Break**
All posters present 10:30 am - 12:00 pm & 1:00 - 2:30 pm.

12:00 - 1:00 pm **Networking Session in the Poster-Exhibit Hall**
Hispanics and Latinx in MS

TUESDAY, JUNE 3, 2025, *continued*

2:30 - 4:30 pm **Oral Sessions (eight parallel sessions)**

- TOA pm: Data-Independent Acquisition: Acquisition and Multiplexing, Hall AB
- TOB pm: Instrumentation: Ambient Ionization and Applications, Room 307-308
- TOC pm: Microbes and the Microbiome, Room 309-310
- TOD pm: Fundamentals: Chemistry of Gas-Phase Ions (Honoring Veronica Bierbaum), Room 314-317
- TOE pm: Protein-Ligand and Protein-Protein Interactions, Ballroom II
- TOF pm: Glycopeptides, Glycoproteins, Ballroom I
- TOG pm: Nucleic Acids and Nucleotides, Ballroom III
- TOH pm: Metabolomics Untargeted Approaches, Ballroom IV

4:45 - 5:30 pm **Plenary Session, Joseph A. Loo presiding**
Presentations for Research Awards and PUI Research Award followed by Award Lecture by Livia Schiavinato Eberlin for the Biemann Medal

5:45 - 7:00 pm **Evening Workshops (hosted by ASMS Interest Groups or Independent organizers)**

- 01 De Novo Peptide Sequencing: Ready For Prime Time? (Independent), Room 307-308
- 02 Art, Museums and Archaeology (Art, Museums and Archaeology Interest Group), Room 309-310
- 03 Spectral Library Basics - What is an Identification? (Mass Spectral Libraries Interest Group), Room 314-317
- 04 Native MS: Strategies for Advancing Protein Characterization in Industry and Academia. (Native Mass Spectrometry Interest Group), Ballroom II
- 05 Young Mass Spectrometrist Workshop: Graduate School Through Early Career Forum (Young Mass Spectrometrists Interest Group), Ballroom I
- 06 Unlocking the Full Potential of Discovery and Early Development DMPK Support: Revolutionizing Efficiency, Innovation, and Integration with Mass Spectrometry (DMPK Interest Group), Ballroom III
- 08 FTMS Community Resources: Access, Education, and Data Analysis (FTMS Interest Group), Room 336
- 09 Process Considerations for Current Nucleic Acid Therapeutics and Emerging Modalities (Oligonucleaotides and Nucleic Acids Interest Group), Room 339-340
- 10 Fundamentals of Electrospray Ionization (Fundamentals Interest Group), Room 341-342
- 11 Plastics, Polymers and Replacement Chemicals Part 1: Recycling, Deconstruction, and Redesign of Polymeric Materials (Polymeric Materials Interest Group), Room 343-344
- 12 Proteomics Data Analysis: From Identification to Quantification (Bioinformatics MS Interest Group), Room 345-346
- 13 Lab Management Software: Necessity or Luxury? (Analytical Lab Managers Interest Group), Room 347-348

8:00 - 11:00 pm **Corporate Member Hospitality Suites, Hilton Baltimore**

WEDNESDAY, JUNE 4, 2025

7:30 am - 5:00 pm **Check-in and badge printing**

7:00 - 8:15 am **Corporate Member Breakfast Seminars, Convention Center AND Hilton Baltimore**

8:30 - 10:30 am **Oral Sessions (eight parallel sessions)**

- WOA am: Single Cell Omics, Hall AB
- WOB am: Structural Biology, Room 307-308
- WOC am: Fundamentals: Ion Structures, Energetics, and Reactions, Room 309-310
- WOD am: Integration of Multi-omics Approaches, Room 314-317
- WOE am: High Throughput MS and Automation, Ballroom II
- WOF am: Food Safety & Chemistry: New Innovations, Ballroom I
- WOG am: Covalent Labeling and Chemical Crosslinking, Ballroom III
- WOH am: Cancer Research, Ballroom IV

10:30 am - 2:30 pm **Poster Session, Exhibits, Lunch Break**

All posters present 10:30 am - 12:00 pm & 1:00 - 2:30 pm.

12:00 - 1:00 pm **Networkings Sessions in separate sections of the Poster-Exhibit Hall**

- Career Opportunities for Chinese Students and Scholars
- SAMs (South Asians in Mass Spec): Career Transitions: Strategies for Growth and Success in Mass Spectrometry

2:30 - 4:30 pm **Oral Sessions (eight parallel sessions)**

- WOA pm: Top-Down Proteomic Analysis, Hall AB
- WOB pm: Food Safety & Chemistry: Foodomics, Allergens, Bacteria, Foods and Supplements, Room 307-308
- WOC pm: Synthetic Polymers and New Materials, Room 309-310
- WOD pm: Small Molecules: Structural Characterization and Quantitation , Room 314-317
- WOE pm: Informatics: Metabolomics, Lipidomics and Glycomics, Ballroom II
- WOF pm: Imaging Instrumentation & Method Development, Ballroom I
- WOG pm: Ion Mobility: Structure Determination & Applications, Ballroom III
- WOH pm: Clinical Analysis: Innovations, Ballroom IV

4:45 - 5:30 pm **ASMS Meeting, Joe Loo presiding**

5:45 - 7:00 pm **Evening Workshops (hosted by ASMS Interest Groups or Independent organizers)**

- 01 The Complementary Role of Ambient Ionization Methods in Analytical Science (Ambient Sampling & Ionization Interest Group), Room 307-308
- 02 The Interface of Biomarker Discovery, Clinical Algorithm Development and Regulatory Oversight (Clinical Chemistry Interest Group), Room 309-310
- 03 Overcoming Challenges in Modern Ion Mobility (Ion Mobility MS Interest Group), Room 314-317
- 04 Single-Cell Proteomics by Mass Spectrometry: Best Practices and Current Challenges (Independent), Ballroom II
- 05 Ion Trap MS: Returning to Fundamentals (Ion Trap MS Interest Group), Ballroom I
- 06 Harmonizing Lipidomics through an Interactive Checklist (Lipids & Lipodomics Interest Group), Ballroom III
- 07 MS Imaging: Challenges and Recent Developments in Sample Preparation (Imaging MS Interest Group), Ballroom IV
- 08 Metaproteomics: Less is (Balti)more (Independent), Room 336
- 09 Cutting-Edge Structural Proteomics and Interactome Analysis: Advances in Covalent Labeling, Crosslinking, and Emerging Technologies (Covalent Labeling & Cross-Linking Interest Group), Room 339-340
- 10 Entrepreneurship in Mass Spectrometry: Non-Traditional Pathways for Scientific Innovation (Independent), Room 341-342

WEDNESDAY, JUNE 4, 2025, *continued*

- 11 Plastics, Polymers, and Replacement Chemicals Part 2 - Tracking the Right Compounds in Humans and the Environment (Exposomics Interest Group), Room 343-344
- 12 Forensics & Homeland Security: Emerging Technology for the Forensic Chemist (Forensics & Homeland Security Interest Group), Room 345-346
- 13 Current hot topics in bioanalysis from hybrid assays, biomarker assay validation to AI (Regulated Bioanalysis Interest Group), Room 347-348
- 14 JASMS - The Life Cycle of a Manuscript and Joining the Reviewer Pipeline (Independent), Room 349-350

8:00 - 11:00 pm **Corporate Member Hospitality Suites, Hilton Baltimore**

THURSDAY, JUNE 5, 2025

7:00 - 8:15 am **Corporate Member Breakfast Seminars, Convention Center**

8:30 - 10:30 am **Oral Sessions (eight parallel sessions)**

- ThOA am: Informatics: Multiomics Integration and Applications, Hall AB
- ThOB am: Clinical Analysis: Applications, Room 307-308
- ThOC am: Fundamentals: Ion Activation and Dissociation, Room 309-310
- ThOD am: Ion Mobility: Instrumentation & Method Development, Room 314-317
- ThOE am: Posttranslational Modifications: Qualitative and Quantitative Analysis, Ballroom II
- ThOF am: Instrumentation: New Developments in Ionization and Sampling, Ballroom I
- ThOG am: Environmental: Non-Target Analysis and Emerging Contaminants, Ballroom III
- ThOH am: H/D Exchange: Innovations and Applications, Ballroom IV

10:30 am - 2:30 pm **Poster Session, Exhibits, Lunch Break**
All posters present 10:30 am - 12:00 pm & 1:00 - 2:30 pm.

2:30 - 4:30 pm **Oral Sessions (eight parallel sessions)**

- ThOA pm: Informatics: Peptide and Protein Identification and Quantification, Hall AB
- ThOB pm: Exposomics, Toxicology and Health Outcomes, Room 307-308
- ThOC pm: Imaging: Spatially Resolved Omics (Honoring Richard Caprioli), Room 309-310
- ThOD pm: Carbohydrates: From Mono to Poly, Room 314-317
- ThOE pm: Instrumentation: High-Resolution Mass Spectrometry, Ballroom II
- ThOF pm: Neuroscience and Neurological Disorders Research, Ballroom I
- ThOG pm: Drug Metabolism and Pharmacokinetics, Ballroom III
- ThOH pm: Fundamentals: Native MS and Structures of Large Ions, Ballroom IV

4:45 - 5:45 pm **Closing Session, Carlito Lebrilla, presiding**
Closing Plenary Lecture: Melissa Trainer (NASA Goddard Space Flight Center), The Dragonfly Mission to Saturn's Moon Titan

7:00 - 10:00 pm **Closing Event at the National Aquarium - ADVANCE PURCHASE TICKET REQUIRED**
Ticket sales close Monday June 2 at 12pm NOON or when tickets sell out. There is a capacity limit of 1,500 attendees for this event.

MONDAY ORALS

MOA AM: QUANTITATIVE PROTEOMICS: INSTRUMENTATION AND APPLICATIONS

Hall AB

Session Chair: Renee Ruhaak (Leiden University Medical Center)

MOA am 08:30 **Modified Orbitrap Astral MS allows for higher scan rates without compromising spectral quality and sensitivity in proteomics**; Martin Rykar[1]; Ivo A. Hendriks[1]; Ulises H. Guzman[1]; Hamish Stewart[2]; Eduard Denisov[2]; Bernd Hagedorn[2]; Tabiwang N. Arrey[2]; Eugen Damoc[2]; Christian Hock[2]; Jesper V. Olsen[1]; *[1]Novo Nordisk Foundation Center for Protein Research, University of Copenhagen, Denmark; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

MOA am 08:50 **Ultra-sensitive quantitation and rapid method development for targeted immunopeptidomics using the Stellar Mass Spectrometer**; Ellen Casavant[1]; Lilian Heil[2]; Cristina Jacob[3]; Scott M. Peterman[4]; Fernanda Salvato[4]; Qingling Li[4]; Amirmansoor Hakimi[4]; Tonya Pekar Hart[3]; *[1]Thermo Fisher Scientific, Palo Alto; [2]Thermo Fisher Scientific, San Jose, CA; [3]Thermo Fisher Scientfic, San Jose, CA; [4]Thermo Fisher Scientific, San Jose, California*

MOA am 09:10 **Identification and Absolute Quantitation of Cysteine Peptides and Proteins via Coulometric Mass Spectrometry and Ferrocene-Based Thiol Alkylation**; Mengyuan Xiao[1]; Yongling Ai[1]; Muhammad Aminu Auwalu[1]; Yuanwei Zhang[1]; Shawn Li[2]; Harsha P. Gunawardena[3]; Hao Chen[1]; *[1]New Jersey Institute of Technology, Newark, NJ; [2]Merck & Co., Inc., West Point, PA; [3]JOHNSON AND JOHNSON, Spring House, PA*

MOA am 09:30 **The Role of Measurement Science in Standardizing Urine Albumin Results for Kidney Disease Assessment**; Ashley Beasley Green[1]; Johanna Camara[1]; N. Alan Heckert[1]; *[1]National Institute of Standards and Technology, Gaithersburg, MD*

MOA am 09:50 **Data-Driven Modeling of the Mouse Macrophage Toll-like Receptor Signaling Pathway**; Nathan P Manes[1]; Sergio A Hassan[1]; Anthony A Armstrong[1]; Fengkai Zhang[1]; Rachel A Gottschalk[2]; Matthew J Marino[1]; Iain DC Fraser[1]; Ronald N Germain[1]; Martin Meier-Schellersheim[1]; Aleksandra Nita-Lazar[1]; *[1]National Institutes of Health, Bethesda, MD; [2]University of Pittsburgh, Pittsburgh, PA*

MOA am 10:10 **Global mass spectrometric profiling of T cell surface proteins and their N-linked glycosylation landscape**; Andrew H Reiter[1, 2]; David S Roberts[2, 3]; Dina Schuster[2]; Carolyn R Bertozzi[2, 3, 4]; *[1]Department of Biology, Stanford University, Stanford, California; [2]Sarafan ChEM-H, Stanford University, Stanford, California; [3]Department of Chemistry, Stanford University, Stanford, California; [4]Howard Hughes Medical Institute, Stanford University, Stanford, California*

MOB AM: PLANTS AND NATURAL PRODUCTS

Room 307-308

Session Chair: Ying Sheng (Regeneron Pharmaceuticals)

MOB am 08:30 **Using multi-omics to explore the uncharted realm of mitochondrial diversity**; Mario Waespy[1]; Magdalene Reinkensmeier[2]; Aiko Barsch[2]; Stefanie Wernisch[2]; Markus Lübeck[2]; Matthew Lewis[2]; Rita Groß-Hardt[1]; *[1]University of Bremen, Bremen, Germany; [2]Bruker Daltonics GmbH & Co.KG, Bremen, Germany*

MOB am 08:50 **Quantitative Peptidomics Revealed a Novel Peptide Cytokine for Eliciting Plant Immunity by Pathogen-Associated Molecular Pattern**; Sheng-Chi Hung[1]; Yet-Ran Chen[1]; *[1]Agricultural Biotechnology Research Center, Academia Sinica, Taipei, Taiwan*

MOB am 09:10 **Unravelling lignin structure with mass spectrometry and generative modelling**; Eliise Tammekivi[1]; Avinash R. Pai[1]; Joseph S. M. Samec[1]; Anneli Kruve[1]; *[1]Stockholm UNIVERSITY, Stockholm, Sweden*

MOB am 09:30 **Optimization of spatial metabolomics and proteomics analyses from a single section of poplar root tissue**; Marija Velickovic[1]; Le Z Day[1]; Kevin J Zemaitis[1]; Isaac Kwame Attah[1]; Christopher Anderton[1]; Dusan Velickovic[1]; *[1]Pacific Northwest National Laboratory (PNNL), Richland, WA*

MOB am 09:50 **Developing Library-Based Methods for Identifying Metabolites in Plants**; Concepcion Africano Remoroza[1]; Nirina Rabe Adriamahavaro[1]; Yamil Simon Manso[1]; Tytus Mak[1]; Yuri Mirokhin[1]; Steve Stein[1]; *[1]NIST, Gaithersburg, MD*

MOB am 10:10 **Identification of bioactive Yucca schidigera saponins via LC–MS and machine learning for antimicrobial applications in animal health**; Maria Federica Marchesi[1]; Martina Felici[2]; Jaewoo Choi[3]; Roberta Majer[2]; Andrea Piva[2]; Jan F. Stevens[3, 4]; Ester Grilli[1]; *[1]Dipartimento di Scienze Mediche Veterinarie (DIMEVET), Università di Bologna, Ozzano dell'Emilia, Italy; [2]Vetagro S.p.A., Reggio Emilia, Italy; [3]Linus Pauling Institute, Oregon State University, Corvallis, OR; [4]Department of Pharmaceutical Sciences, Oregon State University, Corvallis, OR*

MOC AM: INSTRUMENTATION: DETECTION OF HIGH-MASS ANALYTES

Room 309-310

Session Chair: Ryan Leib (Stanford University)

MOC am 08:30 **Development of a Miniaturized Poschenrieder CDMS ion trap for increased charge accuracy and throughput**; Alexey Barkhanskiy[1]; Elvin Cabrera[2]; Ellen Liggett[3]; Thomas D Hoare[2]; Yuko Ishikawa[4]; Richard C Chapman[1]; John Hoyes[1]; Brian Biggar[4]; Perdita E Barran[3]; *[1]True Mass, Rowath, United Kingdom; [2]Manchester Institute of Biotechnology, University of Manchester, Manchester, United Kingdom; [3]The University of Manchester, Manchester, United Kingdom; [4]The University of Edinburgh, Edinburgh, United Kingdom*

MOC am 08:50 **The Design and Characterisation of a New Charge Detection Mass Spectrometry (CDMS) Instrument for the Analysis of Megadalton-Sized Molecules**; Jakub Ujma[1]; Chris Wheeldon[1]; Alistair Schofield[1]; Michael Danby[1]; David Eatough[1]; David Bruton[1]; Anisha Haris[1]; Keith Richardson[1]; David Langridge[1]; Andy Jarrell[2]; Benjamin E Draper[3]; Martin Jarrold[3]; Kevin Giles[1]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Waters Corporation, Milford, MA; [3]Megadalton Solutions, Bloomington, Indiana*

MOC am 09:10 **Mass Determination of Filled and Empty Adeno-associated Virus serotype 5 via Proton Transfer Charge Reduction**; Nicolas J. Pizzala[1]; Boukar K.S. Faye[1]; Hangtian Song[2]; Li Tao[2]; Scott A. McLuckey[1]; *[1]Purdue University, West Lafayette, IN; [2]Bristol-Myers Squibb.Co, Lawrence, NJ*

MOC am 09:30 **Charge Detection Mass spectrometry (CDMS) for the characterization of recombinant adeno associated virus (rAAV) at different manufacturing stages**; Stacey Nash[1]; Jin Park[1]; *[1]Ultragenyx, Woburn, MA*

MOC am 09:50 **Advanced single bioparticle mass analysis : nanospray ionization coupled to a linear charge detection array ion trap spectrometer**; Tessa Reinert[1]; Sylvain Maclot[1]; Lilou Duplantier[1]; Guillaume Montagne[1]; Christian Clavier[1]; Xavier

Dagany[1]; Clothilde Comby-Zerbino[1]; Michel Kerleroux[1]; Anton Kozhinov[2]; Konstantin Nagornov[2]; Yury Tsybin[2]; Rodolphe Antoine[1]; *[1]Institut Lumière Matière, Université Claude Bernard Lyon1, Villeurbanne, France; [2]Spectroswiss, EPFL Innovation Park, Lausanne, Switzerland*

MOC am 10:10 **To Teradaltons (TDa) and Beyond: Extending Mass Spectrometry to Micrometer-Scale Analytes with Laser Assisted in-Vacuum Electrospray Ionization**; Zachary M Miller[1]; Evan R Williams[1]; *[1]University of California, Berkeley, Berkeley, CA*

MOD AM: METABOLOMICS AND LIPIDOMICS: NEW TECHNOLOGIES AND APPLICATIONS

Room 314-317

Session Chair: Gary Siuzdak (Scripps Research)

MOD am 08:30 **Comparative Analysis of Single-Phase and Dual-Phase Extraction Methods for Metabolomics**; Erica Kim[1]; Tao Huan[1]; *[1]University of British Columbia, Vancouver, BC*

MOD am 08:50 **Parallel targeted and untargeted metabolite analysis of mouse plasma samples using a benchtop multi-reflecting time of flight mass spectrometer**; Adam M King[1]; Lee A Gethings[2]; Richard Lock[2]; Ian Wilson[3, 4]; James Langridge[5]; *[1]Waters corporation, Wilmslow, United Kingdom; [2]Waters Corporation, Wilmslow, United Kingdom; [3]Imperial College London, Division of Systems Medicine, London, United Kingdom; [4]University of Liverpool, Liverpool, United Kingdom; [5]Waters Corporation, Wilmslow, United Kingdom*

MOD am 09:10 **CD38 as a Key Regulator of NAD+ and Lipid Metabolism in the CNS: Implications for Brain Aging**; Prasanna Vadhana Ashok Kumaar[1]; Jingqi Fang[1]; Benjamin D. Ambrose[1]; Andrea Roberts[1]; Genesis Hormazabel[1]; Rebeccah Riley[1]; Birgit Schilling[1]; Lisa M. Ellerby[1]; Eric Verdin[1]; *[1]Buck Institute for Research on Aging, Novato, CA*

MOD am 09:30 **Towards Single-Droplet Blood Metabolomics: Small-Scale Highly Accurate and Reproducible Platform (SHARP) for Blood Analysis**; Xian Luo[1]; Shuang Zhao[1]; Kaitlyn Melo[1]; Liang Li[1, 2]; *[1]The Metabolomics Innovation Centre, Edmonton, AB; [2]Department of Chemistry, University of Alberta, Edmonton, AB*

MOD am 09:50 **Quantitative and qualitative analysis of bile acids by high-resolution mass spectrometry using electron-based fragmentation**; Paul RS Baker[1]; Santosh Kapil Kumar[2]; Dilip Kumar K Kandula[2]; Robert Proos[2]; Maxim D Seferovic[3]; Thomas D Horvath[3, 4]; *[1]SCIEX, Homewood, AL; [2]Sciex, Framingham, MA; [3]Baylor College of Medicine, Houston, TX; [4]Texas Children's Hospital - Microbiome Center, Houston, TX*

MOD am 10:10 **Targeted Metabolite Quantification in Trace Cancer Cell Samples**; Katelyn G McMurray[1, 2]; Darryl Hardie[2]; Bo Ren[1, 2]; Jun Han[2, 3]; Julian J Lum[1, 4]; David R Goodlett[1, 2]; *[1]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC; [2]Genome BC Proteomics Centre, University of Victoria, Victoria, BC; [3]Division of Medical Sciences, University of Victoria, Victoria, BC; [4]Deeley Research Centre, BC Cancer Research Institute, Victoria, BC*

MOE AM: DRUG DISCOVERY AND DEVELOPMENT: QUALITATIVE AND QUANTITATIVE

Ballroom II

Session Chair: Benqian Wei (Merck & Co., Inc.)

MOE am 08:30 **Ubiased identification and validation of degrader drug targets by high-throughput deep proteomic screening and high-sensitivity ubiquitinomics**; Uli Ohmayer[1]; Martin Steger[1]; Bachuki Shashikadze[1]; Kevin McGowan[2]; Qiong Wu[3]; Björn Schwalb[1]; Anastasia Bednarz[1]; Sophie Machata[1]; Tobias Graef[1]; Denis Bartoschek[1]; Zhe Shi[2]; Jeanine Price[2]; Anand Mayasundari[2]; Lei Yang[2]; Jun Yang[3]; Vadim Demichev[4]; Gisele Nishigushi[2]; Zoran Rankovic[5, 6]; Henrik Daub[1]; *[1]NEOsphere Biotechnologies GmbH, Planegg, Germany; [2]Department of Chemical Biology and Therapeutics, St. Jude Children's Research Hospital, Memphis, TN; [3]Department of Surgery, St. Jude Children's Research Hospital, Memphis, TN; [4]Department of Biochemistry, Charité - Universitätsmedizin Berlin, Berlin, Germany; [5]Centre for Protein Degradation, The Institute of Cancer Research, London, United Kingdom; [6]Department of Chemical Biology and Therapeutics, Memphis, TN*

MOE am 08:50 **Multiplexed Quantitation of Antibodies and Biomarkers Using Parallel Reaction Monitoring (PRM) Coupled with FAIMS and DuoESI Source**; Isabel Wang[1]; Hilda Hernandez-Barry[1]; Phillip Chu[1]; John Tran[1]; Rachel Liuqing Shi[1]; *[1]Genentech Inc., South San Francisco, CA*

MOE am 09:10 **Phosphoproteomic Landscape of Osimertinib-Tolerant Persister Cells Reveals Targetable Kinase-Substrate Signatures**; Hsiang-En Hsu[1]; Matthew J Martin[2]; Shao-Hsing Weng[1]; Reta Birhanu Kitata[1]; Srikar Nagelli[2]; Chiung-Yun Chang[3]; Sonja Hess[3]; Yu-Ju Chen[1, 4]; *[1]Academia Sinica, Taipei, Taiwan; [2]AstraZeneca, Cambridge, United Kingdom; [3]AstraZeneca Pharmaceuticals LP, Gaithersburg, MD; [4]National Taiwan University, Taipei City, Taiwan*

MOE am 09:30 **High-throughput screening of HDAC inhibitors for quantification of low abundant histone acetylation and acylation marks using mass spectrometry**; Rashmi Karki[1]; Francisca NDL Vitorino[1]; Richard M. Searfoss[1]; Benjamin A. Garcia[1]; *[1]Washington University School of Medicine, St. Louis, MO*

MOE am 09:50 **MS imaging in drug development: The clinical-stage antibiotic BTZ-043 accumulates and efficiently acts against Mycobacterium tuberculosis in tuberculosis lesions**; Andreas Roempp[1]; Axel Treu[1]; Julia Kokesch-Himmelreich[1]; Leon Groeschel[1]; Franziska Marwitz[2]; Nadine Aboutara[2]; Julia Dreisbach[3]; Dominik Schwudke[2]; Michael Hölscher[3]; Christoph Hölscher[4]; Kerstin Walter[4]; *[1]Bioanalytical Sciences and Food Analysis, University of Bayreuth, Bayreuth, Germany; [2]Division of Bioanalytical Chemistry, Research Center Borstel, Leibniz Lung Center, Borstel, Germany; [3]Institute of Infectious Diseases and Tropical Medicine, LMU University Hospital, University of Munich (LMU), Munich, Germany; [4]Division of Infection Immunology, Research Center Borstel, Leibniz Lung Center, Borstel, Germany*

MOE am 10:10 **The Tissue Protein Library Platform for Accelerated Bioanalytical Method Development and Target Assessment**; Gene Ciccimaro[1]; Joshua Nicklay[1]; Jingjing Deng[1]; Jacob Zalaznick[1]; Bogdan Sleczka[1]; Petia Shipkova[1]; *[1]Bristol Myers Squibb, Princeton, NJ*

MOF AM: BIOMARKERS: QUANTITATIVE ANALYSIS

Ballroom I

Session Chair: Richard R. Drake (Medical University of South Carolina)

MOF am 08:30 **Combined glycomic and glycoproteomic platform for sera and brain tissues reveals biomarkers for Glioblastoma, Meningioma, and High-Grade Meningioma**; Atit Silsirivanit[1]; Michael Russelle S Alvarez[2]; Sheryl Joyce Grijaldo-Alvarez[3]; Riya Gogte[3]; Anirudh Yadlapati[3]; Edwin Grey[3]; Amnat Kitkhuandee[1]; Nontaphon

Piyawattanametha[1]; Wunchana Seubwai[1]; Sukanya Luang[1]; Orasa Panawan[1]; Panupong Mahalapbutr[1]; Kulthida Vaeteewoottacharn[1]; Kanlayanee Sawanyawisuth[1]; Worachrt Let-itthiporn[1]; Charupong Saengboonmee[1]; Pichayen Duangthongphon[1]; Kritsakorn Jingjit[1]; Anuchit Pankongsap[1]; Sakda Waraasawapati[1]; Chaiwat Aphivatanasiri[1]; Carlito Lebrilla[3]; *[1]Khon Kaen University, Khon Kaen, Thailand; [2]University of California Davis, Davis, CA; [3]University of California, Davis, Davis, CA*

MOF am 08:50 **Digital Proteome: A comprehensive multi-tissue and multi-species proteome expression atlas supporting target discovery and therapeutic development**; Sandra Schär[1]; Jan Muntel[1]; Polina Shichkova[1]; Marco Tognetti[1]; Christopher Below[1]; Yuehan Feng[1]; Roland Bruderer[1]; Lukas Reiter[1]; Igor Sobanski[1]; Matevz Stefancic[1]; Simona Candea[1]; *[1]Biognosys AG, Schlieren, Switzerland*

MOF am 09:10 **Proteome profiling of rabies positive and negative samples isolated from canine brain tissues, cerebrospinal fluid and sera**; Ukamaka Uchenna Eze[1]; Rethabile Mokoena[2]; Kenneth Ikejiofor Ogbu[3]; Sinegugu Dubazana[2]; Ernest C Ngoepe[4]; Mparamoto Munangatire[4]; Romanus C Ezeokonkwo[5]; Boniface M Anene[1]; Sindisiwe Buthelezi[2]; Claude T Sabeta[6]; *[1]Department of Veterinary Medicine, University of Nigeria, Nsukka, Nigeria; [2]Council for scientific and industrial research, Pretoria, South Africa; [3]Department of Animal Health, Federal College of Animal Health and Production Technology, National Veterinary Research Institute, Vom, Nigeria; [4]Agricultural Research Council, Onderstepoort Veterinary Reasearch, Pretoria, South Africa; [5]Department of Veterinary Parasitology and Entomology, University of Nigeria, Nsukka, Nigeria; [6]Department of Veterinary Tropical Diseases, University of Pretoria, Pretoria, South Africa*

MOF am 09:30 **Integrated metabolomic and lipidomic approaches to elucidate rapamycin-induced metabolic dysregulation**; Jericha Mill[1]; Ryan Marshall[2]; Dudley Lamming[2]; Judith Simcox[1, 3]; *[1]Department of Biochemistry, University of Wisconsin-Madison, Madison, Wisconsin; [2]Department of Medicine, Division of Diabetes, Endocrinology and Metabolism, University of Wisconsin-Madison, Madison, Wisconsin; [3]Howard Hughes Medical Institute, Chevy Chase, Maryland*

MOF am 09:50 **Proteomic platform comparison in search of novel and robust protein biomarkers for Lewy body dementia (LBD) in cerebrospinal fluid (CSF)**; Caroline M Watson[1]; Higginbotham A Higginbotham[1]; Shantaraman Shantaraman[1]; Edward J Fox[1]; Pritha Bagchi[1]; Fang Wu[1]; James J Lah[1]; Allan I Levey[1]; Nicholas T Seyfried[1]; *[1]Emory University School of Medicine, Atlanta, GA*

MOF am 10:10 **SysQuan: Revolutionizing Large-Scale Absolute Quantitative Liver Proteomics with an Affordable Single-Injection Workflow using Stable Isotope-Labeled Mouse**; Timon Geib[1]; Yassene Mohammed[2, 3, 4]; Vincent R. Richard[1, 2]; M. Immanuel Reyes Madlangsakay[5]; Ying Lao[5]; Victor Spicer[5]; Claudia Gaither[6, 7]; Pradyumn Maheshwari[6]; Linfeng Wu[8]; Robert Popp[6]; John Sausen[8]; René P. Zahedi[5, 9, 10, 11]; Christoph H. Borchers[1, 2, 3, 12, 13]; *[1]McGill University - Lady Davis Institute, Montréal, QC; [2]Segal Cancer Proteomics Centre, Jewish General Hospital, Montreal, QC; [3]Gerald Bronfman Department of Oncology, Montreal, QC; [4]Leiden University Medical Center, Leiden, Netherlands; [5]Manitoba Centre for Proteomics and Systems Biology, Winnipeg, MB; [6]MRM Proteomics Inc, Montreal, Quebec; [7]Faculty of Veterinary Medicine, Department of Clinical Sciences, University of Montreal, Montreal, QC; [8]Agilent Technologies, Santa Clara, CA; [9]Department of Internal Medicine, University of Manitoba, Winnipeg, MB; [10]Department of Biochemistry and Medical Genetics, University of Manitoba, Winnipeg, MB; [11]Paul Albrechtsen Research Institute, CancerCare Manitoba, Winnipeg, MB; [12]Division of Experimental Medicine, McGill University, Montreal, QC; [13]Department of Pathology, McGill University, Montreal, QC*

MOG AM: GC-MS INSTRUMENTATIONS INSTRUMENTATION AND APPLICATION

Ballroom III

Session Chair: Jorge Smith (Waters Corporation)

MOG am 08:30 **Molecular Characterization of Heteroatom-Containing Compounds in Tactical Fuels by Using Two-Dimensional Gas Chromatography/Methane Chemical Ionization/Time-of-Flight Mass Spectrometry**; Grace Greene[1]; Jacob Guthrie[2]; Caroline Rowell[2]; Philip Duvall[2]; Marielle Jackson[2]; N. Scott Bergey[3]; Richard Bell[3]; Gozdem Kilaz[2]; Michael E. Peretich[3]; Hilkka I Kentämaa[2]; *[1]Purdue University, West Lafayette, IN; [2]Purdue Univeristy, West Lafayette, IN; [3]Naval Air Systems Command, Patuxent River, MD*

MOG am 08:50 **Chemical Analysis of Rapid vs Traditionally Aged Whiskeys via Gas Chromatography – Mass Spectrometry**; David P Schafer[1]; Troy Bencoe[1]; Josiah Phillips[1]; Nathan Bays[1]; Ryan D Davis[1]; Jessica Ròman-Kustas[1]; *[1]Sandia National Laboratories, Albuquerque, NM*

MOG am 09:10 **Mass spectrometry analytical tools in the dating of the Chinese scrolls from the Inner Mongolia**; Olga V Polyakova[1]; Maria Kondratieva[1]; Zhuangzhi Li[1]; Viatcheslav Artaev[2]; Jonelle Shiel[2]; Scott Pugh[2]; Albert T Lebedev[1]; *[1]Shenzhen MSU-BIT University, Shenzhen, China; [2]LECO, St. Joseph, MI*

MOG am 09:30 **Life, Death & Cannibalism in Fruit Flies – a GCMS supported odor analysis**; Fabian S Menges[1]; Emily J Siff[1]; Gustavo Madeira Santana[1]; Frédéric Marion-Poll[2]; John R Carlson[1]; *[1]Yale University, New Haven, CT; [2]Universite Paris Saclay, Paris, France*

MOG am 09:50 **Characterization of Subterrestrial Volatile Organic Compounds (VOCs) from native soils and Terraforms**; Chaevien S Clendinen[1]; Vimal Kumar Balasubramanian[1]; Arunima Bhattacharjee[1]; Karl K. Weitz[1]; Nathalie Munoz[1]; Kylee Tate[1]; Heather M. Olson[1]; *[1]Pacific Northwest National Laboratory, Richland, Washington*

MOG am 10:10 **Highly parallel metabolite profiling of yeast extracts using GC-MS/MS technology with automated method development and TBDMS derivatization**; Vladimir Shulaev[1]; Debasish Ghosh[1]; Amit Gujar[2]; *[1]University of North Texas, Denton, TX; [2]Thermo Fisher Scientific, Austin, TX*

MOH AM: CHALLENGES IN MS ANALYSIS OF COMPLEX MIXTURES

Ballroom IV

Session Chair: Adriana Zardini Buzatto (University of Calgary)

MOH am 08:30 **Exploring Samples Relevant to Titan via Dragonfly Mass Spectrometer (DraMS)-Like Laser Desorption Mass Spectrometry and Pyrolysis/Derivatization Gas Chromatography Mass Spectrometry**; M Joseph Pasterski[1]; Caroline Freissinet[2]; Arnaud Buch[3]; Cyril Szopa[2]; David Boulesteix[4]; Thomas Gautier[2]; Sarah Horst[5]; Cara Pesciotta[5]; Marco E. Castillo[1, 6]; Friso Van Amerom[1, 7]; Desmond A. Kaplan[1, 8]; Jacob D Graham[1]; Ryan M Danell[1, 9]; William B Brinckerhoff[1]; Andrej Grubisic[1];

Melissa G. Trainer[1]; Xiang Li[1]; *[1]NASA Goddard Space Flight Center, Greenbelt, MD; [2]LATMOS, Guyancourt, France; [3]LGPM - Process Engineering and Materials Laboratory, Gif-sur-Yvette, France; [4]LGPM - Process Engineering and Materials Laboratory, Gif-sur-Yvette, France; [5]Department of Earth and Planetary Sciences Johns Hopkins University, Baltimore, MD; [6]Aerodyne, Cape Canaveral, FL; [7]Mini-Mass Consulting, Inc, Hyattsville, MD; [8]KapScience, Tewksbury, MA; [9]Danell Consulting, Inc., Winterville, NC*

MOH am 08:50 **A Solid Phase Extraction Capture (SPEC) device for ultra-robust and ultra-sensitive proteomics**; Tim Heymann[1]; Denys Oliinyk[1]; Lukas Henneberg[1]; Thierry Nordmann[1]; Edwin Rodriguez[1]; Marvin Thielert[1]; Kathrin Korff[1]; Vincent Albrecht[1]; Johannes Mueller-Reif[1]; Matthias Mann[1]; *[1]Max Planck Institute of Biochemistry, Martinsried, Germany*

MOH am 09:10 **Deep proteome characterization unveils distinct secretory phenotypes of Wild Type and Familial Alzheimer's Disease organoids**; Natalie P Turner[1]; Anthony Balistreri[1]; John R. Yates III[1]; Jeff W Kelly[1]; *[1]The Scripps Research Institute, La Jolla, CA*

MOH am 09:30 **Deciphering native topology of protein complexes in a cell lysate by combining surface-induced dissociation and native CZE-MS/MS**; Fei Fang[1]; Zihao Qi[2, 3]; Qianjie Wang[1]; Qianyi Wang[1]; William J. Moeller[2, 3]; Vicki H. Wysocki[2, 3]; Liangliang Sun[1]; *[1]Department of Chemistry, Michigan State University, East Lansing, MI; [2]Department of Chemistry and Biochemistry, The Ohio State University, Columbus, Ohio; [3]Native Mass Spectrometry-Guided Structural Biology Center, The Ohio State University, Columbus, Ohio*

MOH am 09:50 **Overcoming Matrix Effects: Using Modified Surfaces for the Analysis of Complex Biofluids with Ambient Ionization Mass Spectrometry**; Elmeri J Latvanen[1]; Yihan Xu[1]; Duncan Roberts[1]; Maria Sani[1]; Petra Paizs[1]; James L Alexander[1]; James Kinross[1]; Lukas Kopecky[1]; Daniel Simon[1, 2]; Timothy M D Ebbels[1]; Elizabeth Want[1]; Panagiotis Manesiotis[3]; Zoltan Takats[1, 2]; Lauren Ford[1]; *[1]Imperial College London, London, United Kingdom; [2]University of Regensburg, Department of Immune Medicine Multimodal Imaging of Intracellular Communication, Regensburg, Germany; [3]Queens University Belfast, Belfast, United Kingdom*

MOH am 10:10 **Expediting metabolomics-based discovery with the Human Metabolome Atlas**; Jeremy K Chan[1]; William D Gwynne[1]; Nicholas S Ly[1]; Brandon Y Lieng[1]; Olivia Taverniti[1]; Verne T. Urquhart-Cox[1]; Mathula Muhundan[1]; Andrew T Quaile[1]; J. Rafael Montenegro-Burke[1]; *[1]University of Toronto, Toronto, ON*

MOA PM: BIOMARKERS: QUALITATIVE ANALYSIS
Hall AB
Session Chair: Maryam Baniasad (InterVenn Biosciences)

MOA pm 02:30 **Pregnancy-associated protein isoforms identified through peptide-level quantification of serum: a tractable model system for cancer biomarker discovery?**; Tammy-Lynn Tremblay[1]; Sue Penny[2]; Jennifer J Hill[1, 3]; *[1]National Research Council Canada, Ottawa, ON; [2]National Research Council of Canada, Halifax, NS; [3]Ottawa Institute of Systems Biology, Ottawa, ON*

MOA pm 02:50 **Highly Precise Absolute Quantification of Plasma Proteins in the Human Disease Blood Atlas**; Fredrik Edfors[1]; David Kotol[2]; Andrea Villanueva Raisman[1]; *[1]SciLifeLab, KTH Royal Institute of Technology, Solna, Sweden; [2]ProteomEdge, Stockholm, Sweden*

MOA pm 03:10 **High-Resolution Liquid Chromatography-Tandem Mass Spectrometry Enables Characterization of Protein Glycosylation Heterogeneity in Pancreatic Cyst Fluid**; Kathryn L. Kapp[1]; Fernando J. Garcia Marques[1]; Abel Bermudez[1]; Nikhiya Shamsher[1]; Sharon Pneh[2]; Walter G. Park[2]; Sharon J. Pitteri[1]; *[1]Canary Center at Stanford for Cancer Early Detection, Department of Radiology, Stanford University School of Medicine, Palo Alto, CA; [2]Division of Gastroenterology and Hepatology, Department of Medicine, Stanford University School of Medicine, Stanford, CA*

MOA pm 03:30 **Longitudinal Proteomic Changes in HCT 116 Colon Cancer Spheroids During Growth**; Catherine B Whitney[1]; Nicole C Beller[2]; Brian D Fries[3]; Arbil Lopez[1]; Amanda B. Hummon[1]; *[1]Department of Chemistry and Biochemistry, The Ohio State University, Columbus, Ohio; [2]Bioanalytical Department Charles River Laboratories, Mattawan, MI; [3]The Ohio State Campus Chemical Instrument Center (CCIC), Columbus, OH*

MOA pm 03:50 **A Diverse Proteomic Catalog of Senescent Cells Enables Development of Improved Cell Type-Specific Senescence Biomarkers in Humans**; Bradley Olinger[1]; Carlos Anerillas[1, 2]; Allison B Herman[1]; Reema Banarjee[1]; Julian Candia[1]; Toshiko Tanaka[1]; Ying Hao[1]; Ziyi Li[1]; Dimitrios Tsitsipatis[1]; Andrew B Singleton[1]; Keenan A Walker[1]; Eleanor M Simonsick[1]; Yue Andy Qi[1]; Myriam Gorospe[1]; Nathan Basisty[1]; *[1]National Institute on Aging, Baltimore, MD; [2]Centro de Biologia Molecular Severo Ochoa, CBMSO, Madrid, Spain*

MOA pm 04:10 **Simultaneous Quantitation and Discovery (SQUAD) of fecal bile acids and conjugates in adults with autism spectrum disorder**; Bashar Amer[1]; Alexey V Melnik[2]; James B. Adams[3]; Rosa Krajmalnik-Brown[3]; Khemlal Nirmalkar[3]; Brandon Bills[4]; Rafael D Melani[4]; Thomas Moehring[5]; Susan S Bird[4]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]BileOmix Inc., Farmington, Connecticut; [3]Arizona State University, Tempe, AR; [4]ThermoFisher Scientific, San Jose, CA; [5]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

MOB PM: STABLE ISOTOPE LABELING APPLICATIONS
Room 307-308
Session Chair: Rahul Ravi Deshpande (Thermo Fisher Scientific)

MOB pm 02:30 **The Protein Turnover Atlas: A Comprehensive Resource for Drug Development**; Barbara Schnitzer[1]; Kathrin Grundner-Culemann[2]; Leonie Reichert[1]; Alexander Betz[1]; Maria Faria[1]; Serhat Beyaz[1]; Götz Hagemann[1]; Christin Zasada[1]; Hannes Hahne[1]; *[1]OmicScouts GmbH, Freising, Germany; [2]Omicscouts GmbH, Freising, Germany*

MOB pm 02:50 **Parallel quasi-simultaneous EI and CI-TOFMS detection with a novel flexible CI source for GC-based isotopologue ratio analysis in metabolomics**; Pegah Mousazadehfazeli[1]; Christina Troyer[1]; Teresa Steininger-Mairinger[1]; Michael Groessl[2]; Sonja Klee[3]; Arnd Ingendoh[4]; Matthew R. Lewis[4]; Stephan Hann[1]; *[1]BOKU University, Department of Natural Sciences and Sustainable Resources, Institute of Analytical Chemistry, Muthgasse 18, 1190 Vienna, Austria; [2]Tofwerk AG, Thun, Switzerland; [3]Tofwerk AG, 3645 Thun, Switzerland; [4]Bruker Daltonics GmbH & Co.KG, Bremen, Germany*

MOB pm 03:10 **In Vivo, Time-Dependent Metabolic Flux Analysis of Normal and Tumor Tissue Using MasSpec Pen Technology**; Michael Tuck[1]; Yasmin Shanneik[1]; Harinarayanan Janakiraman[1]; Zachary Gao[1]; Faith Jackobs[1]; Trevor Godfrey[1]; E. Ramsay Camp[1]; Livia

S. Eberlin[1]; *[1]Department of Surgery, Baylor College of Medicine, Houston, Texas*

MOB pm 03:30 **Developing a DIA-Based Approach to Decipher Protein Degradation and Synthesis Dynamics in Unfolded Protein Response (UPR)**; YUE DOU[1]; Tian Zhang[1]; *[1]University of Virginia, Charlottesville, VA*

MOB pm 03:50 **High-throughput identification of isotopically depleted proteoforms without deconvolution using a proteoform-centric analysis workflow**; David S Butcher[1]; Lissa C Anderson[1, 2]; *[1]National High Magnetic Field Laboratory, Tallahassee, FL; [2]Florida State University, Tallahassee, FL*

MOB pm 04:10 **Triple Safeguard-Enhanced Chemoproteomic Platform for Reliable Citrullination Mapping with Staggered DIA Detection in Alzheimer's Disease**; Wei Wilson Li[1]; Zexin Zhu[1]; Lauren Fields[2]; Haiyan Lu[1]; Zicong Wang[1]; Kelly H. Lu[2]; Lingjun Li[1, 2]; *[1]School of Pharmacy, University of Wisconsin-Madison, Madison, WI; [2]Department of Chemistry, University of Wisconsin–Madison, Madison, WI*

MOC PM: INDUSTRY: TRACE ANALYSIS, QUALITY CONTROL, AND AUTOMATION

Room 309-310

Session Chair: Caroline E.R. Rowell (NASA Goddard Space Flight Center)

MOC pm 02:30 **AAV6 VP3-Only Capsids for Standardization in Ion-Exchange Chromatography, Native Mass Spectrometry, and Charge Detection Mass Spectrometry**; Weijing Liu[1]; Julia Braun[2]; Ke Ma[3]; Joanna Geddes[4]; Kay Opperman[4]; Bhavin Patel[4]; Rosa Viner[5]; Thomas Moehring[6]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Carlsbad, CA; [3]Thermo Fisher, Sunnyvale, CA; [4]Thermo Fisher Scientific, Rockford, IL; [5]ThermoFisher Scientific, San Jose, CA; [6]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

MOC pm 02:50 **Intelligent BioAnalysis (iBA) System: Pioneering the Future of Bioanalysis**; Romina Schnegotzki[1]; Christian Spaeth[2]; Christoph Disch[3]; Siegfried Wild[1]; Svenja Mayer-Wrangowski[4]; Wolfgang Joerg[3]; Jürgen Weber[3]; Michael Haas[3]; Andreas Harald Luippold[1]; *[1]Drug Discovery Sciences, DDS, Boehringer Ingelheim Pharma GmbH & Co. KG, Biberach, Germany; [2]Lab Automation and Robotic Solutions, LARS, Boehringer Ingelheim Pharma GmbH & Co. KG, Biberach, Germany; [3]Lab Automatin and Robotic Solutions, LARS, Boehringer Ingelheim Pharma GmbH & Co. KG, Biberach, Germany; [4]DEV NCS & DMPK, Boehringer Ingelheim Pharma GmbH & Co. KG, Biberach, Germany*

MOC pm 03:10 **High-speed adaptive re-calibration of mass spectra for process monitoring**; Konstantin O. Nagornov[1]; Anton N. Kozhinov[1]; Yury O. Tsybin[1]; *[1]Spectroswiss, Lausanne, Switzerland*

MOC pm 03:30 **Amplify laboratory efficiency by Simultaneous QUAntitation and Discovery: SQUAD can elevate high-resolution MS analysis of known and unknown nitrosamines**; Tobias Lieblein[1]; Sven Hackbusch[2]; Jon Bardsley[3]; Christian Laue[1]; Andrea Nees[1]; Sebastien Morin[4]; Min Du[5]; Valeria Van Axel[6]; *[1]Merck Healthcare KGaA, Darmstadt, Germany; [2]Thermo Fisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific, Hemel Hempstead, United Kingdom; [4]Thermo Fisher Scientific, Mississauga, ON; [5]Thermo Fisher Scientific, Lexington, MA; [6]Merck Serono S.p.A, Guidonia Montecelio, Italy*

MOC pm 03:50 **Unified Triple Quadrupole LC/MS Method for Comprehensive PFAS Analysis Across Diverse Matrices**; Aimei Zou[1]; Siji Joseph[2]; *[1]Agilent Technologies Singapore, Singapore, Singapore; [2]Agilent Technologies, Singapore, Singapore*

MOC pm 04:10 **Real-Time Monitoring of Odorous VOCs from Industrial Facilities Using SIFT-MS**; Nathan C Hoppens[1]; Tucker Kitchengs[1]; Eric Winegar[2]; Daniel Kleist[3]; Ron Kleist[3]; Leslie Silva[1]; *[1]Syft Technologies, Inc., Anaheim, CA; [2]Winegar Air Services, Sacramento, CA; [3]VortX Kleen Air Systems, Inc., San Rafael, CA*

MOD PM: FUNDAMENTALS: IONIZATION METHODS

Room 314-317

MOD pm 02:30 **A New 'Proton Attraction' Model for Ambient Gas Adsorption to Spray Solution During Electrospray Ionization**; Khadija Khetabi[1]; Amy Le[1]; Andre R Venter[2]; Richard B Cole[1, 3]; *[1]Sorbonne Université - Faculté des Sciences et Ingénierie, Paris Cedex 05, France; [2]Western Michigan University, Kalamazoo, MI; [3]University of New Orleans, New Orleans, LA*

MOD pm 02:50 **Direct extraction and ionization of intact proteins from aqueous environment using desorption by impulsive vibration excitation**; Khaled Madhoun[1]; Pei Su[2]; Alexander A.C. Wainwright[1]; Samuel E. Janisse[2]; Neil Kelleher[2]; Jared O. Kafader[2]; R.J. Dwayne Miller[1]; *[1]University of Toronto, Toronto, ON; [2]Northwestern University, Evanston, IL*

MOD pm 03:10 **Probing Charge State Limits and Spatial Distribution on ESI-MS Analytes: Quantifying Effects of Shape, Size, and Surface Chemistry**; Cleo S McLaughlin[1]; David Z Keifer[1]; *[1]Salisbury University, Salisbury, MD*

MOD pm 03:30 **Uranium-Containing Anions Studied by Photoelectron Spectroscopy**; Burak Tufekci[1]; Kathryn Foreman[1]; Ashley Hunt[2]; Evangelos Miliordos[3]; Lan Cheng[1]; Kirk Peterson[2]; Kit Bowen[1]; *[1]The Johns Hopkins University, Baltimore, MD; [2]Washington State University, Pullman, WA; [3]AUBURN UNIVERSITY, Auburn, AL*

MOD pm 03:50 **SICRIT® analysis of pesticides and environmental pollutants in complex matrices using a standard ESI workflow on Shimadzu LCMS- 9030 QTOF**; Ciara Conway[1, 2]; Divya RAMESH[1]; Markus Weber[1, 2]; Jan-Christoph Wolf[1]; Jan Bucek[1]; *[1]Plasmion GmbH, Augsburg, Germany; [2]Technical University of Munich, Garching, Germany*

MOD pm 04:10 **3D-Image-guided laser for precision sampling of individual patient-derived organoids with different morphology and treatment response for proteomic and transcriptomic analysis**; Ayham Moustafa[1, 2, 3, 4]; Manuela Moritz[1]; Thomas Mair[1]; Mohamed E. Elsesy[2]; Wael Y. Mansour[2, 3, 4, 5]; Hartmut Schlüter[1, 4]; Jan Hahn[1, 3, 4]; *[1]Section Mass Spectrometry and Proteomics, Center for Diagnostics, University Medical Center Hamburg-Eppendorf, Hamburg, Germany; [2]Department of Radiotherapy and Radiation Oncology, Center for Oncology, Hamburg, Germany; [3]Mildred Scheel Cancer Career Center Hamburg HaTriCS4, University Medical Center Hamburg-Eppendorf, Hamburg, Germany; [4]University Cancer Center Hamburg (UCCH), University Medical Center Hamburg-Eppendorf, Hamburg, Germany; [5]II. Medical Oncology Clinic and Polyclinic, University Medical Center Hamburg-Eppendorf, Hamburg, Germany*

MOE PM: ARTIFICIAL INTELLIGENCE IN MS IN INSTRUMENTATION AND APPLICATIONS

Ballroom II

Session Chair: Gaurav Chopra (Purdue University)

MOE pm 02:30 **AI-Controlled Autonomous Proteomics**; Soroush Hajizadeh[1, 2, 3, 4, 5]; Eric F Zaniewski[1, 2]; Johannes

Kreuzer[1, 2, 3]; Daniel A. Haber[1, 2, 3]; Dennis Sgroi[1, 2, 3]; Lecia V. Sequist[1, 3]; Michael S. Lawrence[1, 2, 3, 4]; Wilhelm Haas[1, 2, 3]; *[1]Massachusetts General Hospital Cancer Center, Boston, MA; [2]Krantz Family Center for Cancer Research, Boston, MA; [3]Harvard Medical School, Boston, Massachusetts; [4]Broad Institute of MIT and Harvard, Cambridge, MA; [5]University of Graz, Graz, Austria*

MOE pm 02:50 **MHCBooster: An AI-powered Software to Boost DDA-based Immunopeptide Identification**; RUIMIN WANG[1]; Saketh Kapoor[1]; Jing Sun[1]; Etienne Caron[1]; *[1]Yale School of Medicine, NEW HAVEN, CT*

MOE pm 03:10 **From RP to HILIC: Graph Transformers Power Method-Independent Prediction of Retention Times for Metabolomics Annotation**; Cailum MK Stienstra[1, 2]; Emir Nazdrajić[1]; Tao Huan[2]; Scott Hopkins[1]; *[1]University of Waterloo, Waterloo, ON; [2]University of British Columbia, Vancouver, BC*

MOE pm 03:30 **Towards AI Agents that Accelerate and Democratize PTM detection and Interpretation of Mass Spectrometry-Based Multiomics Synthetic Biology Data**; Aivett Bilbao[1]; Yuqian Gao[1]; Erin Bredeweg[1]; Nathalie Munoz[1]; Ashfiqur Rahman[1]; Andrea Harrison[1]; Young-Mo Kim[1]; Gregg T. Beckham[2]; Gayle J. Bentley[3]; Sarah M. Stow[4]; Joonhoon Kim[1]; Kyle R. Pomraning[1]; Kristin E. Burnum-Johnson[1]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]National Renewable Energy Laboratory, Golden, CO; [3]US Department of Energy, Bioenergy Technologies Office, Golden, CO; [4]Agilent Technologies, Santa Clara, CA*

MOE pm 03:50 **Applying deep learning model 'LightGlue' to MALDI imaging in single cell level for label free photograph alignment**; Xinfeng Zhou[1]; Zhenhe Chen[2]; Xiaodong Li[2]; Wenjian Sun[1]; *[1]Shimadzu Reseach Laboratory (Shanghai) Co., Ltd., Shanghai, China; [2]Shimadzu China Innovation Center, Shimadzu Corporation, Beijing, China*

MOE pm 04:10 **Integrating Model-Based Reconstruction and Deep Learning for Accelerating Mass Spectrometry Imaging**; Mithunjha Anandakumar[1, 2]; Timothy J Trinklein[2, 3]; Jonathan V Sweedler[1, 2, 3]; Fan Lam[1, 2]; *[1]Department of Bioengineering, University of Illinois Urbana-Champaign, Urbana, IL; [2]Beckman Institute for Advanced Science and Technology, University of Illinois Urbana-Champaign, Urbana, IL; [3]Department of Chemistry, University of Illinois Urbana-Champaign, Urbana, IL*

MOF PM: LIPIDOMICS: NEW MS TECHNOLOGIES AND APPLICATIONS

Ballroom I

Session Chair: Brittney L. Gorman (Pacific Northwest National Lab)

MOF pm 02:30 **Distinguishing Oxylipin Isomers with High Resolution Ion Mobility Spectrometry and Mass Spectrometry Separations**; Amie M. Solosky[1]; James N. Dodds[1]; Gerhard Hagn[2]; Craig E. Wheelock[2, 3]; Erin S. Baker[1]; *[1]University of North Carolina Chapel Hill, Chapel Hill, NC; [2]Karolinska Institutet, Solna, Sweden; [3]Karolinska University Hospital, Stockholm, Sweden*

MOF pm 02:50 **Tandem mass spectrometry imaging of low abundance ether phospholipids guided by bulk lipidomics analysis**; Tommy Zhang[1]; Sara Amer[1]; Julia Laskin[1]; *[1]Purdue Univeristy, West Lafayette, IN*

MOF pm 03:10 **OzSmart-MRM: AI-Powered Ozone Electrospray Ionization for Isomer-Specific MRM Profiling of Fatty Acids in Health and Disease**; Caitlin Randolph[1]; Connor H Beveridge[2]; Sanjay Iyer[2]; Palak Manchanda[2]; Stephen J. Blanksby[3]; Shane Tichy[4]; Gaurav Chopra[2, 5, 6, 7, 8]; *[1]Purdue University, West Lafayette, IN; [2]Purdue Univeristy, West Lafayette, IN; [3]School of Chemistry and Physics, Queensland University of Technology, Brisbane, Australia; [4]Agilent Technologies, Santa Clara, CA; [5]Purdue Institute for Integrative Neuroscience, West Lafayette, IN; [6]Purdue Institute for Inflammation, Immunology, and Infectious Disease, West Lafayette, IN; [7]Purdue Institute for Cancer Research, Purdue University, West Lafayette, IN; [8]Purdue Institute for Drug Discovery, West Lafayette, IN*

MOF pm 03:30 **High-Throughput and Highly Selective Quantitative Lipidomics Approach with the Stellar Mass Spectrometer – a Novel Hybrid Nominal Mass Instrument**; Brittany Lee[1]; Cristina C. Jacob[2]; Rahul Deshpande[1]; Susan Bird[3]; Magdalena Vagnerova[4]; Hector Gallart Ayala[4]; Julijana Ivanisevic[4]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientfic, San Jose, CA; [3]Thermo Fisher Scientific, Boston, MA; [4]University of Lausanne, Lausanne, Switzerland*

MOF pm 03:50 **OzMALDI: A Gas-Phase, In-Source Ozonolysis Reaction for Efficient Double-Bond Assignment in Mass Spectrometry Imaging with Matrix-Assisted Laser Desorption/Ionization**; Josiah Rensner[1]; Hyojin Kim[2]; Edgar Cahoon[2]; Kiyoul Park[2]; Young Jin Lee[1]; *[1]Iowa State University, Ames, IA; [2]University of Nebraska-Lincoln, Lincoln, NE*

MOF pm 04:10 **Enhanced Lipid Structural Characterization in Human Plasma Using Automated Micro-SPE Extraction and Multimodal (CID, EAD, UVPD) LC-MS**; Laura Gisela González Iglesias[1]; Romain Giraud[1]; Hagen M. Gegner[2]; Renzo Picenoni[2]; Guenter Boehm[2]; Gerard Hopfgartner[1]; *[1]University of Geneva, LSMS, Geneva, Switzerland; [2]CTC Analytics AG, Zwingen, Switzerland*

MOG PM: INSTRUMENTATION: NEW HYBRID AND MULTIMODAL APPROACHES

Ballroom III

Session Chair: Scott R. Kronewitter (Thermo Fisher Scientific)

MOG pm 02:30 **Evaluation of a modified Orbitrap Astral mass spectrometer for quantitative proteomics – beyond identification lists**; Michael J MacCoss[1]; Chris Hsu[1]; Nicholas Shulman[1]; Anna Pashkova[2]; Deanna L Plubell[1]; Eugen Damoc[2]; Hamish Stewart[2]; Johannes Petzoldt[2]; Brendan MacLean[1]; Philip Remes[3]; Andrew N Hoofnagle[4]; Alexander Makarov[2]; Christian Hock[2]; Vlad Zabrouskov[3]; Christine C Wu[1]; *[1]University of Washington - Genome Sciences, Seattle, WA; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [3]Thermo Fisher Scientific, San Jose, California; [4]University of Washington, Seattle, WA*

MOG pm 02:50 **Fully Parallelized Tandem MS on a 21 T FT-ICR/Orbitrap/Quadrupole/Ion Trap Hybrid Mass Spectrometer**; Chad R. Weisbrod[1]; Jesse D. Canterbury[2]; Mike Senko[3]; Lydia Babcock-Adams[1]; Marek Polak[1]; Nathan K. Kaiser[1]; Lissa C. Anderson[1, 4]; Kristina Hakansson[1, 4]; Christopher L Hendrickson[1]; *[1]National High Magnetic Field Laboratory, Tallahassee, FL; [2]ThermoFisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific, San Jose, California; [4]Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL*

MOG pm 03:10 **Isotopic Resolution from an Open-Source Digitally Driven Linear Ion Trap**; Adam P Huntley[1]; Gordon A. Anderson[2]; Peter T.A. Reilly[1]; Brian H. Clowers[1]; *[1]Washington State University Department of Chemistry, Pullman, WA; [2]GAA Custom Electronics, LLC, Kennewick, WA*

MOG pm 03:30 **Mass and mobility selective ion soft-landing and TEM structural analysis of conformationally dynamic protein assemblies**; Hari R Newnham[1, 2, 3]; Niklas Geue[1, 2, 3]; Elvin Cabrera[1, 2, 3]; Ellen Liggett[1, [2, 3]; Alexey Barkhanskiy[1, 2, 3]; Irene Del Mar Farinas Lucas[2, 3]; Richard Collins[3]; Alan Roseman[3]; Jakub Ujma[4]; Perdita E Barran[1, 2, 3]; *[1]Michael Barber Centre for Collaborative Mass Spectrometry, Manchester, United Kingdom; [2]Manchester Institute of Biotechnology, University of Manchester, Manchester, United Kingdom; [3]The University of Manchester, Manchester, United Kingdom; [4]Waters Corporation, Wilmslow, United Kingdom*

MOG pm 03:50 **Improving single-cell visualization through multi-modal mass spectrometry imaging and electron microscopy**; John Sentmanat[1]; Kisurb Choe[1]; Mazdak Taghioskoui[2]; Andrei Fedorov[1]; *[1]Georgia Institute of Technology, Atlanta, GA; [2]Trace Matters Scientific, Bethesda, MD*

MOG pm 04:10 **Computational and Data-Driven Approaches for Advancing Pesticide Detection through Chemical Ionization Mass Spectrometry (CIMS): A Multidisciplinary Approach**; Fariba Partovi[1, 2]; Joona Mikkilä[2]; Siddharth Iyer[1]; Federica Bortolussi[3]; Suvi Ojanperä[4]; Hilda Sandström[5]; Patrick Rinke[5]; Aleksei Shcherbinin[2]; Matti Rissanen[1, 3]; *[1]Aerosol Physics Laboratory, Physics Unit, Faculty of Engineering and Natural Sciences, Tampere University, Tampere, Finland; [2]Karsa Ltd, Helsinki, Finland; [3]Departement of Chemistry, University of Helsinki, Helsinki, Finland; [4]Finnish Customs, P.O. Box 512, FI-00101, Helsinki, Finland; [5]Department of Applied Physics, Aalto University, Espoo, Finland*

MOH PM: BIOTHERAPEUTICS: CHARACTERIZATIONS AND QUANTITATION

Ballroom IV

Session Chair: Josue Baeza (Merck)

MOH pm 02:30 **Addressing Challenges in Large Biomolecule Analysis using Charge Detection Mass Spectrometry**; Anisha Haris[1]; Rebecca J D'Esposito[2]; David Bruton[1]; Keith Richardson[1]; Jakub Ujma[1]; Chris Wheeldon[1]; Alistair Schofield[1]; Michael Danby[1]; David Eatough[1]; Kevin Giles[1]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Waters, Milford, MA*

MOH pm 02:50 **Characterization of mRNA Vaccines with Mass Photometry: Method Development and Technical Perspectives**; Lauren F Barnes[1]; Brenda Watt[2]; Josephine Rood[1]; Salma Jalal[3]; Gogulan Karunanithy[3]; Sarita Hebbar[3]; Leah Wang[1]; Jason Rouse[4]; *[1]Pfizer, Chesterfield, MO; [2]Refeyn Inc., Waltham, MA; [3]Refeyn Inc., Oxford, United Kingdom; [4]Pfizer Inc., Andover, MA*

MOH pm 03:10 **Ion Mobility-Mass Spectrometry and Collision Induced Unfolding Capture Antibody-Cytokine Complexes Revealing Polydisperse Oligomers and Structures**; Alyssa M. Erlenbeck[1]; Brandon T. Ruotolo[1]; *[1]University of Michigan-Ann Arbor, Ann Arbor, MI*

MOH pm 03:30 **Assessment of MAM vs Conventional QC Methods for Quantitative Analysis of PQAs of mAbs**; Jingzhong (Tim) Guo[1]; Sheila Mugabe[2]; Vishal Amancha[2]; Nithin Singam[2]; Sameer Kumar GS[2]; Li Jing[2]; Niomi Peckham[2]; Jarkko Huuskonen[2]; Dipankar Das[2]; Diane McCarthy[2]; *[1]US Pharmacopeia, Rockville, MD; [2]United States Pharmacopeia, Rockville, MD*

MOH pm 03:50 **Identification of Isobaric Mass Differences on Bispecific Monoclonal Antibodies by LC-MS Analysis**; Robert J Schuster[1]; Paul MacGregor[1]; Lana Fabia[1]; Nicole A Schneck[1]; *[1]GSK, Collegeville, PA*

MOH pm 04:10 **Rapid analysis of therapeutic antibodies by direct infusion peptide mapping**; Austin Z. Salome[1]; Alexander S. Hebert[1]; Craig D. Wenger[1]; Joomi Ahn[2]; Alayna M. George Thompson[3]; Harsha Gunawardena[4]; John S. Chlystek[1]; Pavel Sinitcyn[1]; Marcel Morgenstern[1]; Lia R. Serrano[1]; Keaton L. Mertz[1]; Scott T. Quarmby[1]; Joshua J. Coon[1, 5, 6]; *[1]University of Wisconsin-Madison, Madison, WI; [2]Eli Lilly, San Diego, CA; [3]AbbVie, Inc., North Chicago, IL; [4]JOHNSON AND JOHNSON, Spring House, PA; [5]Morgridge Institute for Research, Madison, WI; [6]CeleramAb Inc., Middleton, WI*

TUESDAY ORALS

TOA AM: BIOTHERAPEUTICS: PROTEINS, ANTIBODIES, AND ANTIBODY DRUG CONJUGATES
Hall AB
Session Chair: Shuai Wu (Amgen)

TOA am 08:30 **Collision Induced Unfolding Detects Shifts in Higher Order Structure within Antibody Polymer Conjugates**; Tiam Farajzadeh[1]; Devin M. Makey[1]; Brandon T. Ruotolo[1]; *[1]University of Michigan-Ann Arbor, Ann Arbor, MI*

TOA am 08:50 **Comprehensive Characterization of Disulfide Linkages in a Cysteine-Engineered Bispecific Antibody Using EThcD-on a modified Orbitrap Hybrid Mass Spectrometry**; Elsa Gorre[1]; Reiko Kiyonami[2]; Abby Chiang[3]; Alexander Barnakov[1]; Min Du[2]; Cong Wang[4]; Peter Krueger[4]; Andy Mahan[1]; Hirsh Nanda[1]; *[1]Johnson and Johnson Innovative Medicine, Spring House, PA; [2]Thermo Fisher Scientific, Lexington, MA; [3]Protein Metrics, LLC, Boston, Massachusetts; [4]Thermo Fisher Scientific, Bremen, Germany*

TOA am 09:10 **Characterizing O-glycosylation in the hinge region of immunoglobulin A by bottom-up and middle-up MS with electron activated dissociation**; Jonathan Dhenin[1]; Edwige Beng-Louka[1]; Heloise Hensinger[1]; Patrick Schindler[1]; *[1]Novartis Pharma AG, Basel, Switzerland*

TOA am 09:30 **Investigating the Complexity of Fc Fusion Proteins using a Modified Hybrid Orbitrap Mass Spectrometer**; Corentin Beaumal[1]; Sara Carillo[1]; Kai Scheffler[2]; Cong Wang[3]; Peter Krueger[3]; Heiner Koch[3]; Kelly Broster[4]; Jonathan Bones[1, 5]; *[1]Nat'l Inst. for Bioprocessing Research & Training, Dublin, Ireland; [2]Thermo Fisher Scientific, Germering, Germany; [3]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [4]Thermo Fisher Scientific, Hemel Hempstead, United Kingdom; [5]University College Dublin, Belfield, Ireland*

TOA am 09:50 **Ultrafast Microdroplet Digestion of Antibodies with Fc-Silencing Mutations**; Yongqing Yang[1]; Mengyuan Xiao[1]; Jim Lau[2]; Michael D Knierman[2]; Hui Zhao[2]; Xi Qiu[2]; Karen Luo[2]; Harsha Gunawardena[3]; Hao Chen[1]; *[1]New Jersey Institute of Technology, Newark, NJ; [2]Agilent Technologies, Wilmington, DE; [3]Janssen Pharmaceuticals, Spring House, PA*

TOA am 10:10 **Multi-activation middle-down mass spectrometry approach to relatively quantify positional isomers in oxidized therapeutic mAb samples**; Sarah Nguyen[1, 2, 3]; Armelle Martelet[3]; Severine Clavier[3]; Sarah Cianferani[1, 2]; Oscar Hernandez-Alba[1, 2]; *[1]LSMBO, IPHC, CNRS, Strasbourg, France; [2]Infrastructure Nationale de Protéomique ProFI, Strasbourg, France; [3]Sanofi R&D, Vitry-sur-Seine, France*

TOB AM: INSTRUMENTATION: INNOVATIVE SEPARATION APPROACHES COUPLED TO MS
Room 307-308
Session Chair: Michael L. Easterling (Bruker Daltonics, Inc.)

TOB am 08:30 **Fast LC Coupled to MS and IM-MS for High-Throughput Reaction Screening and Peptide Mapping**; Devin M. Makey[1]; Brandon T. Ruotolo[1]; Robert T. Kennedy[1]; *[1]University of Michigan, Ann Arbor, MI*

TOB am 08:50 **Alternative Structures for Lossless Ion Manipulations**; Cullen Greer[1]; Brian H. Clowers[1]; *[1]Washington State University, Pullman, WA*

TOB am 09:10 **Ultra-low flow porous layer open tubular liquid chromatography columns enable sensitive top-down and bottom-up proteomic analysis of limited samples**; Michal Gregus[1]; Yunfan Gao[1]; Somak Ray[1]; Anne-Lise Marie[1]; Alexander R. Ivanov[1]; *[1]Northeastern University, Boston, MA*

TOB am 09:30 **Nano flow ion-pairing LCMS for polar metabolomics**; Abigail E Ellis[1]; Rahul Deshpande[2]; Susan Bird[2]; Ryan D Sheldon[1]; *[1]Van Andel Institute, Grand Rapids, MI; [2]Thermo Fisher Scientfic, San Jose, CA*

TOB am 09:50 **Separation and Analysis of High Mass Virus-Like Particles by SEC-CD-MS**; Lohra M Miller[1]; Martin Jarrold[1, 2]; Benjamin E Draper[1]; Raj A Parikh[2]; Lavelay Kizekai[3]; Bala Addepalli[3]; Michelle Chen[4]; Matthew Lauber[3]; *[1]Megadalton Solutions, Bloomington, Indiana; [2]Indiana University, Bloomington, IN; [3]Waters Technology Corporation, Milford, MA; [4]Waters Technology Corporation, Goleta, CA*

TOB am 10:10 **High-Throughput Structural Analysis of Endogenous Protein Complexes by Native Top-Down Proteomics with Online Two-Dimensional Liquid Chromatography**; Matthew S Fischer[1]; Holden T Rogers[1]; Emily A Chapman[1]; Ying Ge[1]; *[1]University of Wisconsin-Madison, Madison, WI*

TOC AM: ENVIRONMENTAL: INNOVATIVE APPROACHES AND INSTRUMENTATION
Room 309-310
Session Chair: Trevor Glaros (Los Alamos National Laboratory)

TOC am 08:30 **Field Portable AFT-MS for Vapor Detection of Drugs and Explosives at Parts-Per-Trillion Levels of Vapor and Picograms of Residue**; Krisztian G. Torma[1]; Mike Chai[1]; William Yang Terziyan[1]; Robert G. Ewing[2]; Elizabeth H. Denis[2]; Shannon E. Schrader[2]; Garret L. Hart[2]; Megan K. Nims[2]; *[1]BaySpec Inc., San Jose, CA; [2]Pacific Northwest National Laboratory, Richland, WA*

TOC am 08:50 **Development of a Novel Aerosol and Vapor Chemical Threat Characterization Platform**; Ashish Chaudhary[1]; Gregory Vasquez[2]; Gottfried Kibelka[2]; *[1]Detect-ION, Tampa, FL; [2]Detect-Ion, Tampa, FL*

TOC am 09:10 **Protein biomarkers discovery of lead (Pb) toxicity and adaptive response in House Sparrows from Australian Mining Towns**; Zeshan Ali[1]; Riccardo Ton[1]; Rhiannon Schembri[1]; Sudip Bhandari[1]; Simon C Griffith[1]; Paul A. Haynes[1]; *[1]1School of Natural Sciences, Faculty of Science and Engineering, Macquarie University, North Ryde, Australia*

TOC am 09:30 **Continuous monitoring of PFAS degradation using boron nitride nanotube fabric photocatalysts**; Eleanor Castracane[1]; Benjamin G. Harvey[1]; Joseph E. Estevez[1]; Patrick W. Fedick[1]; *[1]Naval Air Warfare Center Weapons Division, China Lake, CA*

TOC am 09:50 **2025 Los Angeles Wildfires: VOC measurements from air, soil and rainwater using SIFT-MS**; Leslie Silva[1]; Heath Timmons[2]; *[1]Syft Technologies, Inc., Anaheim, CA; [2]University of California, Los Angeles, Los Angeles, CA*

TOC am 10:10 **Taking Science Anywhere: Portable, Real-Time Detection of PFOA and PFOS in Environmental and Biological Samples Using Multiple Ionization Methods**; Frank S Yenchick[1]; Dushan Kovacevic[1]; Milan Pophristic[2, 3]; Sarah Trimpin[1, 2]; *[1]Wayne State University, Detroit, MI; [2]MSTM, Newark, DE; [3]Saint Joseph's University, PHILADELPHIA, PA*

TOD AM: LIPODOMICS: TARGETED AND UNTARGETED
Room 314-317
Session Chair: Rafael Montenegro-Burke (University of Toronto)

TOD am 08:30 **How Endurance Exercise Training Alters the Rat Lipidome Profile of Plasma and Eight Tissues - a MoTrPAC Study**; David A Gaul[1]; Zhenxin Hou[2]; Chih-Yu Chen[2]; Tiantian Zhang[2]; Samuel G Moore[1]; Evan Savage[1]; Alexis Bennett[1]; Xueyun Liu[2]; Anna Ivanova[2]; Kristal Maner-Smith[2]; Christopher Newgard[3]; Sue C Bodine[4]; Eric A Ortlund[2]; Facundo M Fernández[1]; *[1]Georgia Institute of Technology,* *Atlanta, GA; [2]Emory University, Atlanta, GA; [3]Duke University, Durham, NC; [4]University of Iowa, Iowa City, IA*

TOD am 08:50 **Susceptibility of Glycerophospholipids to Non-Enzymatic Lipid Peroxidation**; Sazia Arefin Kachi[1]; Yulemni Morel[1]; Amir Mehrabani Tabari[1]; Chinmoy Sarkar[1]; Marta M. Lipinski[1]; Jace W. Jones[1]; *[1]University of Maryland, Baltimore, MD*

TOD am 09:10 **Structural elucidation of ganglioside isomers via high-resolution ion mobility-MS/MS**; Shuling Xu[1]; Zhijun Zhu[1]; Peng-Kai Liu[1]; Penghsuan Huang[1]; Zicong Wang[1]; Gaoyuan Lu[1]; Lingjun Li[1]; *[1]University of Wisconsin-Madison, Madison, WI*

TOD am 09:30 **Lipid Adaptations in Escherichia coli as a Mechanism of Antimicrobial Resistance**; Adriana Zardini Buzatto[1, 2]; Krupali Patel[1]; *[1]University of Calgary, Calgary, AB; [2]Calgary Metabolomics Research Facility, Calgary, AB*

TOD am 09:50 **Spatial Mapping of Isomeric Inflammation-Mediating Biomolecules Using Additive-Enhanced Nano-DESI Mass Spectrometry Imaging**; Syeda Nazifa Wali[1]; Manxi Yang[2, 3]; Miranda Weigand[2]; Zhong-Yin Zhang[2]; Julia Laskin[2]; *[1]Purdue University, West Lafayette, IN; [2]Purdue Univeristy, West Lafayette, IN; [3]Merck & Co., Rahway, NJ*

TOD am 10:10 **Highly Sensitive Targeted Method for Single Cell Lipidomics on Stellar MS– a Hybrid Nominal Mass Instrument**; Rahul Ravi Deshpande[1]; Ying Liu[2]; Bashar Amer[1]; David A. Gaul[2, 3]; Cristina Jacob[1]; Facundo Fernandez[2, 3]; Susan Bird[1]; *[1]Thermo Fisher Scientific, San Jose, California; [2]Systems Mass Spectrometry Core, Petit Institute of Bioengineering and Bioscience, Georgia Institute of Technology, Atlanta, GA; [3]School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, Georgia*

TOE AM: INFORMATICS: INNOVATIONS

Ballroom II

Session Chair: Aline Martins (University of California, San Diego)

TOE am 08:30 **Integration of longitudinal quality metrics enhances differential analysis in noisy large-scale Mass Spectrometry(MS)-based proteomics experiments acquired with DIA**; Devon Kohler[1]; Eralp Dogu[2]; Manuel Magana[3]; Mrittika Bhattacharya[4]; Veronica G Anania[3]; Olga Vitek[1]; *[1]Northeastern University, Boston, MA; [2]Mugla Sitki Kocman University, Köstekli, Turkey; [3]Genentech Inc., South San Francisco, CA; [4]Genentech, Inc., South San Francisco, CA*

TOE am 08:50 **FLASHApp: Interactive Data Analysis and Visualization for Top-Down Proteomics**; Tom D Müller[1, 2]; Jihyung Kim[1, 2]; Andrew Almaguer[3]; Ayesha Feroz[1, 2]; Axel Walter[1, 2]; Jaekwan Kim[4]; Wonhyeuk Jung[5]; Oliver Kohlbacher[1, 2, 6]; Kyowon Jeong[1, 2]; *[1]Applied Bioinformatics, Department for Computer Science, University of Tübingen, Tübingen, Germany; [2]Institute for Bioinformatics and Medical Informatics, University of Tubingen, Tubingen, Germany; [3]jambit GmbH, Stuttgart, Germany; [4]Fullseeomics, Seoul, South Korea; [5]Clinical Pharmacology and Safety Sciences, Astrazeneca, Gaithersburg, MD; [6]Translational Bioinformatics, University Hospital Tübingen, Tübingen, Germany*

TOE am 09:10 **A Task-Specific Transfer Learning Approach to Enhancing Small Molecule Retention Time Prediction with Limited Data**; Yuhui Hong[1]; Haixu Tang[1]; *[1]Indiana University, Bloomington, IN*

TOE am 09:30 **Foundation Model for Mass Spectrometry-Based Proteomics - Enabling Interpretable Open and Error-Tolerant Searching and More**; Tom Altenburg[1]; Thilo Muth[2]; Patrick Van Zalm[3, 4]; Hanno Steen[3, 4]; Bernhard Y Renard[1, 3, 5]; *[1]Hasso Plattner Institute, Potsdam, Germany; [2]Robert Koch Institute, Berlin, Germany; [3]Boston children's hospital, Boston, MA; [4]Harvard Medical School, Boston, MA; [5]Icahn School of Medicine at Mount Sinai, New York City, NY*

TOE am 09:50 **One model to predict them all - accurate and fast zero-shot peptide spectrum prediction for any post-translational modification**; Lizi Mamisashvili[1]; Igor Brohnshtein[2]; Vishal Sukumar[1]; Daniel P. Zolg[1]; Florian Seefried[1]; Tobias Schmidt[1]; Siegfried Gessulat[2]; Martin Frejno[1]; *[1]MSAID, Garching b. München, Germany; [2]MSAID, Berlin, Germany*

TOE am 10:10 **image2image: An Open-Source Framework for Multi-Modal Image Registration of Imaging Mass Spectrometry, Spatial Transcriptomics, and Microscopy Data**; Lukasz G Migas[1, 2]; Angela R. S. Kruse[2, 3]; John W. Hickey[4]; David M.G. Anderson[2, 5]; Melissa A Farrow[2, 3]; Roy Lardenoije[6]; Madeline E Colley[2, 3]; Joana P. Gonçalves[6]; Jeffrey M Spraggins[2, 3, 5, 7]; Raf Van De Plas[2, 8]; *[1]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [2]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [3]Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; [4]Department of Biomedical Engineering, Duke University, Durham, NC; [5]Department of Biochemistry, Vanderbilt University, Nashville, TN; [6]Department of Intelligent Systems, Delft University of Technology, Delft, Netherlands; [7]Department of Chemistry, Vanderbilt University, Nashville, TN; [8]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands*

TOF AM: IMAGING: PHARMACEUTICALS, METABOLITES, LIPIDS, AND GLYCANS

Ballroom I

Session Chair: Nannan Tao (Bruker)

TOF am 08:30 **Multimodal imaging reveals lipidomic differences in renal cell types between deep and superficial glomeruli**; Allison B Esselman[1, 2]; Felipe A Moser[3]; Léonore E M Tideman[3]; Lukasz G Migas[1, 3]; Thai Pham[1, 4]; Anna Smith[1, 4]; Jacqueline M Van Ardenne[1, 2]; Madeline E Colley[1, 4]; Melissa A Farrow[1, 4]; Haichun Yang[5, 6]; Agnes B Fogo[5, 6, 7, 8]; Mark DeCaestecker[7]; Raf Van De Plas[1, 3, 9]; Jeffrey M Spraggins[1, 2, 4, 5, 9]; *[1]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [2]Department of Chemistry, Vanderbilt University, Nashville, TN; [3]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [4]Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; [5]Department of Pathology, Microbiology, and Immunology, Vanderbilt University Medical Center, Nashville, TN; [6]Department of Pediatrics, Vanderbilt University Medical Center, Nashville, TN; [7]Division of Nephrology and Hypertension, Vanderbilt University Medical Center, Nashville, TN; [8]Department of Medicine, Vanderbilt University Medical Center, Nashville, TN; [9]Department of Biochemistry, Vanderbilt University, Nashville, TN*

TOF am 08:50 **Evaluation of NAD/NADH levels in a CD38 knockout mouse model following NAM treatment by MALDI Mass Spectrometry imaging**; Junhai Yang[1]; Andrew Bowman[1]; Christopher Good[1]; Emine Can Hamel[2]; Maria Quinton[1]; Jens Hamann-Fenton[2]; David S Wagner[1]; *[1]Abbvie Inc, Waukegan, IL; [2]Calico Science LLC, South San Francisco, CA*

TOF am 09:10 **From Biopsy to Biofluids: MALDI-MSI N-Glycan Profiling as a Step Toward Non-Invasive Lupus Nephritis Diagnosis and Monitoring**; Aaron Angerstein[1]; Tamara K Nowling[2]; Vishwajeeth

Pasham[3]; Bethany J Wolf[4]; Jim C Oates[2]; Richard R Drake[1]; [1]*Department of Pharmacology and Immunology, Medical University of South Carolina, Charleston, SC;* [2]*Department of Medicine, Rheumatology Division, Medical University of South Carolina, Charleston, SC;* [3]*Department of Pathology and Lab Medicine, Medical University of South Carolina, Charleston, SC;* [4]*Department of Public Health Sciences, Medical University of South Carolina, Charleston, Charleston, SC*

TOF am 09:30 **Mass Spectrometry Imaging of BRG399: Spatial Drug Distribution and Metabolite Profiling in Immunogenic Cell Death for Cancer Therapy**; Sylwia Stopka[1]; Juan J Aristizabal-Henao[1]; Srada Karmacharya[1]; Kaila M Bennett[1]; Jacob P Matson[1]; Archna Ravi[1]; Andressa L Mota[1]; Dinesh Chimmanamada[2]; Vivek K Vishnudas[1]; Stephane Gesta[1]; Niven R Narain[1, 3]; Abbas Khojasteh[4]; Lawrence Recht[4]; Maria-Dorothea Nastke[1]; Michael A. Kiebish[1]; [1]*BPGbio, Framingham, MA;* [2]*Coorg Biosciences, Arlington, MA;* [3]*University of Miami, Miami, Florida;* [4]*Stanford University, Stanford, CA*

TOF am 09:50 **Lipid and neurotransmitter spatial distribution in transgenic rat model of Alzheimer's disease using MALDI MS imaging**; Tong Shen[1]; Pamela Lein[2]; Oliver Fiehn[1]; [1]*West Coast Metabolomics Center, University of California, DAVIS, CA;* [2]*Department of Molecular Biosciences, School of Veterinary Medicine, University of California, Davis, CA*

TOF am 10:10 **Cancer biomarker discovery from FFPE samples by multi-modal integration of Laser Desorption Rapid Evaporation Ionization Mass Spectrometry (LD-REIMS) using LC-MS**; Yuting Lu[1]; Yu Zhang[1]; Daniel Simon[1, 2]; Virag Sagi-Kiss[1]; Rachel Lai[1]; Yuchen Xiang[1]; Zoltan Takats[1, 2]; [1]*Imperial College London, Division of Systems Medicine, London, United Kingdom;* [2]*University of Regensburg, Department of Immune Medicine Multimodal Imaging of Intracellular Communication, Regensburg, Germany*

TOG AM: FORENSICS, INNOVATIONS AND APPLICATIONS
Ballroom III
Session Chair: Danielle Aldredge (Amgen)

TOG am 08:30 **Accelerating Countermeasure Candidate Discovery for Organophosphorus Chemical Warfare Agents**; Nicolas M Morato[1, 2]; Todd H Corzett[3]; Katelyn E Mason[3]; Carlos A Valdez[3]; Teneile M Alfaro[3]; Saphon Hok[3]; Brian P Mayer[3]; R. Graham Cooks[1, 2]; [1]*Department of Chemistry, Purdue University, West Lafayette, IN;* [2]*Purdue Institute for Cancer Research, Purdue University, West Lafayette, IN;* [3]*Forensic Science Center, Lawrence Livermore National Laboratory, Livermore, CA*

TOG am 08:50 **Non-Contact Sampling for Rapid Detection of Chemical Residues on Objects Using High-Resolution Chemical Ionization Mass Spectrometry**; HJ Jost[1]; Joona Mikkilä[1]; Jyri Mikkilä[1]; Paxton Juuti[1]; Jussi Kontro[1]; Aleksei Shcherbinin[1]; [1]*Karsa Ltd, Helsinki, Finland*

TOG am 09:10 **Classifying Physical Activity from Endogenous Fingerprint Lipids with Machine Learning and MALDI-MS**; Daphne R Patten[1]; Raven L Buckman Johnson[1]; Trevor T Forsman[1]; Young Jin Lee[1]; [1]*Iowa State University, Ames, IA*

TOG am 09:30 **A Fast, Validated Oral Fluid Toxicology Screening Workflow With DART-MSMS**; Francois A Espourteille[1]; Terry Bates[1]; Marc Y Chalom[1]; [1]*Bruker Applied Mass Spectrometry, Billerica, MA*

TOG am 09:50 **Let’s get cracking! The detection and identification of cannabidiol pyrolysis products**; Rabi A Musah[1]; Niara A Nichols[1]; A John Dane[1]; Kirk Jensen[2]; [1]*Louisiana State University, Baton Rouge, LA;* [2]*JEOL USA, Inc., Peabody, MA*

TOG am 10:10 **What do Volcanic Eruptions and Urban Fires Have in Common? Ash Clouds filled with BPCAs—Forensic Analysis by LC/QTOF-MS**; Michael Thurman[1]; Imma Ferrer[1]; James Pyke[2]; [1]*University of Colorado, Boulder, CO;* [2]*Agilent Technologies, Melbourne, Australia*

TOH AM: FUNDAMENTALS: UNCONVENTIONAL APPROACHES IN MS
Ballroom IV
Session Chair: Dmitry Eremin (Caltech)

TOH am 08:30 **Mapping Chemical Reaction Networks by Integrating Electrospray Ionization-Mass Spectrometry and Continuous Flow Chemistry**; Quentin Duez[1, 2]; Jeroen Van De Wiel[2]; Bob Van Sluijs[2]; Wilhelm T. S. Huck[2]; Pascal Gerbaux[1]; [1]*University of Mons, Mons, Belgium;* [2]*Radboud University, Nijmegen, Netherlands*

TOH am 08:50 **Probing Reactions at Electrode Interfaces through Electrochemistry Mass Spectrometry**; Bethany A. Phillips[1]; Patrick J. Herchenbach[1]; Jeffrey E. Dick[1]; Julia Laskin[1]; [1]*Purdue University, West Lafayette, IN*

TOH am 09:10 **IMS-MS/MS-microED Pipeline for Structural Elucidation of Small Molecules**; Bela Paizs[1, 2]; Marcus Gallagher-Jones[1]; Stefan Lohmann[1]; Amar Rai[1, 3]; Aleyna Lumsden[1]; Daniel McGill[1]; Zhiyuan Ding[1]; Zoltan Takats[2, 3]; Adam Nelson[1, 4]; Angus Kirkland[5]; [1]*Rosalind Franklin Institute, Didcot, United Kingdom;* [2]*deShape Ltd., London, United Kingdom;* [3]*Imperial College London, London, United Kingdom;* [4]*University of Leeds, Leeds, United Kingdom;* [5]*University of Oxford, Oxford, United Kingdom*

TOH am 09:30 **Mass Spectrometric Validation of Scaled Thin-Film Reactors for the Accelerated Formation of Trinitrotoluene**; Elise E. Tseng[1]; Michael K. Bellas[1]; Patrick W. Fedick[1]; Benjamin G. Harvey[1]; [1]*Naval Air Warfare Center Weapons Division, China Lake, CA*

TOH am 09:50 **Use of Acoustic Ion Manipulation (AIM) for Atmospheric Pressure Ion Gating**; Jake Shelley[1]; Julia L Danischewski[1]; Yi You[2]; Lauren Bauer[1]; Josefin Hufgard[2]; Jens Riedel[2]; [1]*Rensselaer Polytechnic Institute, Troy, NY;* [2]*Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, Germany*

TOH am 10:10 **Mild and efficient coupling reactions enabled by in situ electrolytically generated Cu(I) cation catalyst in nanoelectrospray**; Annesha Sengupta[1]; Disni Gunasekera[1]; Gopal Reddy Ramidi[1]; Mia Beaudoin[1]; Shiqing Xu[1, 2]; Xin Yan[1]; [1]*Department of Chemistry, Texas A&M University, College Station, TX;* [2]*Department of Pharmaceutical Sciences, Texas A&M University, College Station, TX*

TOA PM: DATA-INDEPENDENT ACQUISITION: ACQUISITION AND MULTIPLEXING
Hall AB
Session Chair: Dirk Valkenborg (Hasselt University)

TOA pm 02:30 **Towards Increasing the Throughput of DIA LC-MS/MS Measurement with Novel Nonisobaric Mass Tags**; Madeline J Yeh[1]; Harrison Specht[1]; Sarah N Sipe[1]; Nikolai Slavov[1, 2]; [1]*Parallel Squared Technology Institute, Watertown, MA;* [2]*Northeastern University, Boston, MA*

TOA pm 02:50 **Accurate multiplexing on the Orbitrap Astral with TMTpro complementary ion quantification**; Alex Johnson[1]; Martin Zeller[2]; Hamish Stewart[2]; Pedro Navarro[2]; Bernard Delanghe[2]; Graeme C. McAlister[3]; Martin Wühr[1]; [1]*Princeton University, Princeton, NJ;* [2]*Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany;* [3]*Thermo Fisher Scientific, San Jose, CA*

TOA pm 03:10 **Sensitive detection of cancer neoantigens enabled by user-defined peptide libraries**; Claudia

Ctortecka[1]; Kasidet Manakongtreecheep[1, 2, 3]; Matthew Bakalar[1]; Timothy Zhu[1, 3]; Griffin Lawrence[1]; Isabelle Lippincott[1]; Gabrielle M. Hernandez[1]; Luis O. Correa-Medero[1]; Cleo Forman[2]; Alexey I. Nesvizhskii[4]; Giacomo Oliveira[3]; Karl R Clauser[1]; Siranush Sarkizova[1]; Jennifer G. Abelin[1, 3]; Nir Hacohen[1, 3, 5]; Steven A. Carr[1]; Catherine J. Wu[1, 2, 3]; *[1]Broad Institute of MIT and Harvard, Cambridge, MA; [2]Harvard Medical School, Boston, MA; [3]Dana-Farber Cancer Institute, Boston, MA; [4]University of Michigan, Ann Arbor, MI; [5]Massachusetts General Hospital, Boston, MA*

TOA pm 03:30 **Enhanced Immunopeptide Identification Using MIDIA-PASEF: A Novel timsTOF Scan Mode**; Jonathan R Krieger[1]; Diego Assis[2]; Matthew Willetts[2]; Nicholas Cheung[3]; Robert Salzler[3]; *[1]Bruker Ltd., Milton, ON; [2]Bruker Scientific LLC, Billerica, MA; [3]Regeneron, Tarrytown, NY*

TOA pm 03:50 **Closing the gap between targeted and untargeted measurements using intelligent data acquisition on Stellar MS**; Lilian Randolph Heil[1]; Cristina Jacob[2]; Nicholas Shulman[3]; Brendan X. MacLean[3]; Michael J. MacCoss[3]; Philip Remes[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]ThermoFisher Scientific, San Jose, CA; [3]University of Washington, Seattle, WA*

TOA pm 04:10 **Double dipping: confirmation bias inflates DIA data completeness**; Michelle T. Berger[1]; Alexander Hogrebe[2]; Daniel P Zolg[1]; Florian Seefried[1]; Martin Heinrich Frejno[1]; *[1]MSAID, Garching b.München, Germany; [2]MSAID, Berlin, Germany*

TOB PM: INSTRUMENTATION: AMBIENT IONIZATION AND APPLICATIONS
Room 307-308
Session Chair: Liang Li (University of Alberta)

TOB pm 02:30 **Fit-for-Purpose Ionization on Portable Instruments for Comprehensive, Fast, Accurate, Affordable and User-friendly Analyses within Seconds**; Sarah Trimpin[1, 2]; Frank Yenchick[1]; Ravin Rayes[1]; Dushan Kovacevic[1]; Sullivan Stimac[3]; Jessalyn Aquilino[2, 4]; Paul Stemmer[1]; John Tomsho[4]; Barbara Larsen[5]; Kevin Rackers[6]; Ken Mackie[7]; Ellen Inutan[2, 8]; Charles N McEwen[2, 4]; Milan Pophristic[2, 4]; *[1]Wayne State University, Detroit, MI; [2]MSTM, Newark, DE; [3]Churchill High School, Livonia, Michigan; [4]Saint Joseph's University, PHILADELPHIA, PA; [5]Larsen Scientific Consulting, West Chester, Pennsylvania; [6]Automation Techniques, Greensboro, North Carolina; [7]Indiana University, Bloomington, IN; [8]Mindanao State University - Iligan Institute of Technology, Illigan City, Philippines*

TOB pm 02:50 **Coaxial Conductance Probe for Uneven Clinical/Biological Sample Investigation with Mass Spectrometry**; Rachel K. Wood[1]; Malek Hassan[1]; Rachel E. Rubino[2]; Madeleine Carew[3]; Christopher J.B. Nicol[2, 3]; Richard D. Oleschuk[1]; *[1]Department of Chemistry, Queen's University, Kingston, Ontario; [2]Sinclair Cancer Research Institute, Queen's University, Kingston, Ontario; [3]Department of Pathology and Molecular Medicine, Queen's University, Kingston, Ontario*

TOB pm 03:10 **An in-depth Study of the Desorption Characteristics of Infrared Lasers Utilized for Ambient Mass Spectrometry**; Daniel Simon[1, 2]; Yu Wang[3]; Yuchen Xiang[2]; Gabriel Stefan Horkovics-Kovats[1]; Istvan Pap[1]; Robert Murray[3]; Zoltan Takats[1, 2]; *[1]University of Regensburg, Department of Functional Genomics, Regensburg, Germany; [2]Imperial College London, Division of Systems Medicine, London, United Kingdom; [3]Imperial College London, Department of Physics, London, United Kingdom*

TOB pm 03:30 **Site Selective and Tunable Chlorination of Arenes and Heteroarenes in Charged Microdroplets**; Owen L Looker[1]; Rebekah E Strong[1]; Abraham K. Badu-Tawiah[1]; *[1]The Ohio State University, Columbus, OH*

TOB pm 03:50 **Identification of Chemical Warfare Agents in Soil Using 3D-printed Cone Spray Ionization on a Portable Mass Spectrometer**; Daniel O. Carmany[1]; Brian Molnar[2]; Ebenezer Bondzie[3]; Hilary M. Brown[2]; Paul S Demond[1]; Elizabeth Dhummakupt[1]; Christopher Mulligan[3]; Patrick W Fedick[2]; *[1]DEVCOM Chemical Biological Center, Aberdeen Proving Ground, MD; [2]Naval Air Warfare Center Weapons Division, China Lake, CA; [3]Illinois State University, Normal, IL*

TOB pm 04:10 **Revealing the Glycosaminoglycan Signature in Ischemic Stroke Brain Using IR-MALDESI Mass Spectrometry Imaging**; Tana Palomino[1]; Tatiana Segura[2]; David C Muddiman[1]; *[1]Biological Imaging Laboratory for Disease and Exposure Research (BILDER), Department of Chemistry, North Carolina State University, Raleigh, NC; [2]Department of Biomedical Engineering, Duke University, Durham, NC*

TOC PM: MICROBES AND THE MICROBIOME
Room 309-310
Session Chair: Peder Lund (Case Western Reserve University)

TOC pm 02:30 **Plasma metabolomics uncovers characteristic metabolic aberrancies and predictive biomarkers in early-onset Pediatric Crohn's Disease**; Zhiwei Zhou[1]; Yuanyuan Liu[1]; Ruben Colman[1]; Michael Rosen[1]; Michael Fischbach[1]; Dylan Dodd[1]; *[1]Stanford University, Palo Alto, CA*

TOC pm 02:50 **High-precision in vivo model to identify a causative, microbiome-dependent metabolite in animals genetically predisposed to autism-spectrum disorders**; Byoungsook Goh[1]; Yunjin Lee[2]; Sang-Mok Lee[1, 2]; Jinseok Park[2]; Minjin Kim[2]; Jun R Huh[2]; Sungwhan F Oh[1, 2]; *[1]Brigham and Women's Hospital, Boston, MA; [2]Harvard Medical School, Boston, Massachusetts*

TOC pm 03:10 **Elucidating bacterial mechanisms of antifungal activity towards fungal pathogens with spatial multiomics**; Kevin J Zemaitis[1]; Audrey G Thomas[2]; Dora Farago[3]; Pranav Dawar[4]; Theresa F Law[2, 5]; Qun Liu[3]; Louis K Prom[6]; Jeffrey L Dangl[2, 5]; Ljiljana Pasa-Tolic[1]; *[1]Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA; [2]Department of Biology, University of North Carolina at Chapel Hill, Chapel Hill, NC; [3]Biology Department, Brookhaven National Laboratory, Upton, NY; [4]Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, Washington 99354; [5]Howard Hughes Medical Institute, University of North Carolina at Chapel Hill, Chapel Hill, NC; [6]United States Department of Agriculture Agricultural Research Service, Southern Plains Agricultural Research Center, College Station, TX*

TOC pm 03:30 **The mleN enzyme in ceftriaxone-resistant Neisseria gonorrhoeae impacts fitness through a putative lysine transport-mediated mechanism**; Stephanie L. Bishop[1]; Maria X. Cardenas-Alvarez[2]; Kate Newns[2, 3]; Julia Adug[4]; Yonatan H. Grad[5]; Robert A. Nicholas[2]; Ian A. Lewis[4]; *[1]University of Western Ontario, London , ON ; [2]University of North Carolina at Chapel Hill, Chapel Hill, NC; [3]Envision Pharma Group, Raleigh, North Carolina; [4]University of Calgary, Calgary, AB; [5]Harvard T. H. Chan School of Public Health, Boston, Massachusetts*

TOC pm 03:50 **Exploring the influence of S. aureus lipase activity on intra- and extracellular lipid**

composition; David T Brewer[1]; Kelly M Hines[1]; *[1]University of Georgia, Athens, GA*

TOC pm 04:10 **Native top-down proteomics reveals a novel mechanism of heme acquisition in model Gram+ pathogenic bacteria Corynebacterium diphtheriae and Staphylococcus aureus**; Andrew K Goring[1]; Jordan Ford[2]; Brendan J. Mahoney[2]; Rachel R. Loo[2]; Robert T. Clubb[2]; Joseph A. Loo[2]; *[1]University of California, Los Angeles, Los Angeles, CA; [2]UCLA, Los Angeles, CA*

TOD PM: FUNDAMENTALS: CHEMISTRY OF GAS-PHASE IONS (HONORING VERONICA BIERBAUM)

Room 314-317

Session Chair: Charles M. Nichols (AOA Dx)

TOD pm 02:30 **Oxygen Attachment Dissociation of Protonated Alkaloids**; Jack Li[1]; Chris Bowen[2]; Bun Chan[3]; Hidenori Takahashi[4]; Richard A. J. O'Hair[5]; *[1]University of Melbourne, Melbourne, Australia; [2]Shimadzu Scientific, Bio21 Institute of Molecular Science and Biotechnology, The University of Melbourne, Melbourne, Australia; [3]Nagasaki University, Nagasaki, Japan; [4]Koichi Tanaka Mass Spectrometry Research Laboratory, Shimadzu Corporation, Kyoto, Japan; [5]University of Melbourne, Victoria, Australia*

TOD pm 02:50 **Identification of Aromatic Aldehyde and Keto Functionalities via Gas-phase Ion-molecule Reactions and Collision-activated Dissociation in Linear Quadrupole Ion-Trap Mass Spectrometer**; Jaskiran Kaur[1]; Ruth O. Anyaeche[2]; Yue Fu[2]; Landon Wence[1]; John Nash[1]; Hilkka I Kenttamaa[1]; *[1]Purdue Univeristy, West Lafayette, IN; [2]Corteva Agriscience, Indianapolis, IN*

TOD pm 03:10 **Characterizing mechanisms of proton, metal, and methyl transfer in gas-phase charge inversion ion/ion reactions involving lipids and diacids**; Yingchan Guo[1]; Jonathan T Specker[1]; Ramón Alain Miranda-Quintana[1]; Boone M Prentice[1]; *[1]University of Florida, Department of Chemistry, Gainesville, FL*

TOD pm 03:30 **SIFT-MS: Ion-Molecule Reaction Coupled with Mass Spectrometry for Real-World Applications**; Gary Williams[1]; Leslie Silva[2]; Vaughan Langford[3]; Daniel Milligan[3]; *[1]Syft, ithaca, NY; [2]Syft Technologies, Anaheim, CA; [3]Syft Technologies, Inc., Anaheim, CA*

TOD pm 03:50 **IR Predissociation of Acetaldehyde-Oxirane Radical Cation Reaction Product: Methylenating Agents in Astronomical Environments**; Davide Corinti[1]; Maria Elisa Crestoni[1]; Simonetta Fornarini[1]; Sandra Brünken[2]; Marius D. Gerlach[2]; Daniel B. Rap[2]; Paul Michael Mayer[3]; *[1]Sapienza - University of Rome, Rome, Italy; [2]Radboud University, Nijmegen, Netherlands; [3]University of Ottawa, Ottawa, ON*

TOD pm 04:10 **Gas-Phase Reactivity and Photochemistry of Halogen Oxide Anions: Atmospheric Implications**; Samuel C. Brydon[1]; Berwyck L. J. Poad[1, 2]; David L. Marshall[2]; Paddy D. Kelly[3]; Boris Ucur[3]; Benjamin I. McKinnon[3]; Samuel J. P. Marlton[4]; Jack Buntine[4]; Péter Szabó[5]; Jeremy N. Harvey[5]; Evan J. Bieske[4]; Adam J. Trevitt[3]; Stephen J. Blanksby[1, 2]; *[1]School of Chemistry and Physics, Queensland University of Technology, Brisbane, Australia; [2]Central Analytical Research Facility, Queensland University of Technology, Brisbane, Australia; [3]Molecular Horizons and School of Chemistry and Molecular Bioscience, University of Wollongong, Wollongong, Australia; [4]School of Chemistry, The University of Melbourne, Parkville, Australia; [5]Department of Chemistry, Katholieke Universiteit, Leuven, Belgium*

TOE PM: PROTEIN-LIGAND AND PROTEIN-PROTEIN INTERACTIONS

Ballroom II

Session Chair: Si Wu (University of Alabama)

TOE pm 02:30 **Concurrent Affinity Selection Mass Spectrometry (ASMS) Screening of GLP1R and CLDN4: A Higher-Throughput Method for the Screening of Membrane-bound Proteins**; Zane Thistleford[1]; Donald Green[1]; Patrick O'Loughlin[1]; Daniel Cohen[1]; Jan Kubicek[2]; Barbara Maertens[2]; Can Jon Ozbal[1]; *[1]Momentum Biotechnologies, Billerica, MA; [2]Cube Biotech, Monheim, Germany*

TOE pm 02:50 **Unraveling the dynamics of mitochondrion-lysosome interactions using a new automated proximity labeling proteomics workflow**; Haorong Li[1]; Noah Smeriglio[2]; Jiawei Ni[2]; Shiori Sekine[3]; Yan Wang[4]; Ling Hao[2]; *[1]George Washington University, Washington, DC; [2]University of Maryland, College park, Hyattsville, MD; [3]University of Pittsburgh, Pittsburgh, PA; [4]National Institutes of Health, Bethesda, MD*

TOE pm 03:10 **BioPlex: Experimental Profiling and Structural Modeling of Protein Interactions for Drug Discovery**; Edward L. Huttlin[1]; Laura Pontano Vaites[1]; Miljan Kuljanin[1]; Jiaming Li[1]; Nathan Zuniga Pena[1]; Lana D'Addieco[1]; Austin Fergusson[1]; Fana Gebreab[1]; Emily Hill[1]; Karina Martinez Perez[1]; Ramin Rad[1]; Joao Paulo[1]; Ernst Schmid[1]; Johannes Walter[1]; David P Nusinow[2]; Donald S. Kirkpatrick[2]; Tyrone Lee[1]; Ludwig Geistlinger[1]; J Wade Harper[1]; Steven P Gygi[1]; *[1]Harvard Medical School, Boston, MA; [2]Xaira Therapeutics, South San Francisco, CA*

TOE pm 03:30 **Evaluating Lipid Selectivity of G Protein-Coupled Receptors Using Untargeted Native Top-Down Mass Spectrometry**; Sophie A. S. Lawrence[1, 2]; Carla Kirschbaum[1, 2]; Haigang Song[1, 2]; Joshua D. Hinkle[3]; Christopher Mullen[3]; John E. P. Syka[3]; Corinne A. Lutomski[1, 2]; Tarick J. El-Baba[1, 2]; Carol V. Robinson[1, 2]; *[1]Kavli Institute for Nanoscience Discovery, University of Oxford, Oxford, United Kingdom; [2]Department of Chemistry, University of Oxford, Oxford, United Kingdom; [3]ThermoFisher Scientific, San Jose, CA*

TOE pm 03:50 **Uncovering the Higher-Order Structural Characteristics, Protein-Ligand Binding, and Proteoform Heterogeneity of AMP-Activated Protein Kinase Complex by Integrated Top-Down Mass Spectrometry**; Hsin-Ju Chan[1]; Boris Krichel[2, 3, 4]; Liam J. Bandura[1]; Emily A. Chapman[1]; Man-Di Wang[1]; Emily A. Reasoner[1]; Ying Ge[1, 2, 5]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [2]Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI; [3]CSSB Centre for Structural Systems Biology, Deutsches Elektronen-Synchrotron DESY & Leibniz Institute of Virology (LIV) & University of Lübeck, Notkestraße, Hamburg, Germany; [4]Institute of Chemistry and Metabolomics, University of Lübeck, Lübeck, Germany; [5]Human Proteomics Program, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI*

TOE pm 04:10 **Effects of post-translational modifications on mAb target binding and blocking of weak ligand-receptor interactions assessed by SEC and LC-MS**; Daniel W Woodall[1]; Joshua Tokuda[1]; Nicholas Clark[1]; Andrew Dykstra[1]; Athena Sudom[2]; Kelli Matthies[1]; Brian Bennett[1]; Jonathan Phillips[1]; Pavel V Bondarenko[1]; *[1]Amgen, Thousand Oaks, CA; [2]Amgen, South San Francisco, CA*

TOF PM: GLYCOPEPTIDES, GLYCOPROTEINS

Ballroom I

Session Chair: Hyun Joo An (Chungnam National University)

TOF pm 02:30 **Human Plasma Glycopeptide Libraries for Human Plasma Glycoproteome Profiling**; Yi Liu[1]; Meghan C. Burke[1]; Yuri Mirokhin[1]; Sergey Sheetlin[1];

Yuxue Liang[1]; Xiaoyu Yang[1]; Guanghui Wang[1]; Zheng Zhang[1]; Zach Goecker[1]; Connie Remoroza[1]; Dmitrii Tchekhovskoi[1]; Steve Stein[1]; *[1]NIST, Gaithersburg, MD*

TOF pm 02:50 **Pan-cancer N-glycoproteomic atlas of patient-derived xenografts uncovers FAT2 as a therapeutic target for head and neck cancers**; Thomas Kislinger[1]; Meinusha Govindarajan[2]; Salvador Mejia-Guerrero[1]; Shawn Chafe[3]; Shahbaz Khan[1]; Wei Shi[1]; Matthew Waas[1]; Amanda Khoo[2]; Lydia Y. Liu[2]; Vladimir Ignatchenko[1]; Simona Principe[1]; Lusia Sepiashvili[2]; Nazanin Tatari[3]; Chitra Venugopal[3]; Petar Miletic[3]; Maxwell Topley[3]; Shan Grewal[3]; Maria-Jose Sandi[1]; Nhu-An Pham[1]; Alison Casey[1]; Hyeyeon Kim[2]; Peter Bergqvist[4]; Begonia Moreno Silva[4]; Patrick Hau Wing Chan[4]; Liza Cerna-Portillo[4]; Jasmine Ai Wei Chin[4]; Abilasha Rao[4]; Ming-Sound Tsao[1]; Rama Khokha[1]; Susie Su[1]; Wei Xu[1]; David Goldstein[1]; Laurie Ailles[1]; Vuk Stambolic[1]; Fei-Fei Liu[1]; Emma Cummins[4]; Ismael Samudio[4]; Sheila Singh[3]; *[1]Princess Margaret Cancer Centre, Toronto, ON; [2]University of Toronto, Toronto, ON; [3]McMaster University, Hamilton, ON; [4]adMare BioInnovations, Vancouver, BC*

TOF pm 03:10 **Mapping the Site-specific Lifetime and Kinetic Landscape of N-linked Glycoproteins**; Yi Di[1]; Yuzhuo Gu[2]; Wenxue Li[1]; Jicong Zhang[2]; Zhiqiang Xue[2]; Shuo Qian[1]; Chao Liu[2]; Yansheng Liu[1]; *[1]Yale University, West Haven, CT; [2]Beihang University, Beijing, China*

TOF pm 03:30 **High-throughput Quantitative Analysis of O-glycosylation in Diabetes**; Feixuan Wu[1]; Dylan Tabang[2, 3]; Peng-Kai Liu[4]; Connie Chamberlain[5]; Jon Odorico[5]; Lingjun Li[1, 3, 4]; *[1]University of Wisconsin-Madison School of Pharmacy, Madison, WI; [2]Department of Pathology, Boston Children's Hospital & Harvard Medical School, Boston, MA; [3]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [4]Biophysics Graduate Program, University of Wisconsin-Madison, Madison, WI; [5]Department of Surgery, Division of Transplantation, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, Wisconsin*

TOF pm 03:50 **Discovery and characterization of tyrosine O-GlcNAcylation as a novel type of glycosylation on many proteins**; Junfeng Ma[1]; Chunyan Hou[1]; Jingtao Deng[1]; Ci Wu[1]; *[1]Georgetown University Medical Center, Washington, DC*

TOF pm 04:10 **Chemical Proteomics for Unraveling the Crosstalk between Protein O-GlcNAcylation and N-Glycosylation**; Longping Fu[1]; Kejun Yin[1]; Xing Xu[1]; Ronghu Wu[1]; *[1]Georgia Tech, Atlanta, GA*

TOG PM: NUCLEIC ACIDS AND NUCLEOTIDES

Ballroom III

Session Chair: Camila A. Ortega Ramirez (TriLink Biotechnologies)

TOG pm 02:30 **Elucidation of the importance of hydrogren bonding of amines for the characterization of crispr RNA**; J. Michael Sutton[1, 2]; Rob Ross[3]; Min Du[3]; *[1]Tome Bio, watertown, MA; [2]Eli Lilly, Lilly Seaport Innovation Center, Boston, Massachusetts; [3]Thermo Fisher Scientific, Lexington, MA*

TOG pm 02:50 **New Oligonucleotide Mode on Orbitrap Tribrid Instruments Enables Optimized Tandem MS Analysis of Oligonucleotide Anions**; Josh Hinkle[1]; Chirstopher Mullen[1]; Scott R. Kronewitter[2]; Ping Yip[2]; Rafael D Melani[1]; John E. P. Syka[1]; Jim L Stephenson[2]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Lexington, MA*

TOG pm 03:10 **seaMass-alpha: Sparse Signal Deconvolution for Quantification and Impurity Detection in Raw Oligonucleotide Mass Spectra**; Harry Tata[1]; Kamila Pacholarz[2]; Andrew Ray[3]; Andrew Dowsey[4]; *[1]School of Mathematics, University of Bristol, Bristol, United Kingdom; [2]Early Chemical Development, Pharmaceutical Sciences, R&D, AstraZeneca, Macclesfield, United Kingdom; [3]New Modalities & Parenteral Development, Pharmaceutical Technology & Development, Operations, AstraZeneca, Macclesfield, United Kingdom; [4]Department of Population Health Sciences, Bristol Medical School, University of Bristol, Bristol, United Kingdom*

TOG pm 03:30 **Integrating RNA modification information from LC-MS/MS and nanopore sequencing**; Maria Cristina Petrella[1, 2]; Laia Llovera[1]; Guadalupe Espadas[1, 2]; Alexane Ollivier[1]; Leszek Piotr Pryszcz[1]; Eva Maria Novoa[1, 2, 3]; Eduard Sabido[1, 2]; *[1]Centre for Genomic Regulation (CRG), Barcelona, Spain; [2]Universitat Pompeu Fabra (UPF), Barcelona, Spain; [3]Catalan Institution for Research and Advanced Studies (ICREA), Barcelona, Spain*

TOG pm 03:50 **Annotating the Secondary Structure Contributions of Ribonucleic Acids in Collision Induced Unfolding Fingerprints**; Courteney R Dufrene[1]; Brandon T. Ruotolo[1]; *[1]University of Michigan, Ann Arbor, MI*

TOG pm 04:10 **Characterization of mRNA medicines using LC MS: Powerful tools for the analysis of mRNA critical quality attributes**; Gareth R Owen[1]; Caroline A Evans[1]; Jessica S Dale[1]; Emma N Welbourne[1]; Mark J Dickman[1]; *[1]University of Sheffield, Sheffield, United Kingdom*

TOH PM: METABOLOMICS UNTARGETED APPROACHES

Ballroom IV

Session Chair: Dinesh Barupal (Icahn School of Medicine at Mount Sinai)

TOH pm 02:30 **ZT Scan DIA with Two-Dimensional Deconvolutions for Untargeted Metabolomics**; Hiroshi Tsugawa[1]; Gordana Ivosev[2]; David Cox[2]; Jason Causon[2]; Paul Baker[2]; Anjali Chelur[2]; Nic Bloomfield[2]; Lu Deng[2]; Yuki Matsuzawa[1]; Kanako Tokiyoshi[1]; Bujinlkham Buyantogtokh[1]; *[1]Tokyo University of Agriculture and Technology, Tokyo, Japan; [2]SCIEX, Concord, ON*

TOH pm 02:50 **Novel trapped ion mobility spectrometry (tims)TOF MS approaches to boost annotation confidence in metabolomics**; Denis A. Ispan[1, 2]; Boris Dymov[1, 2]; Patrick Boschmann[1, 2]; Stefanie Wernisch[3]; Lucia Laugwitz[4]; Lisa Sevenich[1, 5]; Sven Meyer[3]; Matthew R. Lewis[3]; Jannik Sprengel[1, 2]; Christoph Trautwein[1, 2]; *[1]M3 Research Center, Medical Faculty University of Tübingen, Tübingen, Germany; [2]Core Facility Metabolomics, Medical Faculty University of Tübingen, Tübingen, Germany; [3]Bruker Daltonics GmbH & Co.KG, Bremen, Germany; [4]Department of Neuropediatrics, University Hospital Tübingen, Tübingen, Germany; [5]Department of Interdisciplinary Neurooncology, University Hospital Tübingen, Tübingen, Germany*

TOH pm 03:10 **Orbitrap Head-to-Head: How Fast is Fast Enough for CE-MS Metabolomics?**; Corinne E Moss[1]; J. Will Thompson[2]; Erin Redman[2]; J. Scott Mellors[2]; Emily Lohr[1]; Katherine A. Overmyer[1, 3]; Joshua J. Coon[1, 3]; *[1]University of Wisconsin-Madison, Madison, WI; [2]908 Devices, Inc., Morrisville, NC; [3]Morgridge Institute for Research, Madison, WI*

TOH pm 03:30 **Targeted Data Processing of Untargeted Metabolomics Data via MassQLab Augments Untargeted Metabolomics Processing Workflows and Interpretation**; Dylan Johnson[1]; Kaylie I Kirkwood-Donelson[1]; Danielle A Lehman[1]; Kirsten E Overdahl[1]; Ruthie L Stokes[1]; Heather L Winter[1]; Alan K. Jarmusch[1]; *[1]National Institute of Environmental Health Sciences, Research Triangle Park, NC*

TOH pm 03:50 **SICRIT®-HRMS for Metabolic Profiling for Biomarker Analysis through Direct Breath Measurements**; Ciara Conway[1, 2]; Divya RAMESH[1]; Jan-Christoph Wolf[1]; Markus Weber[1, 2]; *[1]Plasmion GmbH, Augsburg, Germany; [2]Technical University of Munich, Garching, Germany*

TOH pm 04:10 **Unbiased Metabolite Profiling of Bladder Cancer Tissues Using Thermo Orbitrap IQ-X Mass Spectrometry**; Vasanta Putluri[1]; Abu Hena Mostafa Kamal[1, 2]; Chandra Shekar R Ambati[1]; Chandra Sekhar Amara[1, 2]; Karthik Reddy Kami Reddy[2]; Tanmay Gandhi[1]; Danthasinghe Waduge Badrajee Piyarathna[2]; Livia S Eberlin[3]; Cristian Coarfa[1, 2]; Seth P Lerner[4]; Arun Sreekumar[2]; Nagireddy Putluri[1, 2]; *[1]1Advanced Technology Core, Dan L Duncan Comprehensive Cancer Center, Baylor College of Medicine, Houston, Texas, United States, Houston, Texas; [2]Department of Molecular and Cell Biology, Baylor College of Medicine, Houston, Texas, United States, Houston, Texas; [3]Department of Surgery, Baylor College of Medicine, Houston, Texas, United States, Houston, Texas; [4]Scott Department of Urology, Baylor College of Medicine, Houston, Texas, United States, Houston, Texas*

WEDNESDAY ORALS

WOA AM: SINGLE CELL OMICS
Hall AB
Session Chair: Kevin D. Clark (Tufts University)

WOA am 08:30 **Multiplexed proteomic analysis of 19,000 single primary immune cells using a prioritized acquisition approach**; Sarah N Sipe[1]; Thibault Colombani[1]; Lina Warinner[1]; Nikolai Slavov[1, 2]; *[1]Parallel Squared Technology Institute, Watertown, MA; [2]Northeastern University, Boston, MA*

WOA am 08:50 **Array-Based Multimodal Mass Spectrometry Imaging Enables Single-Cell Profiling of Circulating Immune Cells**; Lyndsay Young[1]; James W Dressman[1]; Muhammed F Bayram[1]; Richard R Drake[1]; Anand S Mehta[1]; *[1]Medical University of South Carolina, Pharmacology & Immunology, Charleston, South Carolina*

WOA am 09:10 **Evaluation of a novel HRIM-QTOF operating mode with 100% ion utilization for ultra-low load and single cell proteomics**; Benjamin Orsburn[1]; Daniel DeBord[2]; Leonard Rorrer[2]; Liulin Deng[2]; Isabel Uribe[2]; Lauren Royer[2]; Frederick Strathmann[2]; *[1]University of Pittsburgh, Pharmacology and Chemical Biology, Pittsburgh, PA; [2]Mobilion Systems Inc., Chadds Ford, PA*

WOA am 09:30 **AI-assisted Electrophoresis Correlative Mass Spectrometry (Eco-AI) for Ultra-Fast Single-Cell Proteomics**; Fei Zhou[1]; Bowen Shen[1]; Peter Nemes[1]; *[1]University of Maryland, College Park, MD*

WOA am 09:50 **Patching Proteomes: A Guide for Effectively Combining Patch Clamp Electrophysiology With Single-Cell Proteomics**; Larry Rodriguez[1]; Aline Martins[1]; Blake Tsu[2]; Stefanie Kairs[2]; Christopher A. Barnes[2]; Marisa Roberto[1]; John R. Yates[1]; *[1]Scripps Resarch, La Jolla, CA, CA; [2]NGeneBioAI, San Diego, CA*

WOA am 10:10 **Scaling Single-Cell Proteomics Beyond 1,000 Samples Per Day Using MS2 Multiplexing and Fast Chromatography on the timsTOF Ultra 2**; Yasat Hacibaloglu[1]; Dorte B. Bekker-Jensen[2]; Ole Bjeld Hørning[2]; Nicolai Bache[2]; Markus Lubeck[3]; Maike Sander[1]; Stefan Kempa[1, 4]; Christoph Krisp[4, 5]; *[1]Max Delbrück Center – Berlin Institute for Medical Systems Biology, Berlin, Germany; [2]Evosep Biosystems, Odense, Denmark; [3]Bruker Daltonics GmbH & Co.KG, Bremen, Germany; [4]MDC-Bruker Center of Excellence for Single Cell Omics, Max Delbrück Center – Berlin Institute for Medical Systems Biology, Berlin, Germany; [5]Bruker Daltonics GmbH & Co.KG, Bremen, Germany*

WOB AM: STRUCTURAL BIOLOGY
Room 307-308
Session Chair: Carla Schmidt (Johannes Gutenberg University Mainz)

WOB am 08:30 **Identifying Endogenous Ligands of 'Orphan' Receptors by Native Top-Down Mass Spectrometry**; Corinne Lutomski[1]; Frances I Butroid[2]; Jack L Bennett[2]; Sophie A. S. Lawrence[2]; Tarick J El-Baba[2]; Carol V Robinson[2]; *[1]University of Oxford, Oxford, United Kingdom; [2]University of Oxford, Oxford, United Kingdom*

WOB am 08:50 **Integrating CryoEM and Native Mass Spectrometry to Study Complex Interactions and Beam-Induced Chemical Modifications**; Cameron W Flowers[1]; Joseph A. Loo[1]; Jose A. Rodriguez[1]; Niko W Vlahakis[1]; *[1]UCLA, Los Angeles, CA*

WOB am 09:10 **Mass spectrometry characterization of active 20S proteasomes, freely circulating in the bloodstream**; Yegor Leushkin[1]; Gili Ben-Nissan[1]; David Morgenstern[1]; Michal Sharon[1]; *[1]Weizmann Institute of Science, Rehovot, Israel*

WOB am 09:30 **LiP-MS Analysis Supports Kinetic Trapping as a Mechanism for Thermotolerance Across the Thermus thermophilus Proteome**; Haley M Moran[1]; Sreemantee Sen[1]; Yang Jiang[2]; Marie Pearce[1]; Edgar Manriquez Sandoval[1]; Leeker Lin[1]; Ernesto Alvarez[1]; Edward O'Brien[2]; Stephen Fried[1]; *[1]Johns Hopkins University, Baltimore, MD; [2]Penn State University, State College, PA*

WOB am 09:50 **What makes a good CAR? Probing the functional significance of clinically relevant CAR-T epitopes using structural MS**; Joey Sheff[1, 2]; Scott McComb[1, 2]; *[1]National Research Council Canada, Ottawa, ON; [2]University of Ottawa, Ottawa, ON*

WOB am 10:10 **Structural Mass Spectrometry Uncovers how ALS-associated Mutations Shape TDP-43 Conformation, Amyloid Fibril Formation and Liquid-Liquid Phase Separation**; Emily J. Byrd[1]; Joel A. Crossley[1]; Antonio N. Calabrese[1]; *[1]The University of Leeds, Leeds, United Kingdom*

WOC AM: FUNDAMENTALS: ION STRUCTURES, ENERGETICS, AND REACTIONS
Room 309-310
Session Chair: Rachel O. Loo (UCLA)

WOC am 08:30 **On the determination of the activation energies for the thermal relaxation of photoisomers by state-of-the-art mass spectrometry methods**; Thomas Robert[1]; Gwendal Henrard[1]; Benjamin Tassignon[1]; Ari Serez[1]; Julien De Winter[1]; Philippe Dugourd[2]; Jérôme Cornil[1]; Fabien Chirot[2]; Pascal Gerbaux[1]; *[1]University of Mons (UMons), Mons, Belgium; [2]Université Claude Bernard Lyon 1, LYON, France*

WOC am 08:50 **E/Z Isomerism Alters the Photostablity of Organic Sunscreen Enzacamene Cations**; Boris Ucur[1]; Andrew J Tague[1]; William R. M. Atkinson[1]; Adam J. Trevitt[1]; *[1]University of Wollongong, School of Chemistry, Wollongong, Australia*

WOC am 09:10 **Gas Phase Macrocyclic Rearrangement of Glutathione (GSH) Conjugates of Cyclobutane-Containing Covalent Bruton's Tyrosine Kinase (BTK)-Inhibitors**; Cathy A. Muste[1]; Chungang Gu[1]; H. George Vandeveer[1]; Martin K. Himmelbauer[1]; *[1]Biogen, Cambridge, MA*

WOC am 09:30 **The combination of ion mobility and electron capture dissociation mass spectrometry for native mass spectrometry applications**; Yury V. Vasilev[1]; Michael R. Armbruster[2]; Rachel Franklin[1]; Joseph C. Meeuwsen[1]; Brandon T. Ruotolo[3]; Ruwan Kurulugama[4]; *[1]Agilent Technologies, Inc., Corvallis, OR; [2]University of Michigan, Ann Arbor, MI; [3]University of Michigan, Ann Arbor, Michigan; [4]Agilent Technologies, Santa Clara, CA*

WOC am 09:50 **Myth-Busting Mysterious Chemistry in Microdroplets**; Casey J Chen[1]; Veena S Avadhani[1]; Evan R Williams[1]; *[1]University of California, Berkeley, Berkeley, CA*

WOC am 10:10 **Modeling an ESI Emitter Using Molecular Dynamics Simulations: From Bulk Solution to Gaseous Ions**; Lars Konermann[1]; Mahsa Dolatkhah Ouch Bolagh[2]; *[1]Univ. of Western Ontario, London, ON; [2]Univ of Western Ontario, London, ON*

WOD AM: INTEGRATION OF MULTI-OMICS APPROACHES
Room 314-317
Session Chair: Donghui Yi (Agilent Technologies, Inc.)

WOD am 08:30 **Optimization of combined Metabolomic, Proteomics and Lipidomics Workflow of Extracellular Vesicle-Enriched Plasma from a Single Sample**; Xun Xie[1]; Ran Zhang[1]; Erika Dorado Montezuma[1]; Zoltan Takats[1]; Virag Sagi-Kiss[1]; Clare Ross[2]; Joan Nanan[2]; Susannah Bloch[3]; Richard Lee And LHC TGM[4]; Harry J. Whitwell[1]; *[1]Division of Systems Medicine, Department of Metabolism Disgestion and Reproduction, Faculty of Medicine, Imperial College London, London, United Kingdom; [2]Imperial College Healthcare NHS Trust, London, United Kingdom; [3]Imperial College Respiratory*

Research Unit, ICHNT, London, United Kingdom; [4]*Royal Marsden Hospital, London, United Kingdom*

WOD am 08:50 **Understanding cellular and global molecular dynamics during spleen aging using a multi-omics approach**; Katarina Vlajic[1]; Alison Luciano[2]; Gennifer E Merrihew[1]; Michael Riffle[1]; Kristine A Tsantilas[1]; Michael J MacCoss[1]; Gary A Churchill[2]; Devin K Schweppe[1]; [1]*University of Washington, Seattle, WA;* [2]*The Jackson Laboratory, Bar Harbor, ME*

WOD am 09:10 **Omics profiling of iPSC-derived motor neuron with nuclear loss of TDP-43 reveals early pathological phenotype for ALS**; Nikhil K Tulsian[1]; Tze Khee Chan[1]; Shahriar Niroomand[2]; U-Ming Lim[1]; Rebecca Klien[2]; Aaron Z Fernandis[1]; [1]*MSD International GmBH, Singapore, Singapore;* [2]*Merck & Co., Inc., West Point, PA*

WOD am 09:30 **High-Sensitivity Integrated Multi-omics Enables Deep Molecular Profiling of Small Extracellular Vesicles (sEVs)**; Andrew J Perciaccante[1]; Holden T Rogers[1]; Aditi Barnwal[2]; Suzanne M Ponik[2]; Ying Ge[1, 2, 3]; [1]*Department of Chemistry, University of Wisconsin-Madison, Madison, WI;* [2]*Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI;* [3]*Human Proteomics Program, University of Wisconsin-Madison, Madison, WI*

WOD am 09:50 **Introducing a Novel Multiomics Kit: Pioneering Fast and Reliable Quantitation of Metabolites, Lipids and Proteins Combined**; Yassene Mohammed[1, 2]; Vincent R. Richard[1, 3]; M. Immanuel Reyes Madlangsakay[4]; Ying Lao[4]; Victor Spicer[4]; Claudia Gaither[5, 6]; Pradyumn Maheshwari[5]; Gordian Adam[7]; Kari Arnarson[8, 9, 10]; Timon Geib[11]; Robert Popp[5]; René P. Zahedi[4, 12, 13, 14]; Margret Thorsteinsdottir[8, 10]; Alice Limonciel[7]; Christoph H. Borchers[1, 15, 16, 17]; [1]*Segal Cancer Proteomics Centre, Jewish General Hospital, Montreal, QC;* [2]*Leiden University Medical Center, Leiden, Netherlands;* [3]*McGill University - Lady Davis Institute, Montréal, QC;* [4]*Manitoba Centre for Proteomics and Systems Biology, Winnipeg, MB;* [5]*MRM Proteomics Inc, Montreal, Quebec;* [6]*Faculty of Veterinary Medicine, Department of Clinical Sciences, University of Montreal, Montreal, QC;* [7]*biocrates life sciences ag, Innsbruck, Austria;* [8]*University of Iceland Faculty of Pharmaceutical Sciences, Reykjavík, Iceland;* [9]*Univeristy of Iceland Faculty of Medicine, Reykjavík, Iceland;* [10]*ArcticMass, Reykjavík, Iceland;* [11]*McGill University - Lady Davis Institute, Montreal, QC;* [12]*Department of Internal Medicine, University of Manitoba, Winnipeg, MB;* [13]*Department of Biochemistry and Medical Genetics, University of Manitoba, Winnipeg, MB;* [14]*Paul Albrechtsen Research Institute, CancerCare Manitoba, Winnipeg, MB;* [15]*Gerald Bronfman Department of Oncology, Montreal, QC;* [16]*Division of Experimental Medicine, McGill University, Montreal, QC;* [17]*Department of Pathology, McGill University, Montreal, QC*

WOD am 10:10 **Integrative Analysis of Multi-Omics Data for Biomarker Discovery**; Rency S Varghese[1]; Xinran Zhang[1]; Sarada Giridharan[1]; Hoi Yan Katharine Chau[1]; Md Mamunur Rashid[1]; Muhammad Salman Sajid[1]; Habtom W Ressom[1]; [1]*Georgetown University, Lombardi Cancer Center, Washington, DC*

WOE AM: HIGH THROUGHPUT MS AND AUTOMATION

Ballroom II

Session Chair: Jacob W. McCabe (SCIEX)

WOE am 08:30 **Higher-Throughput Analysis with Parallelized Pre-Accumulation**; Hamish Stewart[1]; Bernd Hagedorn[1]; Eduard Denisov[1]; Yannick Mueller[1]; Johannes Petzoldt[1]; Tabiwang Arrey[1]; Eugen Damoc[1]; Julia Kraegenbring[1]; Kyle L. Fort[1]; Erik Couzijn[1]; Jan-Peter Hauschild[1]; Florian Harking[2]; Ulises H. Guzman[2]; Jesper V. Olsen[2]; Christian Hock[1]; [1]*Thermo Fisher Scientific, Bremen, Germany;* [2]*Novo Nordisk Foundation Center for Protein Research, University of Copenhagen, Denmark*

WOE am 08:50 **High-Throughput Single-Cell Proteoform Imaging Mass Spectrometry (scPiMS) Using Micropatterned Cell Arrays**; Hannah Zhou[1]; Pei Su[1]; Fatma Ayaloglu Butun[1]; Colin L. Hisey[2]; Jared O. Kafader[1]; Neil L. Kelleher[1]; [1]*Northwestern University, Evanston, IL;* [2]*Department of Biomedical Engineering, Northwestern University, Evanston, IL*

WOE am 09:10 **Automated Desalting for the High-Throughput Collision Induced Unfolding Analysis of Biotherapeutics Direct from Formulation**; Amanda Cicali[1]; Michael R. Armbruster[1]; Nicole Rivera-Fuentes[1]; Brandon T. Ruotolo[1]; [1]*University of Michigan-Ann Arbor, Ann Arbor, MI*

WOE am 09:30 **A high-throughput native mass spectrometry-based platform for the screening and characterization of small-molecule drugs**; Kleitos Sokratous[1]; Tatiana Silva[1]; Aisha Ben-Younis[1]; Emma Sisley[1]; Karolina Gherbi[1]; Ken R. Durbin[2]; Philip Compton[3]; Jonathan Hopper[1]; Idlir Liko[1]; [1]*OMass Therapeutics, Oxford, United Kingdom;* [2]*Proteinaceous, Evanston, IL;* [3]*Integrated Protein Technologies, Evanston, IL*

WOE am 09:50 **Automated High-Throughput Electrochemical Reaction Monitoring Using a Liquid Handling Robot and Desorption Electrospray Ionization Mass Spectrometry**; Solita Marie Wilson[1]; Patrick W. Fedick[1]; [1]*Naval Air Warfare Center Weapons Division, China Lake, CA*

WOE am 10:10 **Ultra High Throughput Analysis of Next-Gen Multispecific Biotherapeutic Bioreactors**; Michael Poltash[1]; Andy Mahan[1]; Hirsh Nanda[1]; [1]*Johnson & Johnson Innovative Medicine, Spring House, PA*

WOF AM: FOOD SAFETY & CHEMISTRY: NEW INNOVATIONS

Ballroom I

Session Chair: Garret Couture (Tegmine Therapeutics)

WOF am 08:30 **A novel high resolution multi-residue pesticide workflow for the chromatographer that is comprehensive, selective, productive, and designed for ease-of-use**; Ed George[1]; Julie Moriceau[2]; Valérie Thibert[2]; Aristide Ganci[2]; Jean-François Garnier[2]; [1]*ThermoFisher Scientific, San Jose, CA;* [2]*Thermo Fisher Scientific, Courtaboeuf, France*

WOF am 08:50 **Evaluation of innovative ambient mass spectrometry tools for rapid and accurate authentication of the botanical origin of honey**; Alessandra Tata[1]; Carmela Zacometti[1]; Andrea Massaro[1]; Jan Buček[2]; Ane Arrizabalaga-Larrañaga[3]; Martin Alewijn[3]; Marco Blokland[3]; Roberto Stella[1]; [1]*Istituto Zooprofilattico Sperimentale Delle Venezie, Legnaro, Italy;* [2]*Plasmion GmbH C/o, Augsburg, Germany;* [3]*Wageningen Food Safety Research (WFSR), Wageningen, Netherlands*

WOF am 09:10 **Olive Oil Quality Analysis and The Detection of Fakes by GC-MS with Cold EI**; Benny Neumark[1]; Oneg Elkabets[1]; Aviv Amirav[1, 2]; [1]*Tel Aviv University, Tel Aviv, Israel;* [2]*Aviv Analytical, Hod Hasharon, Israel*

WOF am 09:30 **High-throughput and accessible glycomics methods for characterizing natural carbohydrates reveal the incredible diversity of our edible world**; Katharine M. Ng[1]; Alexandria M. S. Conner[1]; Megan Ellis[1]; Dan Snarski[1]; Jada Kate Garcia[1]; Jenna L. Treon[1]; Riley A Drexler[1]; Jessica E. Prenni[2]; Tracy Shafizadeh[3]; Selena Ahmed[4]; Matthew J. Amicucci[1]; Steve M. Watkins[1, 3]; [1]*One Bio Inc, Sacramento, CA;* [2]*Colorado State University,* *Fort Collins, CO; [3]Verso Biosciences, Inc., Davis, CA; [4]American Heart Association, Dallas, TX*

WOF am 09:50 **Flux Balance Analysis Predicts Cardio-Metabolic Benefits of Foods in Cancer Patients**; Kyoungmin Kim[1]; Yagi Gao[1]; Ian Williamson[1]; Anja Karlstaedt[2]; *[1]Cedars Sinai Medical Center, Los Angeles, CA; [2]Smidt Heart Institute, Cedars-Sinai Medical Center, Los Angeles, CA*

WOF am 10:10 **Quantitative food biomarkers readout allows accurate reference of dietary ontology**; Julius Agongo[1]; Harsha Gouda[1]; Aubrey McMaugh[1]; Jennifer Cao[1]; Gail Ackermann[1]; Mehrnaz S Aghili[1]; Brigid Boland[1]; Tiffany Holt[1]; Rob Knight[1]; Monica Guma[1]; Pieter C Dorrestein[1]; *[1]University of California San Diego, San Diego, CA*

WOG AM: COVALENT LABELING AND CHEMICAL CROSSLINKING

Ballroom III

Session Chair: Francis O'Reilly (National Cancer Institute, NIH)

WOG am 08:30 **Refining structural surfaceomics to further characterize tumor specific surface protein conformations**; Audrey Kishishita[1]; Clinton Yu[2]; Fenglong Jiao[2]; Michael R. Hoopmann[3]; Yi He[4]; Rosa Viner[4]; Lan Huang[2]; Robert L. Moritz[3]; Arun P. Wiita[1]; *[1]UCSF, San Francisco, CA; [2]UC-Irvine, Irvine, CA; [3]Institute for Systems Biology, Seattle, WA; [4]Thermo Fisher Scientific, San Jose, California*

WOG am 08:50 **Leveraging the Senescent Cell Surfaceome to Characterize the Heterogeneity of Senescent Cells**; Reema M Banarjee[1]; Mansi Shrivastava[1]; Linna Cui[1]; Thedoe Nyunt[1]; Anjana Ram[1]; Dimitrios Tsitsipatis[1]; Amit Dey[1]; Christopher Dunn[1]; Myriam Gorospe[1]; Nathan Basisty[1]; *[1]NIH National Institute of Aging, Baltimore, MD*

WOG am 09:10 **Mapping Methionine Oxidation Susceptibility in MsrA-Deficient E. coli Using Synchrotron X-ray Footprinting and Mass Spectrometry**; Ezaz Ahmed[1, 2]; Daniela Schlatzer[3]; Rohit Jain[2, 4]; Filipa Blasco Tavares Pereira Lopes[2, 3]; Janna Kiselar[2, 3]; David T. Lodowski[2, 3]; Mark R Chance[2, 3, 4]; Erik R. Farquhar[2, 4]; *[1]Center for Synchrotron Biosciences, Case Western Reserve University, School of Medicine, 10900 Euclid Avenue, Cleveland, OH; [2]Department of Nutrition, Case Western Reserve University, School of Medicine, 10900 Euclid Avenue, Cleveland, Ohio; [3]Center for Proteomics and Bioinformatics, Case Western Reserve University, School of Medicine, 10900 Euclid Avenue, Cleveland, Ohio; [4]Center for Synchrotron Biosciences, Case Western Reserve University, School of Medicine, 10900 Euclid Avenue, Cleveland, Ohio*

WOG am 09:30 **Reducing N: Click-Linking allows for sample and search complexity reduction and improves PPI sampling of structurally preserved interactomes by XL-MS**; Bruno C. Amaral[1]; D. Alex Crowder[1]; Benjamin L. Muselius[1]; Pauline Douglas[1]; David C. Schriemer[1]; *[1]University of Calgary, Calgary, AB*

WOG am 09:50 **A high-efficiency Azide-A-DSBSO crosslinking-MS protocol for identifying thousands of in vivo protein interactions within 8 hours**; Pin-Lian Jiang[1]; Ying Zhu[1]; Cong Wang[1]; Jiaxin Tsai[1]; Fan Liu[1]; *[1]Forschungsverbund Berlin e. V., Berlin, Germany*

WOG am 10:10 **Integrative Cross-linking Mass Spectrometry (XL-MS) Approach for Large-Scale Mapping of Protein-Protein Interactions in Cellular Environments**; Giovanna Lopes De Araujo[1]; Guilherme Reis De Oliveira[2]; Robyn Kaake[3]; Danielle Swaney[3]; Nevan Krogan[3]; Antoine Forget[3]; Fabio Gozzo[1]; *[1]University of Campinas (Unicamp), Campinas, Brazil; [2]Centro de Pesquisa Boldrini, Campinas, Brazil; [3]Quantitative Bioscience Institute - University of California San Francisco, San Francisco, CA, , USA, California*

WOH AM: CANCER RESEARCH

Ballroom IV

Session Chair: Melissa R. Pergande (Boston University)

WOH am 08:30 **Investigating the Role of Mammalian SWI-SNF (BAF) Complexes in the Pathogenesis of Malignant Peripheral Nerve Sheath Tumors**; Kirill Miachin[1]; Benjamin A Garcia[2]; Angela Hirbe[2]; Joanna Lempiainen[2]; *[1]Washington University in St. Louis, St. Louis, MO; [2]Washington University School of Medicine, St. Louis, MO*

WOH am 08:50 **Splicing Factor Mutations Remodel the Leukemia Cell Proteome**; Karl A. T. Makepeace[1, 2]; Pedro Bak-Gordon[1]; David S. Johnson[1, 2]; Chloe J. Jones[1, 2]; Claire E. Sattler[1]; Lewis M. Brown[1, 2]; James L. Manley[1]; *[1]Department of Biological Sciences, Columbia University, New York, NY; [2]Quantitative Proteomics and Metabolomics Center, Columbia University, New York, NY*

WOH am 09:10 **High-Throughput Quantification of Chromatin-Associated Proteins to Advance Neuroblastoma Therapeutic Discovery**; Andrea I Gutierrez[1]; Brian McEllin[1]; Julia Robbins[1]; Daniele Canzani[1]; Sebastian J. Paez[1]; Lillian T.A. Tatka[1]; William E. Fondrie[1]; Alexander J. Federation[1]; Lindsay K Pino[1]; *[1]Talus Bioscience, Seattle, WA*

WOH am 09:30 **Leveraging Glycomics for Improved Biomarker Discovery in Squamous Cell Carcinoma (SCC)**; Sheryl Joyce G. Alvarez[1]; Anastasia Elizabeth Abello[1]; Michael Russelle S. Alvarez[1]; Adeola Kabirat Adeyemi[1]; Xiao-Jing Wang[1]; Carlito B. Lebrilla[1]; *[1]University of California Davis, Davis, CA*

WOH am 09:50 **Native top-down mass spectrometry uncovers novel post-translational modifications of tetraspanins in cancer**; Olivia B Ramsay[1]; Jack L Bennett[2, 3]; Susanne Mesoy[2, 3]; Maya M Miller[4]; Eric O'Neill[1]; Carol V Robinson[2, 3]; *[1]Department of Oncology, University of Oxford, Oxford, United Kingdom; [2]Kavli Institute for Nanoscience Discovery, University of Oxford, Oxford, United Kingdom; [3]Department of Chemistry, University of Oxford, Oxford, United Kingdom; [4]Department of Physiology, Anatomy and Genetics, University of Oxford, Oxford, United Kingdom*

WOH am 10:10 **Decoding adaptive drug resistance to KRAS-G12C inhibition through nascent and single-cell proteomics**; Dr Syed Azmal Ali[1]; Sara Signoretti[1]; Selin Ulukaya[1, 2]; Pablo Henneman[1]; Elena Markeviciute[1, 2]; Prof. Jeroen Krijgsveld[1, 2]; *[1]German Cancer Research Center (DKFZ), Heidelberg, Germany; [2]Heidelberg University, Medical Faculty, Heidelberg, Germany*

WOA PM: TOP-DOWN PROTEOMIC ANALYSIS

Hall AB

Session Chair: Sharon Pitteri (Stanford University)

WOA pm 02:30 **Top-down Proteomics Deciphers Cardiac Proteoform Landscape in Phospholamban R14del Cardiomyopathy for Precision Medicine**; Holden T Rogers[1]; Frederik E Deiman[2]; Zhan Gao[3]; Niels Grote Beverborg[2]; Rachel E Baum[4]; Peter Van Der Meer[2]; Ioannis Karakikes[4]; Peter C Glijnis[5]; Ying Ge[1, 3, 6]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [2]University Medical Center Groningen, Department of Experimental Cardiology, Groningen, Netherlands; [3]Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI; [4]Department of Cardiothoracic Surgery, Stanford School of Medicine, Stanford, CA; [5]PLN Foundation, Wieringerwerf, Netherlands; [6]Human Proteomics Program, University of Wisconsin-Madison, Madison, WI*

WOA pm 02:50 **Characterization of Endangered Coral Acropora cervicornisHistone Variant Proteoforms using Top-down and Bottom-up LC-TIMS-ECD-ToF MS/MS.**; Cassandra N. Fuller[1]; Sabrina Mansoor[2]; Kevin Jeanne Dit Fouque[1]; Lilian Valadares Tose[1]; Javier Rodriguez-Casariego[2]; Mariangela Kosmopoulou[3]; Detlev Suckau[4]; Francisca N De Luna Vitorino[5]; Benjamin A Garcia[5]; Francisco Fernandez-Lima[1, 6]; *[1]Department of Chemistry and Biochemistry, Florida International University, Miami, FL; [2]Environmental Epigenetics Laboratory, Institute of Environment, Florida International University, Miami, FL; [3]Fasmatech Science & Technology, TESPA Lefkippos, NCSR Demokritos, Greece; [4]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [5]Department of Biochemistry and Molecular Biophysics, Washington University School of Medicine, St. Louis, MO; [6]Biomolecular Sciences Institute, Florida International University, Miami, FL*

WOA pm 03:10 **Radical Initiated Photodissociation (RIPD) enables top-down proteoform fingerprinting and PTM localization analysis**; Lin He[1]; Evan Hubbard[1]; Thomas Shoff[1]; Aidan Purcell[1]; Ryan R Julian[1]; *[1]University of California, Riverside, Riverside, CA*

WOA pm 03:30 **Proteoform-Level Analysis of Senescence-Associated Secreted Proteins: Unveiling the Senescent Secretome Using Top-Down Mass Spectrometry**; Mozhgan Boroumand[1]; Amit Dey[1]; Kellye A Sutton[2]; Tomas Pierce[1]; Si Wu[2]; Nathan Basisty[1]; *[1]National Institute on Aging, Baltimore, MD; [2]The University of Alabama, Tuscaloosa, AL*

WOA pm 03:50 **High resolution top-down peptidomics of salivary secretion from the human malaria vector, Anopheles gambiae**; Erika Nishiduka[1]; Motoshi Suzuki[2]; Eric Calvo[1]; *[1]Laboratory of Malaria and Vector Research (LMVR), NIAID, Rockville, MD; [2]Research Technologies Branch (RTB), NIAID, Rockville, MD*

WOA pm 04:10 **Top-Down ExD fragmentation of immunoglobulins on a prototype timsOmni enables confident annotation of the hypervariable regions**; Simon OLLIVIER[1, 2]; Dina Schuster[1, 2]; Danique M.H. Van Rijswijck[1, 2]; Athanasios Smyrnakis[3]; Jan Fiala[1, 2]; Stuart Pengelley[4]; Oliver Raether[4]; Mariangela Kosmopoulou[3]; Detlev Suckau[4]; Jean-François Greisch[5]; Dimitris Papanastasiou[3]; Albert J.R. Heck[1, 2]; *[1]Biomolecular Mass Spectrometry & Proteomics, Bijvoet Center for Biomolecular Research & Utrecht Institute for Pharmaceutical Sciences, Utrecht University, Padualaan 8, 3584 CH Utrecht, Netherlands; [2]Netherlands Proteomics Center, Padualaan 8, 3584 CH Utrecht, Netherlands; [3]Fasmatech Science & Technology, Athens, 15233, Greece; [4]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [5]Bruker Switzerland AG, Fällanden, Switzerland*

WOB PM: FOOD SAFETY & CHEMISTRY: FOODOMICS, ALLERGENS, BACTERIA, FOODS AND SUPPLEMENTS

Room 307-308

Session Chair: Matt Amicucci (one.bio)

WOB pm 02:30 **Analysis of Psilocybin Mushroom Edibles Using GC-MS and LC-HRMS Reveals Adulteration with Synthetic Psychedelics ('Syndelics') and Misleading Product Labeling**; Richard B. Van Breemen[1]; Daniel Simchuk[1]; Bjorn Fritzsche[2]; Daniel Huson[2]; Scott A Kuzdzal[3]; Jonathan Ferguson[3]; *[1]Oregon State University, Corvallis, OR; [2]Rose City Laboratories, Portland, OR; [3]Shimadzu Scientific Instruments, Columbia, MD*

WOB pm 02:50 **Validation of a LC-MS/MS method for the quantification of morphine, codeine, and thebaine on poppy seeds**; Katherine L Fiedler[1]; Erica L Bakota[2]; Douglas M Monroe[2]; *[1]U.S. Food and Drug Administration, College Park, MD; [2]U.S. Food and Drug Administration, Lenexa, KS*

WOB pm 03:10 **Perspectives on Navigating the Labyrinth of Omics Standardization in a Global Research Landscape**; Melanie Odenkirk[1]; Margaret L. Read[1]; Selena Ahmed[2]; Jessica Prenni[1]; *[1]Colorado State University, Fort Collins, CO; [2]American Heart Association, Dallas, TX*

WOB pm 03:30 **Identification of gluten target peptides for the development of an MS gluten detection method in fermented and hydrolyzed foods**; Sara K Schlange[1]; Joseph L Baumert[1]; Melanie L Downs[1]; *[1]Food Allergy Research and Resource Program, Department of Food Science and Technology, University of Nebraska-Lincoln, Lincoln, NE*

WOB pm 03:50 **Multi-omics Analyses Reveal the Impact of Agricultural Production Practices on the Molecular Composition of Foods**; Mariana Barboza[1, 2]; Cheng-Yu Charlie Weng[3]; Shawn Ehlers-Cheang[4]; Jiani Jiang[5]; Christopher Suarez[3]; Fangzhou Li[6]; Hunter Jacobs[1, 2]; Bruce German[7]; Ilias Tagkopoulos[6]; Carlito B. Lebrilla[3]; Justin Siegel[2, 3, 8]; *[1]Innovation Institute for Food and Health, University of California Davis, Davis, California; [2]Genome Center, College of Biological Sciences, University of California Davis, Davis, California; [3]Department of Chemistry, University of California Davis, Davis, California; [4]Department of Chemistry, University of California, Davis, Davis, California; [5]Department of Chemistry, University of California, Davis, Davis, CA; [6]Department of Computer Science, University of California Davis, Davis, California; [7]Department of Food Science and Technology, University of California, Davis, Davis, California; [8]Innovation Institute for Food and Health, University of California Davis, Davis, CA*

WOB pm 04:10 **Evolution of Direct Mass Detector and Multivariate Statistical Analysis in Geographical Origin Testing of Spices and Herbs**; Mariajohn Muthaiya[1]; Karen B Olszewski[1]; Robert Cannon[1]; *[1]McCormick and Company, Inc., Hunt Valley, MD*

WOC PM: SYNTHETIC POLYMERS AND NEW MATERIALS

Room 309-310

Session Chair: Christina J. Mastromatteo (Lubrizol)

WOC pm 02:30 **Pushing the Limits of Synthetic Polymer Analysis using Ultra-High Resolution Mass Spectrometry**; Callan Littlejohn[1]; Meng Li[2]; Sam Weekes[1]; Yutong Niu[1]; Stefan Bon[1]; Mark P Barrow[1]; Peter B O'Connor[1, 2]; *[1]Department of Chemistry, University of Warwick, Coventry, United Kingdom; [2]Advanced Mass Spectrometry Research Technology Platform, University of Warwick, Coventry, United Kingdom*

WOC pm 02:50 **Structural Motifs in Crosslinked Polyester Networks Revealed by Thermal Desorption/Pyrolysis Interfaced with Direct Analysis in Real Time Tandem Mass Spectrometry**; Calum Bochenek[1]; Arsalaan Nisar Pathan[1]; James M Eagan[1]; Chrys Wesdemiotis[1]; *[1]The University of Akron, Akron, Ohio*

WOC pm 03:10 **Novel MALDI-TOFMS analysis of nonpolar terpolymers and halogenated nonpolar copolymers using high explosive matrices**; Colleen L Ray; *Los Alamos National Laboratory, Los Alamos, NM*

WOC pm 03:30 **A novel approach for the quantification of the mass of micro and nanoplastic particles from filter samples**; Patrick Martens[1]; Judith C Chow[1]; Monica Arienzo[1]; *[1]Desert Research Institute, Reno*

WOC pm 03:50 **Structural features and conformational changes of multiply entangled macrocycles studied by ion mobility mass spectrometry**; Anniina Kiesilä[1];

Fabien B. L. Cougnon[1]; Elina Kalenius[1]; [1]*University of Jyväskylä, Jyväskylä, Finland*

WOC pm 04:10 **Creation of a searchable pyrolysis GCMS reference library to aid in the identification of polymers and their mixtures**; Edward Erisman[1]; Yamil Yamil Simón-Manso[1]; William E Wallace[1]; [1]*NIST, Gaithersburg, MD*

WOD PM: SMALL MOLECULES: STRUCTURAL CHARACTERIZATION AND QUANTITATION

Room 314-317

Session Chair: Ruth Anyaeche (Corteva Agriscience)

WOD pm 02:30 **MS/MS Spectra Comparison of Cannabinoids Using Collision-Induced Dissociation (CID) and Electron-Activated Dissociation (EAD)**; Elizabeth Rae Milner[1, 2]; Inah Gu[1, 2]; Jaewoo Choi[3, 4]; Claudia S. Maier[2, 3, 4]; Jan F. Stevens[1, 2, 4, 5]; [1]*Department of Pharmaceutical Sciences, Oregon State University, Corvallis, OR;* [2]*Linus Pauling Institute, Oregon State University, Corvallis, OR;* [3]*Department of Chemistry, Oregon State University, Corvallis, OR;* [4]*OSU Mass Spectrometry Center, Oregon State University, Corvallis, OR;* [5]*Global Hemp Innovation Center, Oregon State University, Corvallis, OR*

WOD pm 02:50 **Quantification and impurity analysis of ALC-0315 from LNPs in plasma using the ZenoTOF 7600 system**; Matthew Stone[1]; Daniel Zimmer[2]; Santosh Kapil Kumar Gorti[1]; Mays Al-Dulaymi[3]; Sahana Mollah[4]; Paul Baker[4]; Robert Proos[1]; Christina M Bailey-Hytholt[2]; [1]*Sciex, Framingham, MA;* [2]*Deptartment of Chemical Engineering, Worcester Polytechnic Institute, Worcester, MA;* [3]*SCIEX, Concord, ON;* [4]*Sciex, Redwood City, CA*

WOD pm 03:10 **Top-down LC-MS/MS structure elucidation and quantitation of semaglutide impurities: Enhanced approaches to analytical procedure development for novel complex drug products**; Roberto Mendez[1]; Mack Shih[1]; Nobel O. Sierra Vega[1]; Jianghong Gu[1]; Guozhang Zou[1]; Patrick J. Faustino[1]; Muhammad Ashraf[1]; Xiaoming Xu[1]; Jinhui Zhang[1]; [1]*FDA, Silver Spring, MD*

WOD pm 03:30 **Structural Characterization of Dimeric Perfluoroalkyl Carboxylic Acid Using Experimental and Theoretical Ion Mobility Spectrometry Analyses**; Aurore Lisette Schneiders[1]; Johann Far[1]; Lidia Belova[2]; Allison Fry[3]; Adrian Covaci[2]; Erin S. Baker[3]; Edwin De Pauw[1]; Gauthier Eppe[1]; [1]*Mass Spectrometry Laboratory, Université of Liège, Liège, Belgium;* [2]*Toxicological Centre, University of Antwerp, Wilrijk, Belgium;* [3]*Department of Chemistry, University of North Carolina at Chapel Hill, Chapel Hill, NC*

WOD pm 03:50 **A Straightforward and Derivatization-Free Approach to Identify Carbon-Carbon Double Bond Position Isomer in Unsaturated Lipids by LC-PDA-MS**; Yu Feng[1]; Raymond Gonzalez[1]; Kara Pearson[1]; [1]*Merck & Co., Inc., West Point, PA*

WOD pm 04:10 **High-throughput screening of biaryl isomers from directed evolution by droplet microfluidics coupled to cyclic ion mobility mass spectrometry**; Laura I. Penabad[1]; Roger C. Diehl[1]; Aidan Olman[1]; Tyler D. Somerville[1]; Maxwell J. Unger[1]; Alison R.H. Narayan[1]; Brandon T. Ruotolo[1]; Robert T. Kennedy[1]; [1]*University of Michigan-Ann Arbor, Ann Arbor, MI*

WOE PM: INFORMATICS: METABOLOMICS, LIPIDOMICS AND GLYCOMICS

Ballroom II

Session Chair: Carolina Rojas Ramirez (University of Michigan)

WOE pm 02:30 **MassCube: a Python framework for end-to-end metabolomics data processing from raw files to phenotype classifiers**; Huaxu Yu[1]; Jun Ding[2]; Tong Shen[1]; Min Liu[1]; Yuanye Li[1]; Oliver Fiehn[1]; [1]*University of California Davis, Davis, CA;* [2]*Wuhan Botanical Garden, Chinese Academy of Sciences, Wuhan, China*

WOE pm 02:50 **Source Tracing by Interactive Molecular Networks Combined with metaMASST in mzmine**; Robin Schmid[1, 2, 3]; Steffen Heuckeroth[1]; Simone Zuffa[3]; Ansgar Korf[1]; Corinna Brungs[4]; Daniel Petras[5]; Mingxun Wang[6]; Pieter C. Dorrestein[3]; Tomáš Pluskal[2]; [1]*mzio GmbH, Bremen, Germany;* [2]*Institute of Organic Chemistry and Biochemistry of the Czech Academy of Science, Prague, Czech Republic;* [3]*Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, San Diego, CA;* [4]*Department of Pharmaceutical Sciences, University of Vienna, Vienna, Austria;* [5]*Department of Biochemistry, University of California Riverside, Riverside, CA;* [6]*Department of Computer Science, University of California Riverside, Riverside, CA*

WOE pm 03:10 **Lipid MetabolicTracing Using Biorthogonal Click Chemistryin LC-MS lipidomics: From experiments to high-throughput data processing**; Laura Goracci[1]; Palina Nepachalovich[2]; Stefano Bonciarelli[3]; Gabriele Lombardi Bendoula[2]; Jenny Desantis[1]; Michela Eleuteri[1]; Christoph Thiele[4]; Maria Fedorova[2]; [1]*Department of Chemistry, Biology and Biotechnology, University of Perugia, Perugia, Italy;* [2]*Center of Membrane Biochemistry and Lipid Research, Faculty of Medicine Carl Gustav Carus, Technical University Dresden, Dresden, Germany;* [3]*Mass Analytica, Sant Cugat del Valles, Spain;* [4]*Life & Medical Sciences Institute, University of Bonn, Bonn, Germany*

WOE pm 03:30 **LipidCruncher: an open-source web application for processing, visualizing, and analyzing lipidomic data**; Abdi Hamed[1]; Yohannes Ambaw[1]; Chandramohan Chitraju[1]; Shubham Singh[1]; Weng Zon Lai[2]; Robert V Farese Jr[1]; Tobias C Walther[1]; [1]*Cell Biology Program, Sloan Kettering Institute, Memorial Sloan Kettering Cancer Center, New York, United States, New York, 10065;* [2]*mRNA Center of Excellence, Sanofi, Waltham, 02451*

WOE pm 03:50 **Accurate and Automated Glycan Quantitation by Parallel Reaction Monitoring Based LC-MS/MS**; Vishal Sandilya[1]; Sarah Sahioun[1]; Sherifdeen B Onigbinde[1]; Yehia Mechref[1]; [1]*Texas Tech University, Lubbock, TX*

WOE pm 04:10 **Structural Feature Annotation of Glycomic LC-MS By Supervised Machine Learning Classification**; Xavier A Holmes[1]; Armin Oulomi[1]; Yasmine Bouchibti[1]; Ryan Schindler[1]; Michael Russelle S. Alvarez[1]; Tristan Seales[2]; Sheryl Joyce Grijaldo-Alvarez[1]; Atit Silsirivanit[1, 3]; Carlito B. Lebrilla[1]; [1]*University of California Davis, Davis, CA;* [2]*University of California-Davis, Davis, CA;* [3]*Khon Kaen University, Khon Kaen, Thailand*

WOF PM: IMAGING INSTRUMENTATION & METHOD DEVELOPMENT

Ballroom I

Session Chair: Marissa A. Jones (KBI Biopharma)

WOF pm 02:30 **Cellular Level Mass Spectrometry Imaging Enabled by Picosecond Laser Desorption – Rapid Evaporative Ionization Mass Spectrometry (ps-LD-REIMS)**; Yu Wang[1]; Ronan Battle[1]; Daniel Simon[1, 2]; Yuchen Xiang[1]; Stefania Maneta Stavrakaki[1]; Yayue Song[1]; Timothy Runcorn[1]; Simone Di Giovanni[1]; Zoltan Takats[1, 2]; Robert Murray[1]; [1]*Imperial College London, London, United Kingdom;* [2]*Universität Regensburg, Regensburg, Germany*

WOF pm 02:50 **iprm-PASEF MALDI MS/MS Imaging Reveals Specialized Metabolites Produced by the Cheese Rind Microbiome**; Gordon T Luu[1]; Robert A Shepherd[2]; Sumankalai Ramachandran[1]; Azad

Eshghi[1]; Laura M Sanchez[2]; *[1]Bruker Scientific LLC, Billerica, MA; [2]University of California Santa Cruz, Santa Cruz, CA*

WOF pm 03:10 **Demonstrating Voxel-by-Voxel (V×V) Single-Point Calibration in Heterogeneous Tissues by IR-MALDESI Quantitative Mass Spectrometry Imaging**; Emily R. Bruce[1]; Alena N. Joignant[1]; Stephen J. Vega[1]; Logan Opperman[2]; David C. Muddiman[1]; *[1]Biological Imaging Laboratory for Disease and Exposure Research, Raleigh, NC; [2]Department of Statistics, North Carolina State University, Raleigh, NC*

WOF pm 03:30 **Spatially Mapping Lipid sn-Isomers in the Mouse Brain by Ozone-Induced Dissociation in the HCD region of an Orbitrap Fusion**; Matthew Briggs[1]; Thao Tran[2]; Manita Shakya[3]; Tialfi Bergamin De Castro[3]; Reuben Young[1]; Jesse Michael[1]; Alan Maccarone[1]; Nathan Heath Patterson[2]; Alison Scott[3]; Shane Ellis[1]; *[1]University of Wollongong, Wollongong, Australia; [2]Aspect Analytics, Genk, Belgium; [3]University of Maryland, Baltimore, Maryland*

WOF pm 03:50 **Bringing Annotation in Imaging with Mass Spectrometry to the Next Level through Spatial Correlation of Product Ions**; Ingela Lanekoff[1]; Varun V. Sharma[2]; Johan Lillja[2]; Robert Martinis[2]; Gabor Toth[2]; *[1]Uppsala University, Uppsala, Sweden; [2]Uppsala University, Uppsala , Sweden*

WOF pm 04:10 **A Novel Silicon Photomultiplier-Based Time-of-Flight Detector for Imaging**; Antonio Mariscal-Castilla[1]; Daniel Guberman[2]; David Heathcote[3]; Rafael Ballabriga[4]; Jerome Alozy[4]; Sergio Gomez[5]; David Gascón[2]; Michael Campbell[4]; Claire Vallance[3]; Andreu Sanoy[2]; Joan Mauricio[2]; *[1]Insitut de Ciénces del Cosmos, Universitat de Barcelona, Barcelona, Spain; [2]Institut de Ciénces del Cosmos, Universitat de Barcelona, Barcelona, Spain; [3]University of Oxford, Oxford, United Kingdom; [4]CERN, Geneva, Switzerland; [5]Universitat Politècnica de Catalunya,, Barcelona, Spain*

WOG PM: ION MOBILITY: STRUCTURE DETERMINATION & APPLICATIONS

Ballroom III

Session Chair: Erin Baker (University of North Carolina)

WOG pm 02:30 **On the charge dependence of biomolecule collision cross sections**; Frederic Rosu[1]; Valerie Gabelica[1]; *[1]University of Geneva, Geneva, Switzerland*

WOG pm 02:50 **A Mass Spectrometry Imaging Annotation Workflow Combining Cyclic Ion Mobility and Machine Learning Molecular Predictions**; Dmitry Leontyev[1]; Eric C Gier[1]; Rebecca Arnold[2]; John A Petros[2]; Facundo M Fernández[1]; *[1]Georgia Institute of Technology, Atlanta, GA; [2]Emory University, Atlanta, GA*

WOG pm 03:10 **Novel strategies for the characterization of the early-stages of aggregate formation of α-Synuclein using ion mobility mass spectrometry**; Raya Sadighi[1, 2]; Andrea Istrati[1, 2]; Sigourney Karijodikoro[1, 2]; Melissa Bärenfänger[1, 2]; Anouk. M Rijs[1, 2]; *[1]Division of Bioanalytical Chemistry, Department of Chemistry and Pharmaceutical Sciences, AIMMS Amsterdam Institute of Molecular and Life Sciences, Vrije Universiteit Amsterdam, 1081 HV Amsterdam, The Netherlands, Amsterdam, Netherlands; [2]Centre for Analytical Sciences Amsterdam, 1098XH Amsterdam, The Netherlands, Amsterdam, Netherlands*

WOG pm 03:30 **Chiral Ion Mobility: Towards Broadscale Drug Enantiomer Separations using Ion Mobility-Mass Spectrometry**; Benjamin K Blakley[1]; Valeria Guidolin[2]; Jody C May[1]; Emma R Remish[1]; Eric Dybeck[3]; John A McLean[1]; *[1]Vanderbilt University, Nashville, TN; [2]PharmSci Smal Molecule, Analytical Research and Development, Pfizer, Groton, CT; [3]MedDesign, Pfizer, Cambridge, MA*

WOG pm 03:50 **Study of Conformational Space for Native(-like) Proteins Using Multi-pass Separations in Structures for Lossless Ion Manipulations and Molecular Dynamic Simulations**; Jung Lee[1]; Viraj D. Gandhi[1]; Christopher Harrilal[1]; Amar Parvate[1]; Stephanie M. Thibert[1]; Ashley Ives[1]; Xin Zhang[1]; Gregory K Schenter[1]; Carlos Larriba-Andaluz[2]; James E Evans[1]; Yehia M. Ibrahim[1]; Sandilya Garimella[1]; *[1]Pacific Northwest National Laboratory, Richland, Washington; [2]Purdue Univeristy, West Lafayette, IN*

WOG pm 04:10 **Combining Glycan Engineering with Ion Mobility Selected Collision-Induced Unfolding to Evaluate the Influence of Glycoforms on Monoclonal Antibody Structural Polydispersity**; Addison E. Bergman[1]; Devin M. Makey[1]; Nicole Rivera-Fuentes[1]; Trey Theobald[1]; Brandon T. Ruotolo[1]; *[1]University of Michigan, Ann Arbor, MI*

WOH PM: CLINICAL ANALYSIS: INNOVATIONS

Ballroom IV

Session Chair: Xin Cong (InterVenn)

WOH pm 02:30 **Designing and Constructing Functional, Mass Spectrometry Compatible Medical Devices Using Stereolithographic Array (SLA) 3-D Printing**; Charlie Wolfe[1]; Livia S Eberlin[2]; *[1]Baylor college of medicine, Houston, TX; [2]Baylor College of Medicine, Houston, TX*

WOH pm 02:50 **Peeking Inside a Blackbox LC-MS/MS System: Evaluation of an Automated, Integrated LC-MS/MS Instrument Fit for the Clinical Laboratory**; Matthew L Crawford[1]; Meghan Bradley[1]; Matthew R Chappell[1]; Russell P Grant[1]; Philippe Metz[2]; Sven Groesgen[2]; *[1]LabCorp, Burlington, NC; [2]Roche Diagnostic GmbH, Mannheim, Germany*

WOH pm 03:10 **Complete Molecular Specificity of M-proteins in Multiple Myeloma Patients using Individual-ion Tandem Mass Spectrometry**; Taojunfeng Su[1]; Ryan T. Fellers[2]; Michael A. R. Hollas[2]; Bryan P. Early[2]; Jared O. Kafader[2]; Sabine Allam[3]; Jean-Baptiste Alberge[3]; Floris Chabrun[3]; Irene Ghobrial[3]; Neil L. Kelleher[2]; *[1]Northwestern University, Evanston, IL; [2]Proteomics Center of Excellence, Northwestern University, Evanston, IL; [3]Harvard Medical School, Boston, MA*

WOH pm 03:30 **Intraoperative Metabolomics-based technologies as a bedside tool in real-time diagnosis and treatment of cervical disease**; Apostolia Galani[1]; Stefania Maneta Stavrakaki[2]; Maria Paraskevaidi[2]; Amelia Fraser-Dale[2]; Daniel Simon[2, 3]; Jinshi Zhao[2]; Burak Temelkuran[2]; Yuchen Xiang[2]; Robert Murray[2]; Yu Wang[2]; Deirdre Lyons[2]; Zoltan Takats[2, 3]; Maria Kyrgiou[2]; *[1]Imperial College London, LONDON, United Kingdom; [2]Imperial College London, London, United Kingdom; [3]University of Regensburg, Department of Functional Genomics, Regensburg, Germany*

WOH pm 03:50 **A canonical targeted approach to detect and purify exosomes for proteome analysis and standardized diagnostic workflows**; Olaf G. Wilhelm[1]; Evelyn Hammer[1]; Rudolf Napieralski[1]; Wolfgang Hammerschmidt[2]; Reinhard Zeidler[2]; Alain Brisson[3]; Christoph Krisp[4, 5]; Andreas Schmidt[6]; Gary Kruppa[6]; Gabriele Schricker[7]; Bastian Höchst[8]; Valter Bergant[9]; Andreas Pichlmair[9]; Percy Knolle[8]; *[1]therawis diagnostics GmbH, München, Germany; [2]Research Unit Gene Vectors, Helmholtz Zentrum München, München, Germany; [3]UMR-5248 CBMN CNRS-University of Bordeaux-IPB, Pessac, France, Pessac, France; [4]Bruker Daltonics GmbH & Co.KG, Bremen, Germany; [5]MDC-Bruker Center of Excellence for Single Cell Omics, Max Delbrück*

Center – Berlin Institute for Medical Systems Biology, Berlin, Germany; [6]Bruker Daltonics, Bremen, Germany; [7]therawis diagnostics GmbH, Munich, Germany; [8]Institute of Molecular Immunology, TUM University Hospital, TUM, Munich, Germany; [9]Institute of Virology, Technical University of Munich, Munich, Germany

WOH pm 04:10 **Diagnosis of Human Visceral Leishmaniasis using a 2D Paper-Based Microfluidic Analytical Device as a public health tool in resource-limited settings**; Hianka J. C. De Carvalho[1]; Rana Arebi[1]; Stephanee Joy B. Zerrudo[1]; Ayesha Seth[1]; Ruth M. Speidel[1]; Hélida M. De Andrade[2]; Ana L. Abreu-Silva[3]; Maria A. Miglino[4]; Abraham K. Badu-Tawiah[1]; *[1]The Ohio State University, Columbus, OH; [2]Universidade Federal de Minas Gerais, Belo Horizonte, Brazil; [3]Universidade Estadual do Maranhão, São Luís, Brazil; [4]Universidade de Marília, São Paulo, Brazil*

THURSDAY ORALS

ThOA AM: INFORMATICS: MULTIOMICS INTEGRATION AND APPLICATIONS
Hall AB
Session Chair: Michael J. MacCoss (University of Washington)

ThOA am 08:30 **Elucidating protein glycosylation biosynthetic pathways by integrating RNAseq transcriptomics and LC-MS/MS glycomics**; Michael Russelle S. Alvarez[1]; Xavier A. Holmes[1]; Armin Oloumi[1]; Sheryl Joyce G. Alvarez[1]; Ryan Schindler[1]; Qingwen Zhou[1]; Anirudh Yadlapati[1]; Atit Silsirivanit[2]; Carlito B. Lebrilla[3]; *[1]University of California Davis, Davis, CA; [2]Khon Kaen University, Khon Kaen, Thailand; [3]University of California, Davis, Davis, CA*

ThOA am 08:50 **IsotopeakeR - a novel approach for mapping lipids on single pixel level**; Maciej Dulewicz[1]; Junyue Ge[1]; Lydia Fenson[1]; Jörg Hanrieder[1, 2]; *[1]University of Gothenburg, Gothenburg, Sweden; [2]University College London, London, United Kingdom*

ThOA am 09:10 **Construction of Multi-Modal Transcriptome-Small Molecule Interaction Networks from High-Throughput Measurements for Studying Human Complex Traits**; Vaha Akbary Moghaddam[1]; Sandeep Acharya[1]; Michaela Schwaiger-Haber[1]; Shu Liao[1]; Wooseok J. Jung[1]; Bharat Thyagarajan[2]; Leah P. Shriver[1]; E. Warwick Daw[1]; Nancy L. Saccone[1]; Ping An[1]; Michael R. Brent[1]; Gary J Patti[1]; Michael A. Province[1]; *[1]Washington University in St. Louis, St. Louis, MO; [2]University of Minnesota, Minneapolis, MN*

ThOA am 09:30 **ProteomeGenerator3 for Integrated Long-Read Sequencing and Multi-Dimensional Mass Spectrometry Proteogenomics**; Katarzyna Kulej[1]; Asher Preska Steinberg[1]; Gabriella Casalena[1]; Jinxin Zhang[1]; Eli Havasov[1]; Sohrab P. Shah[1]; Andrew McPherson[1]; Alex Kentsis[1, 2]; *[1]Memorial Sloan Kettering Cancer Center (MSKCC), New York, NY; [2]Weill Cornell Medical College, Cornell University, New York, NY*

ThOA am 09:50 **CONECT (Comprehensive Omics Networking for Exposure to Chemicals & Characterization of Tissues):R Tools for Multi-Omics Integration & Organ Specific Insights**; Raquel Shortt[1]; Conor Jenkins[2]; Gabrielle Rizzo[2]; Allison Clay[2, 3]; Priscilla Lee[2]; Jennifer Horsmon[2]; Dylan Fudge[2]; Daniel Angelini[2]; Elizabeth Dhummakupt[2]; Tyler Goralski[2]; *[1]Excet A Precise Systems Company, Edgewood, MD; [2]DEVCOM CBC, Edgewood, Maryland; [3]Precise Systems, Lexington Park, MD*

ThOA am 10:10 **Molecular Phenotypes and Responses During Human Pregnancy**; Xiaotao Shen[1]; Liang Liang[2]; Yue Wu[3]; Brian Piening[3]; Gucci Gu[3]; Charles Abbott[3]; Songji Chen[3]; Qing Liu[3]; Hanne Röst[3]; Hassan Chaib[3]; Eric Wei[3]; Hanayh Zackriah[4]; Michael Snyder[3]; *[1]Nanyang Technological University, Singapore, Singapore, Singapore; [2]Medical College of Wisconsin, Milwaukee, WI; [3]Stanford University, Palo Alto, CA; [4]University of California, Berkeley, Berkeley, CA*

ThOB AM: CLINICAL ANALYSIS: APPLICATIONS
Room 307-308
Session Chair: Emily R. Sekera (St. Jude Children's Research Hospital)

ThOB am 08:30 **A Novel Method for Urine Drug Screening Based on Desorption ElectroSpray Ionization (DESI) MS Analysis**; Julia Balog[1]; Erika Stark[1]; Eltahir I Elbakri[2]; Rav Sheth[3]; Steven Pringle[4]; Patrice Ohouo[2]; *[1]Waters Immerse, Cambridge, MA; [2]CleanSlate, Holyoke, MA; [3]Waters Corporation, Milford, MA; [4]Waters Corporation, Wilmslow, United Kingdom*

ThOB am 08:50 **Comprehensive Investigation of Bongkrekic Acid Intoxication in Clinical and Post-Mortem Specimens Using Mass Spectrometry**; Guan-yuan Chen[1, 2]; Ying-Tzu Shieh[2]; Ju-yu Chen[2]; Chu-yun Teng[2]; Ya-jin Jheng[2]; Te-I Weng[1, 2]; *[1]Department and Graduate Institute of Forensic Medicine, College of Medicine, National Taiwan University, Taipei, Taiwan; [2]Forensic and Clinical Toxicology Center, College of Medicine, National Taiwan University, Taipei, Taiwan*

ThOB am 09:10 **Proteomics and Ontology-Based Clustering Unveil Insights into Rare Pediatric Diseases**; Ericka CM Itang[1, 2]; Vincent Albrecht[1]; Alicia-Sophie Schebesta[1]; Marvin Thielert[1]; Anna-Lisa Lanz[2, 3]; Katharina Danhauser[2, 3]; Christoph Klein[2, 3]; Matthias Mann[1, 2]; Susanne Pangratz-Fuehrer[2, 3]; Johannes Mueller-Reif[1, 2]; *[1]Max Planck Institute of Biochemistry, Munich, Germany; [2]German Center for Child and Adolescent Health (DZKJ), partner site Munich, Munich, Germany; [3]Department of Pediatrics, Dr. von Hauner Children's Hospital, Ludwig-Maximilians-Universität München, Munich, Germany*

ThOB am 09:30 **Understanding and Targeting Epigenetic Vulnerabilities in Malignant Peripheral Nerve Sheath Tumors**; Joanna K. Lempiainen[1]; Kirill Miachin[1]; Yixuan Xie[1]; Xingyu Liu[1]; Kuangying Yang[2]; Cynthia Horth[3]; Eric Bareke[3]; Jacek Majewski[3]; Angela C. Hirbe[2]; Benjamin A. Garcia[1]; *[1]Department of Biochemistry and Molecular Biophysics, Washington University School of Medicine, St. Louis, MO; [2]Division of Oncology, Washington University School of Medicine, St. Louis, MO; [3]Department of Human Genetics, McGill University, Montreal, Quebec*

ThOB am 09:50 **Sensitive cell surface proteomics tailored for fresh and cryopreserved cell lines and solid tissues**; John R. Thorup[1]; Sarah Johnston[2]; Edwin Sedodo[2]; Kathleen O'Neill[2]; Ronny Drapkin[2]; Namrata Udeshi[1]; Michael A. Gillette[1]; Steven A. Carr[1]; Shankha Satpathy[1]; *[1]Broad Institute of MIT and Harvard, Cambridge, MA; [2]University of Pennsylvania, Perelman School of Medicine, Philadelphia, PA*

ThOB am 10:10 **diaPASEF Proteomics and Phosphoproteomics Elucidate EGFR Signaling Overactivation and Uncover Lipid Metabolic Changes in Pachyonychia Congenita, a Rare Skin Disease**; Sara Ceccacci[1, 2]; Kevin Roger[1]; Lucile Marchal[2]; Hélène Ragot[2]; Janice Schwartz[3]; Alain Hovnanian[2]; Chiara Guerrera[1]; *[1]Necker Proteomics, Université Paris Cité - Structure Fédérative de Recherche Necker, INSERM US24/CNRS UAR3633, Paris, France; [2]Université Paris Cité, Inserm, UMR 1163, Institut Imagine, Laboratory of genetic skin diseases, F-75015, Paris, France; [3]Pachyonychia Congenita Project, Salt Lake City, Utah*

ThOC AM: FUNDAMENTALS: ION ACTIVATION AND DISSOCIATION
Room 309-310
Session Chair: Matthew Bush (University of Washington)

ThOC am 08:30 **Enthalpy vs Entropy: Exploring the Mechanisms Behind Macrocyclic Structure Formation in Peptides Using Collision Induced Dissociation with Pentaglycine**; Evan H Perez[1]; Peter B. Armentrout[1]; *[1]University of Utah, Salt Lake City, UT*

ThOC am 08:50 **Dipolar DC Dissociation Kinetics in Quadrupole Ion Traps: How Detector Response Affects Measured Activation Parameters of Multiply-Charged Peptides**; Samantha A Mehnert[1]; Scott A. McLuckey[2]; *[1]Purdue University, West Lafayette, IN; [2]Purdue Univeristy, West Lafayette, IN*

ThOC am 09:10 **Expedient electron transfer dissociation for improved glycoproteome characterization**; Haley M. Schramm[1]; Tim S Veth[1]; Kayla A. Markuson[1]; Joshua D. Hinkle[2]; John E. P. Syka[2]; Graeme C.

McAlister[2]; Chirstopher Mullen[2]; Nicholas M Riley[1]; *[1]University of Washington, Seattle, WA; [2]Thermo Fisher Scientific, San Jose, CA*

ThOC am 09:30 **Investigating differences in gas-phase protein structure pre/post proton-transfer charge reduction via tandem mass spectrometry**; Marek Polak[1]; Lissa C. Anderson[1, 2]; Christopher L Hendrickson[1]; Kristina Hakansson[1, 2]; Chad R. Weisbrod[1]; *[1]National High Magnetic Field Laboratory, Tallahassee, FL; [2]Department of Chemistry & Biochemistry, Tallahassee, FL*

ThOC am 09:50 **False positives in the assignment of internal ions**; Maxence Derbez-Morin[1]; Brielle L Van Orman[1]; Ryan R Julian[1]; *[1]University of California, Riverside, Riverside, CA*

ThOC am 10:10 **Determining Thermochemical Barriers in Collision Induced Dissociation and Unfolding Experiments in Modern Commercial Instruments**; Austin W Green[1]; Samantha O Shepherd[1, 2]; Evan Wylie[1]; Mary Ruth Shifflett[1]; Kenneth Newton[1]; Ruwan Kurulugama[3]; James S. Prell[1]; *[1]University of Oregon, Eugene, OR; [2]Yale University, New Haven, CT; [3]Agilent Technologies, Santa Clara, CA*

ThOD AM: ION MOBILITY: INSTRUMENTATION & METHOD DEVELOPMENT

Room 314-317

Session Chair: James Dodds (University of North Carolina at Chapel Hill)

ThOD am 08:30 **Showing Off Those Curves: Enabling Low-Mass Analysis with a Novel Rounded Turn SLIM Design**; Heidi Sabatini[1]; Bradley B. Garrison[1]; Copeland Johnson[1]; Cole L Frank[1]; Breland M. Jones[1]; Christopher D. Chouinard[1]; *[1]Clemson University, Clemson, SC*

ThOD am 08:50 **Developing a Cross-Platform Ion Mobility Calibration For Machine Learning: Using Sodium Iodide and Caesium Iodide to Investigate Small Molecule Protomers**; Caitlin Allison[1]; Valeria Guidolin[2]; Eleanor Sinclair[3]; Thomas Hoare[3]; Eric Dybeck[4]; Helene Fain[5]; Agisilaos Chantzis[6]; Steven Corless[7]; Lucy Morgan[8]; Frederick Strathmann[9]; Miriam Fico[9]; Sebastian Ordyniak[10]; Perdita Barran[3]; Carlos Larriba-Andaluz[11]; Frank Sobott[1]; *[1]Molecular and Cellular Biology & Astbury Centre, University of Leeds, Leeds, United Kingdom; [2]PharmSci Small Molecule, Analytical Research and Development, Pfizer, Groton, CT; [3]Chemistry & Michael Barber Centre University of Manchester, Manchester, United Kingdom; [4]MedDesign, Pfizer, Cambridge, MA; [5]Process Technology & Engineering Analytical Solutions, Syngenta, Bracknell, United Kingdom; [6]Computational Chemical Design and Modelling Group, Research Chemistry, Syngenta, Bracknell, United Kingdom; [7]National Measurement Lab (NML) at LGC, Teddington, United Kingdom; [8]Analytical Chemistry and Data Science, Pfizer, Sandwich, United Kingdom; [9]MOBILion Systems, Inc., Chadds Ford, PA; [10]Computer Science, University of Leeds, Leeds, United Kingdom; [11]Mechanical Engineering, Purdue University, Indianapolis, IN*

ThOD am 09:10 **Collisional Cross Section Measurement via Orbitrap Mass Analysis: Figures of Merit for High-throughput Applications**; Kyle Fort[1]; Konstantin Aizikov[1]; Ulises H. Guzman[2]; Tobias Woerner[1]; Shelley Jager[3, 4]; Albert J.R. Heck[3, 4]; Jesper V. Olsen[5]; Alexander Makarov[1]; *[1]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [2]Novo Nordisk Foundation Center for Protein Research, University of Copenhagen, Copenhagen, Denmark; [3]Utrecht University, Utrecht, Netherlands; [4]Netherlands Proteomics Center, Padualaan 8, 3584 CH Utrecht, Netherlands; [5]Novo Nordisk Foundation Center for Protein Research, University of Copenhagen, Denmark*

ThOD am 09:30 **Mobility and Mass Selective Isolation, Separation and Characterization of Macro-Biomolecules**; Jung Lee[1]; Viraj D. Gandhi[1]; Christopher Harilal[1]; Amar Parvate[1]; Stephanie M. Thibert[1]; Ashley Ives[1]; Xin Zhang[1]; Gregory K Schenter[1]; Yehia M. Ibrahim[1]; Carlos Larriba-Andaluz[2]; James E Evans[1]; Sandilya Garimella[1]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]Purdue Univeristy, West Lafayette, IN*

ThOD am 09:50 **Dual-Path TW-SLIM-TOF System for Ion Mobility-Mass Spectrometry with Complete Ion Utilization**; Cullen Greer[1]; Brian H. Clowers[1]; *[1]Washington State University, Pullman, WA*

ThOD am 10:10 **Elucidating Biomolecular Complexity in Alpha-Synuclein Aggregation: Ion Mobility-Mass Spectrometry meets Infrared Action Spectroscopy**; Agathe Depraz Depland[1]; Olivier Verhoev[1]; May Constabel[1, 2]; Steven Daly[1, 2]; Sjors Bakels[1]; Anouk M. Rijs[1]; *[1]Vrije Universiteit Amsterdam, Amsterdam, Netherlands; [2]MS Vision, Almere, Netherlands*

ThOE AM: POSTTRANSLATIONAL MODIFICATIONS: QUALITATIVE AND QUANTITATIVE ANALYSIS

Ballroom II

Session Chair: Sureyya Ozcan (METU)

ThOE am 08:30 **Next-Generation Multiplexed Targeted Pathway Proteomics Quantifies Post-Translational Modifications with High Target Throughput in 3.4 Minutes Per Sample**; Steven Shuken[1]; Charlotte Beard[2]; Shane L. Dawson[3]; Kean Hean Ooi[3]; Jesse D. Canterbury[4]; Nathan R. Zuniga[3]; Brandon M. Gassaway[3]; João A. Paulo[3]; M. Windy McNerney[2]; Qing Yu[3, 5]; Steven P. Gygi[3]; *[1]Harvard Medical School, Boston, MA; [2]Department of Psychiatry and Behavioral Sciences, Stanford University School of Medicine, Stanford, CA; [3]Department of Cell Biology, Harvard Medical School, Boston, MA; [4]Thermo Fisher Scientific, San Jose, California; [5]Department of biochemistry and molecular biotechnology, University of Massachusetts Chan Medical School, Worcester, MA*

ThOE am 08:50 **Orders of magnitude sensitivity improvement in phosphoproteomics via nanoPhos**; Denys Oliinyk[1]; Tim Heymann[1]; Lukas Henneberg[1]; Florian Rosenberger[1]; Matthias Mann[1]; *[1]Max Planck Institute of Biochemistry, Martinsried, Germany*

ThOE am 09:10 **MS-Ion: Unveiling Ion Associations in PTM-Enriched Proteomic Data**; Michelle Fai[1]; Yi-Ju Chen[2]; Hui-Yin Chang[1]; *[1]Department of Biomedical Sciences and Engineering, Institute of Systems Biology and Bioinformatics, National Central University, Taoyuan, Taiwan; [2]Department of Biological Science and Technology, National Yang Ming Chiao Tung University, Hsinchu, Taiwan*

ThOE am 09:30 **Decoding native membrane proteoforms with precisION**; Jack L Bennett[1, 2]; Tarick J El-Baba[1, 2]; Konstantin C Zouboulis[1, 2]; Carla Kirschbaum[1, 2]; Haigang Song[1, 2]; Frances I Butroid[1, 2]; Justin L P Benesch[1, 2]; Corinne A Lutomski[1, 2]; Carol V Robinson[1, 2]; *[1]Kavli Institute for Nanoscience Discovery, University of Oxford, Oxford, United Kingdom; [2]Department of Chemistry, University of Oxford, Oxford, United Kingdom*

ThOE am 09:50 **Exploring Immunogenic Glycosylation and Organ-Specific N-Glycan Diversity in Pigs for Xenotransplantation**; Ji Eun Park[1, 2]; Myung Jin Oh[1, 2]; Joohyun Shim[3]; Kimyung Choi[3]; Hyun Joo An[1, 2]; *[1]Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, South Korea; [2]Asia-Pacific Glycomics Reference Site, Daejeon, South Korea; [3]Department* *of Transgenic Animal Research, Optipharm, Inc., Chungcheongbuk-do, Cheongju-si, South Korea*

ThOE am 10:10 **Optimized Platform for In-depth Characterization of MHC Class I and II Peptides and Phosphorylated Immunopeptides**; Dorothy Ahlf Wheatcraft[1]; Evgenii Tcyganov[2]; Xiaoxu Wang[2]; Jana Zecha[2]; Kristina Archer[2]; Shino Hanabuchi[2]; Matthew Glover[2]; Rajat Varma[2]; Dmitry Gabrilovich[2]; Sonja Hess[2]; *[1]AstraZeneca, Gaithersburg, MD; [2]AstraZeneca, Gaithersburg, Maryland*

ThOF AM: INSTRUMENTATION: NEW DEVELOPMENTS IN IONIZATION AND SAMPLING

Ballroom I

Session Chair: Ethan McBride (Los Alamos National Laboratory)

ThOF am 08:30 **Ion Optics Voltages Change Ion Structure**; Gary L. Glish[1]; Matthew T. Campbell[2, 3]; Russell P Grant[1, 4]; Tyler S. Larson[3]; Conner J. Baucom[1]; *[1]University of North Carolina, Chapel Hill, NC; [2]LabCorp, RTP, NC; [3]University of North Carolina - Chapel Hill, Chapel Hill, NC; [4]LabCorp, Burlington, NC*

ThOF am 08:50 **High Throughput Sensitive Single Cell Analysis using Rapid Droplet Sampling Interface Coupled to Mass Spectrometry**; Vilmos Kertesz[1]; Stephen C Zambrzycki[1]; John F Cahill[1]; *[1]Oak Ridge National Laboratory, Oak Ridge, TN*

ThOF am 09:10 **Analysis of volatile organic compounds using LDI-produced metal ions as ionization agents**; Monika Koktava[1]; Vadym Prysiazhnyi[1]; Jan Preisler[1]; Antonin Bednarik[1]; *[1]Masaryk University, Brno, Czech Republic*

ThOF am 09:30 **Determination of Proteins and Peptides Using Paper Spray-Mass Spectrometry Coupled with Faradaic Ion Concentration Polarization**; Lahiru Wedasingha[1]; Magnus Rydberg[1]; Nicholas E. Manicke[1]; *[1]Department of Chemistry and Chemical Biology, Indiana University, Indianapolis, Indianapolis, Indiana*

ThOF am 09:50 **Enhancing data quality in mass spectrometry imaging through dopant-enriched nitrogen nebulizer gas**; Gábor Tóth[1, 2]; Ingela Lanekoff[1, 2]; *[1]Department of Chemistry - BMC, Uppsala University, Uppsala, Sweden; [2]Center of Excellence for the Chemical Mechanisms of Life, Uppsala University, Uppsala, Sweden*

ThOF am 10:10 **Miniaturized MALDI-2 Imaging Mass Spectrometry for Point-of-Care Diagnostics**; William Yang Terziyan[1]; Krisztian G. Torma[1]; Mike Chai[1]; *[1]BaySpec Inc., San Jose, CA*

ThOG AM: ENVIRONMENTAL: NON-TARGET ANALYSIS AND EMERGING CONTAMINANTS

Ballroom III

Session Chair: Brett R. Blackwell (Los Alamos National Laboratory)

ThOG am 08:30 **Lactational Transfer of Per- and Polyfluoroalkyl Substances (PFAS) in Marine Mammals: Quantitative and Non-Targeted Analyses**; Kara M. Joseph[1]; Ashlee T. Falls[1]; Michael L. Power[2]; Erin S. Baker[1]; *[1]University of North Carolina Chapel Hill, Chapel Hill, NC; [2]Smithsonian's National Zoo and Conservational Biology Institute, Washington, DC*

ThOG am 08:50 **Ultra-Sensitive Identification of 500 Pesticides, Pharmaceuticals in Irrigated Soils Using Reclaimed Water via Direct Injection and Ion Trap-Enhanced Q-TOF-MS**; Amadeo R. Fernández-Alba[1]; Lorena Manzano-Sanchez[1]; Marc Lopez Matarin[1]; Dolores Hernando Guil[2]; Maria Jesus Martinez Bueno; Damia Barceló; *[1]UNIVERSITY OF ALMERIA, Almeria, Spain; [2]Department of Desertification and Geo-ecology, Experimental Station of Arid Zones, CSIC, Almeria, Spain*

ThOG am 09:10 **NIST Mass Spectral Libraries in the Identification of Plastic-Related Compounds: Extractables & Leachables**; Adam Zuber[1]; Yamil Simón-Manso[1]; Edward P Erisman[1]; Tytus D Mak[1]; William E Wallace[1]; *[1]National Institute of Standards and Technology (NIST), Gaithersburg, MD*

ThOG am 09:30 **Compositional and Structural Analysis of Scrubber Water Discharges from Ships Using Liquid Chromatography Fourier Transform Ion Cyclotron Resonance Mass Spectrometry**; Christopher Paul Rüger[1, 2]; Helly Johanna Hansen[1]; Eric Schneider[1]; Martha Liliana Chacón-Patiño[2, 3]; Maxime SUEUR[2, 4, 5]; Germain S. Vallverdu[2, 6]; Julien Maillard[2, 5]; Ryan P Rodgers[2, 3]; Pierre Giusti[2, 5]; Thorsten Streibel[1, 7]; Carlos Afonso[2, 4]; Ralf Zimmermann[1, 7]; *[1]University of Rostock, Chair of Analytical Chemistry and Dept. of Life, Light and Matter, Rostock, Germany; [2]International Joint Laboratory, iC2MC: Complex Matrices Molecular Characterization, Harfleur, France; [3]National High Magnetic Field Laboratory, Tallahassee, FL; [4]Normandie Univ, UNIROUEN, INSA Rouen, CNRS, CARMeN, 76000 Rouen, France, Mont Saint Aignan, France; [5]TotalEnergies Research and Technology Gonfreville, Harfleur, France; [6]Université de Pau et des Pays de l'Adour, IPREM UMR-CNRS, Pau, France; [7]Helmholtz Munich, Munich, Germany*

ThOG am 09:50 **High-Resolution Mass Spectrometry based DNA Adductomics: Application in Environmental Exposure Assessment**; Zareen Saeed Khan[1]; Elena Gorokhova[1]; Justyna Hampel[1]; Bala S. Seetha[1]; Natalia Tretyakova[2]; Pedro F.M. Sousa[1]; Lars Förlin[3]; Hitesh Motwani[1]; *[1]Stockholm University, Stockholm, Sweden; [2]University of Minnesota, Minnneapolis, MN; [3]University of Gothenburg, Gothenburg, Sweden*

ThOG am 10:10 **Impact of urban wildfires on drinking water: Urban structural ash produces more toxic disinfection byproducts than vegetation ash**; Susan Richardson[1]; Patrick Justen[1]; Erin Katie Jaynes[1]; Coley Beavers[1]; Talal Alshehri[1]; Mahbub Alam[1]; Mohammed Baaalousha[1]; *[1]University of South Carolina, Columbia, SC*

ThOH AM: H/D EXCHANGE: INNOVATIONS AND APPLICATIONS

Ballroom IV

Session Chair: Charles Nwosu (Takeda Pharmaceuticals International Co)

ThOH am 08:30 **Enhancement of Protein-Protein Interactions by Destabilizing Mutations Revealed by HDX-MS**; Yoshitomo Hamuro[1]; Richard Huang[1]; *[1]Janssen Pharmaceuticals, Spring House, PA*

ThOH am 08:50 **A fully automated, ultra-sensitive nanoHDX-MS platform for the analysis of megadalton-scale protein complexes**; Shaunak Raval[1]; Yuqi Shi[2]; Julia Morriss[3]; Alexander R. Ivanov[4]; Inna Afasizheva[5]; Ruslan Afasizhev[5]; Brian B. Liau[3]; Steven A. Carr[1]; Malvina Papanastasiou[1]; *[1]Broad Institute of MIT and Harvard, Cambridge, MA; [2]ThermoFisher Scientific, San Jose, CA; [3]Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA; [4]Department of Chemistry & Chemical Biology, Northeastern University, Boston, MA; [5]Department of Molecular and Cell Biology, Boston University Medical Campus, Boston, MA*

ThOH am 09:10 **Integration of online electrochemical reduction to time-resolved HDX-MS for enhanced sequence coverage of heavily disulfide bonded proteins**; Alice Colyer[1]; Joseph Anacleto[1]; Cristina Lento[1]; Dominic Narang[2]; Derek J Wilson[1]; *[1]York U, Toronto, ON; [2]Rapid Novor Inc, Kitchener, ON*

ThOH am 09:30 **Intact SARS CoV-2 VLP dynamics by cyclic IMS-Q-TOF HDXMS reveal large conformational changes and altered epitope landscape in Spike protein**; Amanda J Gramm[1]; Sean M Braet[1]; Bindu Y Srinivasu[2]; Elijah J Bass[3]; Fiona L Kearns[4]; Rommie E Amaro[4]; Robert V Stahelin[3]; Thomas E Wales[2];

Ganesh S Anand[1]; [1]*Pennsylvania State University, University Park, PA; [2]Northeastern University, Boston, MA; [3]Purdue Institute for Inflammation, Immunology, and Infectious Disease, West Lafayette, IN; [4]University of California San Diego, San Diego, CA*

ThOH am 09:50 **Hydrogen-deuterium exchange mass spectrometry with integrated protein thermal depletion reveals differential polyclonal antibody binding in two human AVA vaccinated donors**; Joel B Langford[1]; Mulin Fang[1]; Oliver Wu[1]; Kellye A. Cupp-Sutton[2]; Kathleen Norris[3]; Kenneth Smith[3]; Si Wu[2]; [1]*University of Oklahoma, Norman, OK; [2]University of Alabama, Tuscaloosa, AL; [3]Oklahoma Medical Research Foundation, Oklahoma City, OK*

ThOH am 10:10 **Site specific HDX-MS for characterization of drug-target interactions reveals divergent binding modes for same-site binders**; Joseph Anacleto[1]; Vimanda Chow[1]; Esther Wolf[2]; Suzanne Ackloo[2]; Yves Leblanc[3]; Cristina Lento[1]; Derek Wilson[4]; [1]*York U, Toronto, ON; [2]University of Toronto, Toronto; [3]SCIEX, Concord, ontario; [4]York University, Toronto, ON*

ThOA PM: INFORMATICS: PEPTIDE AND PROTEIN IDENTIFICATION AND QUANTIFICATION

Hall AB

Session Chair: Elizabeth F. Bayne (Merck & Co., Inc.)

ThOA pm 02:30 **Carafe enables high quality in silico spectral library generation for data-independent acquisition proteomics**; Bo Wen[1]; Chris Hsu[1]; Wen-Feng Zeng[2]; Michael Riffle[1]; Alexis Chang[1]; Miranda Mudge[1]; Brook Nunn[1]; David Shteynberg[1]; Brendan MacLean[1]; Matthew D. Berg[1]; Judit Villen[1]; Michael J. MacCoss[1]; William S. Noble[1, 3]; [1]*Department of Genome Sciences, University of Washington, Seattle, WA; [2]Department of Proteomics and Signal Transduction, Max Planck Institute of Biochemistry, Munich, Germany; [3]Paul G. Allen School of Computer Science and Engineering, University of Washington, Seattle, WA*

ThOA pm 02:50 **Multi-dimensional Bayesian Analysis Enhances the Sensitivity of High Throughput Single Cell Proteoform Imaging Mass Spectrometry (scPiMS)**; Michael Hollas[1]; Pei Su[2]; Indira Pla[1]; Stanislav S Rubakhin[3]; Fatma A. Butun[1]; Joseph B. Greer[1]; Bryan P. Early[1]; Ryan Fellers[1]; Jonathan V Sweedler[3]; Jared Kafader[1]; Neil Kelleher[1, 2]; [1]*Proteomics Center of Excellence, Northwestern University, Evanston, IL; [2]Northwestern University, Chicago, IL; [3]university of Illinois-Urbana Champaign, Urbana, IL*

ThOA pm 03:10 **A Robust Computational Workflow for Multiplex-DIA MS Profiles Protein Turnover Regulations Associated with Cisplatin Resistance and Aneuploidy**; Barbora Salovska[1]; Wenxue Li[1]; Oliver M. Bernhardt[2]; Pierre-Luc Germain[3]; Tejas Gandhi[2]; Lukas Reiter[2]; Yansheng Liu[1]; [1]*Yale University, New Haven, CT; [2]Biognosys AG, Schlieren, Switzerland; [3]ETH Zurich, Zurich, Switzerland*

ThOA pm 03:30 **A scalable, cloud-based proteomics platform for the masses**; Layla Eljagh[1]; Markus Schneider[1]; Daniel P. Zolg[1]; Patroklos Samaras[1]; Dulguun Bold[1]; Samia Ben Fredj[1]; Florian Seefried[1]; Tobias Schmidt[1]; Siegfried Gessulat[2]; Martin Frejno[1]; [1]*MSAID, Garching b.München, Germany; [2]MSAID, Berlin, Germany*

ThOA pm 03:50 **Scalable Peptide MRM Transition Prediction for High-Throughput Proteomics via Hashing-Based Sequence Encoding**; Ramon Adàlia[1, 2]; Ismael Zamora[3]; [1]*Universitat Autònoma de Barcelona, Cerdanyola del Vallès, Spain; [2]Lead Molecular Design, SL, Sant Cugat del Vallès, Spain; [3]Mass Analytica, Sant Cugat del Valles, Spain*

ThOA pm 04:10 **FLASHTnT (Tag and exTension): A robust and versatile proteoform identification and characterization tool for top-down proteomic**; Kyowon Jeong[1, 2]; Jaywon Lee[3, 4]; Wonhyeuk Jung[5]; Tom D. Müller[1, 2]; Aniruddha Panda[3, 4]; Ayesha Feroz[2, 6]; Jared B. Shaw[7]; Louise M. Buur[8]; Viktoria Dorfer[8]; Oliver Kohlbacher[2, 6, 9]; Kallol Gupta[3, 4]; [1]*Applied Bioinformatics, Department for Computer Science, University of Tübingen, Tübingen, Germany; [2]Institute for Bioinformatics and Medical Informatics, University of Tubingen, Tubingen, Germany; [3]Department of Cell Biology, Yale School of Medicine, New Haven, CT; [4]nanobiology Institute, Yale University, New Haven, CT; [5]Clinical Pharmacology and Safety Sciences, One Medimmune Way, Astrazeneca, Gaithersburg, MD; [6]Applied Bioinformatics, Department for Computer Science, University of Tübingen, Tübingen, Germany; [7]Department of Chemistry, University of Nebraska-Lincoln, Lincoln, NE; [8]Bioinformatics Research Group, University of Applied Sciences Upper Austria, Hagenberg, Austria; [9]Translational Bioinformatics, University Hospital Tübingen, Tübingen, Germany*

ThOB PM: EXPOSOMICS, TOXICOLOGY AND HEALTH OUTCOMES

Room 307-308

Session Chair: Jiajun Lei (Ellison Medical Institute)

ThOB pm 02:30 **Characterizing Toxic Metabolites and Health Implications of Azobenzene Disperse Dyes: A Toxicometabolomics Approach**; Kirsten E Overdahl[1]; Alan K Jarmusch[1]; [1]*National Institute of Environmental Health Sciences, Research Triangle Park, NC*

ThOB pm 02:50 **Comprehensive Profiling of Human Urinary Phase II Metabolites Using UPLC-QTOF MSE DIA Workflow**; Jin Chen[1]; Saurin Sutaria[2]; Zhengzhi Xie[1]; Manjiri Kulkarni[1]; Rachel J. Keith[1]; Aruni Bhatnagar[1]; Clara G. Sears[1]; Sanjay Srivastava[1]; Pawel Lorkiewicz[1]; [1]*University of Louisville, Louisville, KY; [2]Bellarmine University, Louisville, Kentucky*

ThOB pm 03:10 **Comprehensive Profiling of Mercapturic Acids Conjugates Associated with Exposure to Reactive Chemical Species Using Enzymatic Deacetylation and High-Resolution Mass Spectrometry**; Yuan-Chih Chen[1]; Man-Ni Zhuang[1]; Jen-Yi Hsu[1]; Yi-Chun Lin[1]; Hsin-Yi Wu[2]; Pao-Chi Liao[1]; [1]*National Cheng Kung University, Tainan, Taiwan; [2]National Taiwan University, Taipei, Taiwan*

ThOB pm 03:30 **Comparison of Human Serum Albumin Cys34 Adductomics in Matched Dried Blood Spot and Plasma Samples**; Aishwarya Jala[1]; Fariba Tayyari[1]; Yeunook Bae[1, 2]; James L Burke[1]; Zhu Zou[1]; Kwang-Youn A Kim[1]; Siyuan Dong[1]; William E Funk[1]; [1]*Northwestern University, Feinberg School of Medicine, Chicago, IL; [2]Illinois State University, Normal, IL*

ThOB pm 03:50 **Mitigating Kidney Toxicity Risk and Prioritizing Drug Candidates Using MALDI Mass Spectrometry Imaging**; Bingming Chen[1]; Lisa LaFranco-Scheuch[1]; Shuzhi Dong[2]; Lorraine Hernandez[1]; Hong Mei[1]; Wendy Zhong[2]; Mark Cancilla[1]; Marissa Vavrek[1]; Juliann Ehrhart[1]; Thomas Forest[1]; Yu Tao[2]; Yingkai Liang[1]; Takayuki Tsuchiya[1]; Andrew Leithead[1]; Bennett Ma[1]; [1]*Merck, West Point, PA; [2]Merck, Rahway, NJ*

ThOB pm 04:10 **Experimental Validation of MS2-based Mixture Toxicity Predictions: a Case Study on Synthetic Mixtures**; Helen Sepman[1, 2]; Lisa A. Baumann[3, 4]; Frederic Béen[3, 5]; Anneli Kruve[1, 2]; [1]*Department of Environmental Science, Stockholm University, Stockholm, Sweden; [2]Department of Chemistry,* *Stockholm University, Stockholm, Sweden; [3]Amsterdam Institute for Life and Environment (A-LIFE), Vrije Universiteit Amsterdam, Amsterdam, Netherlands; [4]Centre for Organismal Studies, University of Heidelberg, Heidelberg, Germany; [5]KWR Water Research Institute, Nieuwegein, Netherlands*

ThOC PM: IMAGING: SPATIALLY RESOLVED OMICS (HONORING RICHARD CAPRIOLI)

Room 309-310

Session Chair: Boone M. Prentice (University of Florida)

ThOC pm 02:30 **Richard M. Caprioli's Pioneering Innovations in Mass Spectrometry**; Per E. Andren; *Uppsala University, Uppsala, Sweden*

ThOC pm 02:50 **Novel Molecular Profiles of Outcome in the Triple Negative Breast Cancer Microenvironment by MALDI MSI Spatialomics**; Peggi Angel[1]; Danielle A Scott[2]; Jaclyn Dunne[2]; Taylor Hulahan[2]; Jade K Macdonald[2]; Laura Spruill[2]; Souvik Seal[2]; Yeonhee Park[3]; Bethany Wolf[2]; Graham Colditz[4]; Anand S Mehta[2]; Richard R Drake[2]; Harikrishnan Nakshatri[5]; Marvella Ford[2]; Harrison B. Taylor[2]; *[1]Medical University of South Carolina, Charleston, SC; [2]Medical University of South Carolina, Pharmacology & Immunology, Charleston, SC; [3]Sungkyunkwan University, Seol, South Korea; [4]Washington University in St. Louis, University City, MO; [5]Indiana University School of Medicine, Indianapolis, IN*

ThOC pm 03:10 **Investigation of localised tissue immune response to intramuscular drug treatment with a mass spectrometry imaging-based spatial multi-omics approach**; William M Hardesty[1]; Fang Xie[1]; Heath Patterson[2]; Wanqiu Zhang[2]; Maria Mantas[2]; Eliot t Mckinley[1]; Alice Ly[2]; Nico Verbeeck[2]; Marc Claesen[2]; Reid Groseclose[1]; *[1]GSK, Collegeville, PA; [2]Aspect Analytics, Genk, Belgium*

ThOC pm 03:30 **Localizing Senescence Associated Metabolites in human Skin and in 3Dskin aging models**; Martina Marchetti-Deschmann[1, 2, 3]; Samuele Zoratto[1, 2]; Christoph Kremslehner[2, 4]; Michaela Schirato[2, 4]; Gaëlle Gendronneau[5]; Agnès Tessier[5]; Florian Gruber[2, 3, 4]; *[1]TU Wien, Vienna, Austria; [2]Christian Doppler Laboratory for Multimodal Imaging of Aging and Senescence - SKINMAGINE, Vienna, Austria; [3]ViCEM - Vienna Center for Engineering in Medicine, Vienna, Austria; [4]Medical University of Vienna, Department of Dematology, Vienna, Austria; [5]Chanel PB, Pantin, France*

ThOC pm 03:50 **Mass spectrometry imaging of the gut microbiome**; Samarth Ganjoo[1]; Pierre Chaurand[1]; *[1]University of Montreal, Montreal, QC*

ThOC pm 04:10 **Integrative Technologies for Multimodal Imaging Mass Spectrometry: a Toolbox for Spatial Biology**; Jeffrey M Spraggins[1, 2, 3, 4, 5]; Raf Van De Plas[1, 3, 6]; *[1]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [2]Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; [3]Department of Biochemistry, Vanderbilt University, Nashville, TN; [4]Department of Chemistry, Vanderbilt University, Nashville, TN; [5]Department of Pathology, Microbiology, and Immunology, Vanderbilt University Medical Center, Nashville, TN; [6]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands*

ThOD PM: CARBOHYDRATES: FROM MONO TO POLY

Room 314-317

Session Chair: Juan Castillo (Gilead Sciences Inc.)

ThOD pm 02:30 **A glycomic LC-MS method for characterizing the activity and specificity of gut bacterial glycosyl hydrolases**; Sophia Jiang[1]; Mary Riley[2]; Justin Siegel[1, 3]; David Andrew Mills[4]; Carlito B. Lebrilla[1]; *[1]Department of Chemistry, University of California, Davis, Davis, CA; [2]Microbiology Graduate Group, University of California, Davis, Davis, CA; [3]Department of Biochemistry and Molecular Medicine, University of California, Davis, Davis, CA; [4]Department of Food Science and Technology, University of California, Davis, Davis, CA*

ThOD pm 02:50 **Distinguishing 3-sialyl-N-acetyllactosamine and 6-sialyl-N-acetyllactosamine by combining Co2+ Adduction and Electron-Transfer Higher-Energy Collisional Dissociation**; Holly T Wilson[1]; Darren T Gass[2]; Elyssia S Gallagher[2]; *[1]Baylor university, Waco, TX; [2]Baylor University, Waco, TX*

ThOD pm 03:10 **Glycan Permethylation and Multiplexed Ion Mobility Mass Spectrometry for Sialic Acid Isomer Characterization**; Angel E. Ibarra[1]; Shuling Xu[2]; Zicong Wang[2]; Lingjun Li[1, 2]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [2]School of Pharmacy, University of Wisconsin-Madison, Madison, WI*

ThOD pm 03:30 **How caterpillars are like worms: analysing zwitterionic N-glycans of insects and nematodes**; Iain Wilson[1]; Shi Yan[1, 2]; Jorick Vanbeselaere[1]; Lena Nuschy[1]; Katharina Paschinger[1]; *[1]Universität für Bodenkultur Wien, Vienna, Austria; [2]Veterinärmedizinische Universität Wien, Vienna, Austria*

ThOD pm 03:50 **Facile determination of intact laminarin molecular weight using HILIC-HESI-HRMS**; Clint M Alfaro[1]; Ritesh Sheth[1]; *[1]UPL, Durham, NC*

ThOD pm 04:10 **Complementary Distribution of Glycoconjugates in Glioblastoma Revealed by Multi-Enzyme MALDI Mass Spectrometry Imaging**; Mehrnoush Taherzadeh Ghahfarrokhi[1, 2]; Emily R. Sekera[3]; John J. Bowling[3]; Parastoo Azadi[2]; *[1]University of Georgia, Athens, GA; [2]Complex Carbohydrate Research Center, University of Georgia, Athens, GA; [3]St Jude Children's Research Hospital, Memphis, TN*

ThOE PM: INSTRUMENTATION: HIGH-RESOLUTION MASS SPECTROMETRY

Ballroom II

Session Chair: Christopher L. Hendrickson (National High Magnetic Field Laboratory)

ThOE pm 02:30 **Enhancing the dynamic range of TIMS-FT-ICR MS instruments to extend the frontiers of complex sample analysis**; Christopher Wootton[1]; Alina Theisen[1]; Gregory Brabeck[1]; Pierre Giusti[2]; Carlos Afonso[3]; Madeline E Colley[4]; Jeffrey M Spraggins[4]; *[1]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [2]TotalEnergies Research and Technology Gonfreville, Harfleur, France; [3]University of Rouen Normandy, Mont Saint-Aignan, France; [4]Vanderbilt University, Nashville, TN*

ThOE pm 02:50 **Charting New Paths in Lipidomics: Understanding Caloric Restriction and Aging with Orbitrap Astral MS**; Salma Ibrahim Abouelhassan[1]; Katherine A. Overmyer[1, 2, 3]; Scott T. Quarmby[1, 3]; Josef P. Clark[1]; Rozalyn M. Anderson[1]; Ricki J. Colman[4]; Joshua J. Coon[1, 2, 3]; *[1]University of Wisconsin-Madison, Madison, WI; [2]Morgridge Institute for Research, Madison, WI; [3]National Center for Quantitative Biology of Complex Systems, Madison, WI; [4]Wisconsin National Primate Research Center, Madison, WISCONSIN*

ThOE pm 03:10 **One Ion AT a Million: Characterizing Individual Nanoparticle Ions with m/z ~ 1,000,000 using Charge Detection Mass Spectrometry**; Conner C Harper[1]; Veena S Avadhani[1]; Evan R Williams[1]; *[1]University of California, Berkeley, Berkeley, CA*

ThOE pm 03:30 **CD-MS Charge State Resolution in Under 600 ms**; Raj Parikh[1]; Martin F Jarrold[1]; *[1]Indiana University, Bloomington, IN*

ThOE pm 03:50 **Structural characterization of lignocellulosic-based pyrolysis oil by two-dimensional mass**

spectrometry; Maria Van Agthoven[1, 2]; Julien Maillard[2, 3]; Maxime Sueur[1, 2, 3]; Christopher A Wootton[4]; Pierre Giusti[1, 2, 3]; Carlos Afonso[1, 2]; *[1]University of Rouen Normandy, Mont Saint-Aignan, France; [2]International Joint Laboratory, iC2MC: Complex Matrices Molecular Characterization, Harfleur, France; [3]TotalEnergies Research and Technology Gonfreville, Harfleur, France; [4]Bruker Daltonics GmbH & Co.KG, Bremen, Germany*

ThOE pm 04:10 **Twenty Years of Orbitrap Mass Spectrometry as A Mainstream Technology for High-Resolution Accurate Mass Analysis**; Alexander Makarov; *Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

ThOF PM: NEUROSCIENCE AND NEUROLOGICAL DISORDERS RESEARCH

Ballroom I

Session Chair: Jeffrey N. Savas (Northwestern University, Feinberg School of Medicine)

ThOF pm 02:30 **Quantification of Linoleic acid pro-resolving metabolites in a Paraquat-induced Drosophilamodel of Parkinson's disease using UPLC-HRMS and MALDI imaging**; Swarnali Chatterjee[1, 2]; Qiaoli Liang[3, 4]; Qi Li[5]; Greg J. Szulczewski[3, 4]; Lukasz Ciesla[2, 3]; *[1]The University of Alabama, TUSCALOOSA, AL; [2]Department of Biological Sciences, The University of Alabama, Tuscaloosa, Alabama; [3]University of Alabama, Tuscaloosa, AL; [4]Department of Chemistry and Biochemistry, The University of Alabama, TUSCALOOSA, Alabama; [5]Brigham and Women's Hospital/Harvard Medical Sch, Boston, MA*

ThOF pm 02:50 **In vivo brain metabolomic profiling of substance abuse by LC-MS/MS and non-targeted chemometrics**; Caitlin N Cain[1]; Pavlo Popov[2]; Nicholas M Oliver[1]; Elaine K Hebda-Bauer[3]; Huda Akil[3]; Robert T Kennedy[1, 4]; *[1]Department of Chemistry, University of Michigan, Ann Arbor, MI; [2]Department of Psychology, University of Michigan, Ann Arbor, MI; [3]Michigan Neuroscience Institute, University of Michigan, Ann Arbor, MI; [4]Department of Pharmacology, University of Michigan, Ann Arbor, MI*

ThOF pm 03:10 **Understanding membrane phase separation through lipid vesicle native ion mobility-mass spectrometry: Mechanism of ultrafast neurotransmitter release**; Aniruddha Panda[1]; Iliana Levesque[2]; Jean N.D. Goder[1]; Anna L. Duncan[3]; Frederic Pincet[4]; Brandon T. Ruotolo[2]; Kallol Gupta[1]; *[1]Department of Cell Biology, Yale University, West Haven, CT; [2]Department of Chemistry, University of Michigan, Ann Arbor, MI; [3]Department of Chemistry, Aarhus University, Aarhus, Denmark; [4]Laboratoire de Physique de l'Ecole Normale Supérieure, ENS, CNRS, Université PSL, Sorbonne Université, Université Paris-Cité, Paris, France*

ThOF pm 03:30 **Unveiling Novel Functional Pathways and Biomarkers in Alzheimer's Disease through Ultra-Sensitive Biofluid Proteomic Profiling**; Hendrik Wesseling[1]; Joel Bucci[1, 2]; Pavithra Krishnaswami[1]; Yao Chen[1]; Bo Yang[1]; Martin Kramer[1]; Mikhail Levit[1]; Simon Dujardin[1]; Krishnan Rajaraman[1]; Bailin Zhang[1]; *[1]Sanofi, Cambridge, MA; [2]ThermoFisher Scientific, Lexington, MA*

ThOF pm 03:50 **Profiling the proteoform landscape of tau from the human brain by individual ion mass spectrometry**; Tian Xu[1]; Taojunfeng Su[1]; Benjamin J. Des Soye[1]; Soumya Kandi[1]; Che-Fan Huang[1]; John T. Wilkins[2]; Jared O. Kafader[1]; Steven M. Patrie[1]; Robert Vassar[3, 4]; Neil L. Kelleher[1]; *[1]Proteomics Center of Excellence, Northwestern University, Evanston, IL; [2]Departments of Medicine (Cardiology) and Preventive Medicine, Feinberg School of Medicine, Northwestern University, Chicago, IL; [3]Mesulam Center for Cognitive Neurology and Alzheimer's Disease, Northwestern University Feinberg School of Medicine, Chicago, IL; [4]Department of Neurology, Northwestern University Feinberg School of Medicine, Chicago, IL*

ThOF pm 04:10 **Native and top-down MS reveals remodeling of brain-derived metabotropic glutamate receptors in depression**; Tarick El-Baba[1]; Corinne A Lutomski[1, 2]; Sophie A. S. Lawrence[1, 2]; Jack L Bennett[1, 2]; Sean Burnap[1, 2]; Frances I Butroid[1, 2]; Di Wu[1, 2]; Haigang Song[1, 2]; Kenny L Chan[3, 4]; Lyonna F Parise[3, 4]; Weston Struwe[1, 2]; Scott J Russo[3, 4]; Carol V Robinson[1, 2]; *[1]Kavli Institute for Nanoscience Discovery, University of Oxford, Oxford, United Kingdom; [2]University of Oxford, Oxford, United Kingdom; [3]Nash Family Department of Neuroscience, Friedman Brain Institute, Icahn School of Medicine at Mount Sinai, New York City, NY; [4]Brain and Body Research Center, Icahn School of Medicine at Mount Sinai, New York City, NY*

ThOG PM: DRUG METABOLISM AND PHARMACOKINETICS

Ballroom III

Session Chair: Mark Cancilla (Merck)

ThOG pm 02:30 **High-Throughput Qualitative and Quantitative Assessment of Drug Metabolism and Drug-Drug Interactions using Automated Desorption Electrospray Ionization Mass Spectrometry**; Mousumi Saha[1]; Nicolas M Morato[2]; Nari Talaty[3]; David S Wagner[3]; Robert Graham Cooks[1]; *[1]Purdue University, West Lafayette, IN; [2]Purdue Institute for Cancer Research, Purdue University, West Lafayette, IN; [3]AbbVie, Inc., North Chicago, IL*

ThOG pm 02:50 **Expedited Biotransformation Studies using Vacuum-Jacketed Chromatography (VJC) with Benchtop Multi-Reflecting Time-of-Flight (XevoTMMRT) Mass Spectrometry and Dedicated Data-Mining Software**; Daniel J Weston[1]; Hania Khoury-Hollins[2]; Ismael Zamora[3]; Fabien Fontaine[3]; Matthew Daly[2]; Leah Bottomley[1]; Martin Palmer[2]; Richard Lock[2]; *[1]GSK, Stevenage, United Kingdom; [2]Waters Corporation, Wilmslow, United Kingdom; [3]Mass Analytica, Sant Cugat del Valles, Spain*

ThOG pm 03:10 **Bioanalytical LC-MS Strategies in the Bioanalysis of siRNA with Multiple Deamination Sites**; Xien Yu Chua[1]; Jing Li[1]; Guodong Zhang[1]; *[1]Alnylam Pharmaceuticals, Cambridge, MA*

ThOG pm 03:30 **Cutting-edge Bioanalytical Strategies to Measure ADC Pharmacokinetics Including Concentration and DAR Determination via Intact Mass, Free Payload, and Digestion-based Approaches**; Jaqueline A. Picache[1]; Jake A. Melby[1]; Wonhyeuk Jung[1]; John F. Kellie[1]; *[1]AstraZeneca, Gaithersburg, Maryland*

ThOG pm 03:50 **Novel LC-MS-based Platform for Extensive Investigation on Antibody-Drug Conjugates Induced Ocular Toxicity**; Xiaoyu Zhu[1, 2]; Min Ma[1, 2]; Yingyi Lian[1, 2]; Ming Zhang[1, 2]; Jun Qu[1, 2]; *[1]University at Buffalo, Buffalo, NY; [2]New York State Center of Excellence in Bioinformatics & Life Sciences, Buffalo, NY*

ThOG pm 04:10 **Molecular Structure and Mass Spectral Data Quality Driven Processing of High-Resolution Mass Spectrometry Data for Pharmacokinetics Studies**; Ismael Zamora[1]; Fabien Fontaine[2]; Luca Morettoni[1]; Kevin Bateman[3]; Rahul Baghla[4]; Ebru Selen[4]; *[1]Mass Spec Analytica, Sant Cugat del Vallés, Spain; [2]Lead Molecular Design, SL, Sant Cugat del Vallès, Spain; [3]2KDAM Consulting, Halifax, NS; [4]Sciex, Framingham, MA*

ThOH PM: FUNDAMENTALS: NATIVE MS AND STRUCTURES OF LARGE IONS

Ballroom IV

Session Chair: Lingjun Li (University of Wisconsin)

ThOH pm 02:30	**Integrating Charge Detection with Slow Mixing Mode (SLOMO) Native Mass Spectrometry to Quantify Biomolecular Interactions**; Duong Bui[1]; Ziyu Zhang[1]; Edward N. Schmidt[1]; Elena N. Kitova[1]; Marlene Fortier[2]; Yves St-Pierre[2]; Mathew S. Macauley[1, 3]; Lara K. Mahal[1]; John S. Klassen[1]; *[1]University of Alberta, Faculty of Science, Chemistry Department, Edmonton, AB; [2]Institut National de la Recherche Scientifique (INRS), Université du Québec, Laval, Québec; [3]University of Alberta, Faculty of Medicine & Dentistry - Medical Microbiology and Immunology Dept, Edmonton, Alberta*
ThOH pm 02:50	**Native Top-Down SID and ECD Analysis of the Avidin Glycoprotein Complex**; Andrew J Arslanian[1, 2]; Vicki H Wysocki[1, 2]; *[1]The Ohio State University, Columbus, OH; [2]Native Mass Spectrometry-Guided Structural Biology Center, The Ohio State University, Columbus, Ohio*
ThOH pm 03:10	**Can Enzymes Retain Catalytic Activity in the Gas Phase? Insights from ESI-IMS/MS/MS and Mobile-Proton Molecular Dynamics Simulations**; Yuen Ki Ng[1]; S. Quinn W. Currie[2]; Elnaz Aliyari[1]; Caroline Cui[1]; Siavash Vahidi[2]; Lars Konermann[1]; *[1]University of Western Ontario, London , ON ; [2]University of Guelph, Guelph, ON*
ThOH pm 03:30	**A New SLIM-Based Instrument That Enables Tandem Ion Mobility and Ion Activation Over a Range of Timescales**; AnneClaire Wageman[1]; Yuan (Bruce) Feng[1]; Addison E. Roush[1]; Matthew Bush[1]; *[1]University of Washington, Seattle, WA*
ThOH pm 03:50	**Improving confidence in protein identification in top-down native ambient mass spectrometry using proton transfer charge reduction**; Rebecca L Edwards[1]; Oliver J Hale[1]; Helen J Cooper[1]; *[1]University of Birmingham, Birmingham, United Kingdom*
ThOH pm 04:10	**Breaking Up Is Hard to…Understand: How Gas-Phase Noncovalent Protein Complexes "Fall to Pieces"**; Rachel R. Loo[1]; Joseph A. Loo[1]; *[1]UCLA, Los Angeles, CA*

POSTER OVERVIEW

MONDAY POSTERS

Set-up for all Monday posters
6:30 - 9:00 am

ALL POSTERS PRESENT
10:30 - 12:00 pm AND 1:00 - 2:30 pm

Remove all Monday posters
5:00 - 8:00 pm

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Artificial Intelligence in MS Instrumentation and Applications I	038-060
Biomarkers: Discovery I	061-104
Cancer Research I	105-135
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Drug Discovery: Qualitative and Quantitative Analysis I	204-231
Epigenetic Modifications	232-237
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Fundamentals: Ion Spectroscopy	312-319
Fundamentals: Ionic Clusters, Nanomaterials, and Catalysis	320-323
Fundamentals: Ionization	324-336
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High Mass Accuracy / High Performance MS: Applications, Automation, and Instrumentation	395-411
Imaging MS: Computational Methods, Software, and Analysis	412-424
Imaging MS: Disease Markers	425-440
Informatics: General, SRM, and DIA	441-446
Informatics: Multiomics Integration	447-468
Instrumentation: New Concepts	469-482
Instrumentation: New Developments in Ionization and Sampling	483-512
Ion Mobility: Fundamentals	513-522
Ion Mobility: Structure	523-539
LC/MS: General	540-570
Lipids: Targeted and Quantitative Analysis	571-584
MALDI: Applications	585-603
MALDI: Innovation in Instrumentation and Sample Prep	604-612
Metabolomics: Targeted and Quantitative Analysis	613-645
Nanoscale/Microfluidic and Capillary Electrophoresis Separations and MS	646-655
Natural Products	656-673
Proteins: PTMs	674-702
Proteomics: Intact Proteins and Top Down Analysis I	703-730
Proteomics: Quantitative I	731-757
Systems Biology	758-764

TUESDAY POSTERS

Set-up for all Monday posters
6:30 - 9:00 am

ALL POSTERS PRESENT
10:30 - 12:00 pm AND 1:00 - 2:30 pm

Remove all Monday posters
5:00 - 8:00 pm

Antibodies & Antibody Drug Conjugates II	001-038
Antidoping, Cannabis, and Opioid Detection	039-046
Art, Archaeology & Paleontology	047-051
Artificial Intelligence in MS Instrumentation and Applications II	052-069
Biomarkers: Discovery II	070-113
Cancer Research II	114-143
Clinical Analysis II	144-171
Data-Independent Acquisition	172-207
Drug Discovery, DMPK, ADME	208-221
Drug Discovery: Qualitative and Quantitative Analysis II	222-249
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Environmental: Pharmaceuticals and Pesticides	286-309
Extractables & Leachables	310-327
Fundamentals: Ion Molecule, Ion/Ion, Ion/Electron Interactions	328-336
Fundamentals: Molecular Modeling / Quantum Mechanical Calculations	337-340
Fundamentals: Native MS	341-362
Glycoproteins II	363-387
H/D Exchange: Protein Structure/Function	388-413
Imaging MS: Method Development	414-455
Industry: Trace Analysis, Quality Control, and Automation	456-462
Informatics: Metabolomics, Lipidomics, and Glycomics	463-491
Informatics: Peptide ID and Quantification	492-524
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Metabolomics: General	546-586
Nucleic Acids and Oligonucleotides I	587-614
Peptides: Identification and Fragmentation Mechanisms	615-623
Peptides: PTM Identification	624-644
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Proteins: Complexes/Non-covalent Interactions	657-691
Proteomics: Intact Proteins and Top Down Analysis II	692-719
Proteomics: Quantitative II	720-742
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POSTER OVERVIEW

WEDNESDAY POSTERS

Set-up for all Monday posters
6:30 - 9:00 am

ALL POSTERS PRESENT
10:30 - 12:00 pm AND 1:00 - 2:30 pm

Remove all Monday posters
5:00 - 8:00 pm

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Biomarkers: Quantitative Analysis I	033-059
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Metabolomics: Identification of Unknown Metabolites	439-459
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Proteins: Conformation Analysis and Structural Biology	606-628
Proteomics: Chemoproteomics	629-650
Proteomics: Clinical Applications	651-678
Proteomics: Infectious Diseases	679-693
Proteomics: New Approaches I	694-719
Single Cell MS I	720-747
Stable Isotope Labeling	748-762

THURSDAY POSTERS

Set-up for all Monday posters
6:30 - 9:00 am

ALL POSTERS PRESENT
10:30 - 12:00 pm AND 1:00 - 2:30 pm

Remove all Monday posters
2:30 - 3:00 pm

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Imaging MS: Pharmaceuticals, Metabolites, Lipids, and Glycans II	207-232
Imaging: Spatially-Resolved Omics II	233-254
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Informatics: Workflow and Data Management	271-300
Instrumentation: Mini/Portable/Fieldable MS	301-318
Instrumentation: New Developments in Mass Analyzers and Ion Detection	319-333
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Ion Mobility: FAIMS/DMS	357-362
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Neuroscience and Neurodegenerative Disease Research II	518-541
Nucleic Acids and Oligonucleotides III	542-571
Peptides: Targeted and Quantitative Analysis	572-595
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Single Cell MS II	676-698
Small Molecules: Qualitative and Quantitative Analysis	699-740
Synthetic Polymers and New Materials	741-754
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MONDAY POSTERS

MONDAY POSTERS

Set-up for all Monday posters
6:30 - 9:00 am

ALL POSTERS PRESENT

10:30 - 12:00 pm AND 1:00 - 2:30 pm

Remove all Monday posters
5:00 - 8:00 pm

Antibodies & Antibody Drug Conjugates I 001-037
Artificial Intelligence in MS Instrumentation and Applications I 038-060
Biomarkers: Discovery I 061-104
Cancer Research I 105-135
Clinical Analysis I 136-163
Covalent Labeling and Chemical Crosslinking 164-203
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Fundamentals: Ionic Clusters, Nanomaterials, and Catalysis 320-323
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GC/MS: Instrumentation and Applications 337-369
Glycoproteins I 370-394
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Imaging MS: Disease Markers 425-440
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MALDI: Applications 585-603
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Metabolomics: Targeted and Quantitative Analysis 613-645
Nanoscale/Microfluidic and Capillary Electrophoresis Separations and MS 646-655
Natural Products 656-673
Proteins: PTMs 674-702
Proteomics: Intact Proteins and Top Down Analysis I 703-730
Proteomics: Quantitative I 731-757
Systems Biology 758-764

ANTIBODIES & ANTIBODY DRUG CONJUGATES I
001-037

MP 001 **Advanced Conformational Characterization of Monoclonal Antibodies: A Detailed Study of Molecular Stability and Dynamics Using Cyclic Ion Mobility Mass Spectrometry**; Abhik Mojumdar[1, 2]; Hee-Jin Yoo[1, 3]; Sunhee Choi[1]; Yeowoon Koo[1, 2]; Eunji Jeon[1]; Moonhee Park[1]; Min Sun Kim[1]; Ju-Yong Hyon[1]; Sung-Ho Yun[1]; Kun Cho[1, 2]; *[1]Korea Basic Science Institute (KBSI), Ochang, Cheongju, South Korea; [2]University of Science and Technology (UST), Daejeon, South Korea; [3]Sogang University, Seoul, South Korea*

MP 002 **Comprehensive Structural Characterization of IgG Subclasses and IgA mAbs Using Cyclic Ion Mobility Mass Spectrometry**; Abhik Mojumdar[1, 2]; Hee-Jin Yoo[1, 3]; Sunhee Choi[1]; Yeowoon Koo[1, 2]; Eunji Jeon[1]; Moonhee Park[1]; Min Sun Kim[1]; Ju-Yong Hyon[1]; Sung-Ho Yun[1]; Kun Cho[1, 2]; *[1]Korea Basic Science Institute (KBSI), Ochang, Cheongju, South Korea; [2]University of Science and Technology (UST), Daejeon, South Korea; [3]Sogang University, Seoul, South Korea*

MP 003 **Improving charge variant analysis of complex monoclonal antibodies at intact level using DIA-PTCR**; Corentin Beaumal[1]; Jingjing Huang[2]; Chirstopher Mullen[2]; Rafael Melani[2]; Kristina Srzentic[3]; Silvia Millán-Martin[1]; Sara Carillo[1]; Jonathan Bones[1, 4]; *[1]Nat'l Inst. for Bioprocessing Research & Training, Dublin, Ireland; [2]Thermo Fisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific, Reinach, Switzerland; [4]University College Dublin, Belfield, Ireland*

MP 004 **A comprehensive LC/MS workflow for Host Cell Protein identification utilizing a novel, multi-reflecting ToF Mass Spectrometry providing high confidence characterization**; Jonathan E Fox[1]; Ying Qing Yu[2]; Malcolm Anderson[3]; Catalin E Doneanu[4]; Laetitia Denbigh[3]; *[1]Waters, Wilmslow, United Kingdom; [2]Waters Corporation, Milford, MA; [3]Waters Corporation, Wilmslow, United Kingdom; [4]Waters, Milford, MA*

MP 005 **Exploring ProAlanase as Effective Alternative to Trypsin Microdroplet-Enabled Analysis of mAbs**; Andrew Schladebeck[1, 2]; Timothy Yaroshuk[2]; Yongqing Yang[2]; Mengyuan Xiao[2]; Jim Lau[3]; Michael D Knierman[3]; Xi Qiu[3]; Hui Zhao[3]; Erica Chaban[1]; Harsha Gunawardena[4]; Hao Chen[2]; Ramarao Gollapalli[1]; *[1]Kenvue, Skillman, NJ; [2]New Jersey Institute of Technology, Newark, NJ; [3]Agilent Technologies, Wilmington, DE; [4]JOHNSON AND JOHNSON, Spring House, PA*

MP 006 **Magnetic Nanoparticle-Assisted Ultra-Fast Protein Digestion for Peptide Mapping in Antibody Characterization**; Gong Cheng; *Asimov Inc, Boston*

MP 007 **Identification of differentially recognized epitopes in pregnancy malaria vaccine candidate VAR2CSA**; Santosh A Misal[1]; Robert D Morrison[1]; Jonathan P Renn[1]; Matthew Cowles[1]; Alassane Dicko[2]; Patrick E Duffy[1]; Michal Fried[1]; *[1]National Institutes of Health, Bethesda, MD; [2]University of Sciences Techniques and Technologies of Bamako, Bamako, Mali*

MP 008 **Bioanalytical Challenges in Developing PK Assays Supporting Novel Degrader-Antibody Conjugates (DACs)**; Sylvia C Wong[1]; Violet Lee[1]; Ivy Chen[1]; Surinder Kaur[1]; Ola Saad[1]; *[1]Genentech, South San Francisco, CA*

MP 009 **Integrated Free Thiol Quantitation and Disulfide Mapping Assays for Comprehensive Protein Characterization Using Mass Spectrometry**; Kevin Ray[1]; Pei Liu[1]; Ben Cutak[1]; *[1]milliporesigma, St. Louis, MO*

MP 010 **Ultrafast microdroplet digestion of antibody charge variants**; Praneeth Ivan Joel FNU[1]; Yongqing Yang[1]; Mengyuan Xiao[1]; Jim Lau[2]; Michael D Knierman[2]; Xi Qiu[2]; Hui Zhao[2]; Thomas Walker[3]; Harsha Gunawardena[4]; Hao Chen[1]; *[1]New Jersey Institute of Technology, Newark, NJ; [2]Agilent Technologies, Inc., Wilmington, Delaware; [3]Agilent Technologies, Lexington, MA; [4]JOHNSON AND JOHNSON, Spring House, PA*

MP 011 **What's in a Peak? Enhanced Charge Varient Analysis with Zeno TOF MS Scan Mode**; Riley Schaefer[1]; Megan E Sharma[1]; Kristen Nields[1]; *[1]Johnson & Johnson Innovative Medicine, Spring House, PA*

MP 012 **Middle-level Mass Spectrometry Analysis of Chain Mispairing in Hinge-mutated Bispecific Antibodies**; Philip Widdowson[1]; Magdalena Widgren-Sandberg[1]; Erica Andersson[1]; Desmond Schofield[2]; Andreas Nägeli[1]; John Lindsay[3]; *[1]Genovis AB, Kavlinge, Sweden; [2]evitria AG, Zurich, Switzerland; [3]Genovis Inc., Cambridge, MA*

MP 013 **Host Cell Protein Identification in Biopharmaceuticals Using Mass Spectrometry: An Iterative Acquisition Approach for Comprehensive Profiling**; Shadab Ahmad[1]; Shilpa Gadgil[2]; Vadiraja Bhat[3]; Nirpendra Singh[4]; Wayne Heacock[5]; *[1]Centre for Cellular And Molecular Platforms (C-CAMP), Bangalore, India; [2]Enzene Biosciences Limited, Pune, India; [3]Agilent technologies, Bangalore, India; [4]Institute for Stem Cell Science and Regenerative Medicine, Bangalore, India; [5]Agilent Technologies, Wilmington, DE*

MP 014 **A Dilute-and-Shoot Method for Monitoring mAb PQAs from Spent Media Enhances the Process Analytical Technology (PAT) Toolbox**; Erin Redman[1]; J. Scott Mellors[1]; Stephanie Klaubert[2]; Scott Miller[2]; Graziella Piras[2]; *[1]908 Devices, Inc., Morrisville, NC; [2]908 Devices Inc., Boston, MA*

MP 015 **Identification of Unknown Basic Variants by icIEF-UV/MS in a Biomanufacturing Process of Monoclonal Antibodies**; Ying Long[1]; Veerabhadraiah Palakollu[1]; Monica Accerbi[1]; *[1]National Institute for Innovation in Manufacturing Biopharmaceuticals (NIIMBL), NEWARK, DE*

MP 016 **Complete Characterization of Kadcyla Using a Modified Hybrid Quadrupole-Orbitrap Mass Spectrometry with electron-transfer/higher-energy collision dissociation (EThcD) fragmentation**; Xiaoxi Zhang[1]; Roberto Gamez[2]; Reiko Kiyonami[3]; Cong Wang[4]; Peter Krueger[4]; Heiner Koch[5]; Min Du[3]; *[1]ThermoFisher Scientific, Shanghai, China; [2]Thermo Fisher Scientific, Austin, TX; [3]Thermo Fisher Scientific, Lexington, MA; [4]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [5]Thermo Fisher Scientific, Bremen, Germany*

MP 017 **Conformation-Dependent Stability of Multispecific Antibodies Revealed by Mobility-Resolved Collision-Induced Unfolding (mr-CIU)**; Kaira A. Mayberry[1]; Jusung Lee[1]; Mark E. Ridgeway[2]; Melvin A. Park[2]; Harsha P. Gunawardena[3]; Christian Bleiholder[1]; Fanny C. Liu[1]; *[1]Florida State University, Tallahassee, FL; [2]Bruker Daltonics GmbH & Co. KG, Billerica, MA; [3]Johnson and Johnson Innovative Medicine, Spring House, PA*

MP 018 **What information can a single quadrupole mass spectrometer provide for biopharmaceutical characterization of monoclonal antibodies?**; Stephen Sciuto; *Agilent Technologies, Santa Clara, CA*

MP 019 **Comprehensive analysis of EpiTAC bispecific antibodies using intact mass spectrometry**; Danica-Mae Manalo[1]; Kevin Carlin[1]; Noah Solomon[1]; Andy Goodrich[1]; Maia Vinogradova[1]; Isaac Rondon[1]; Lichao Zhang[1]; *[1]Epibiologics, San Mateo, CA*

MP 020 **Comparative LC-MS Strategies for Comprehensive ADC Quantitation: A Case Study on Telisotuzumab Vedotin**; David Zuluaga[1]; Leif Morin[1]; Min Meng[1]; Aihua Liu[1]; *[1]Resolian, Malvern, PA*

MP 021 **Mass Spectrometry-Based Proteomics Reveals Payload-Induced Perturbations in Biological Pathways of Toxicity-Prone Cells**; Santosh Renuse[1]; Cheng Wang[2]; Colten Eberhard[1]; Linda Irons[1]; Kevin Contrepois[3]; Dhaval K Shah[2]; Holly Kimko[1]; *[1]AstraZeneca, Gaithersburg, Maryland; [2]University at Buffalo, Buffalo, NY; [3]AstraZeneca, South San Francisco, CA*

MP 022 **A Hybrid LBA, LC-MS/MS Assay for the Simultaneous Quantitation of an Antibody-Drug Conjugate and Its Antibody Component**; Joshua Powers[1]; Brian Melo[1]; Ines Santos[1]; Jian Chen[1]; Yongjun Xue[1]; Madhan Masilamani[1]; Jim Shen[1]; *[1]BMS, Lawrence Township, NJ*

MP 023 **Comprehensive Characterization of Monoclonal Antibodies on a Modified Hybrid Orbitrap Mass Spectrometer**; Zoltan Szabo[1]; Kristina Srzentic[2]; Cong Wang[3]; Heiner Koch[3]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Reinach, Switzerland; [3]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

MP 024 **Mobility-resolved collision-induced unfolding in Tandem-TIMS characterizes protein-ligand binding affinity**; Fanny C Liu[1]; Mengqi Chai[1]; Tyler C Cropley[1]; Kaira A. Mayberry[1]; Justis Booth[1]; Mark E. Ridgeway[2]; Melvin A Park[3]; Harsha P. Gunawardena[4]; Christian Bleiholder[1]; *[1]Florida State University, Tallahassee, FL; [2]Bruker Daltonics GmbH & Co. KG, Billerica, MA; [3]Bruker Switzerland AG, Fällanden, Switzerland; [4]Johnson & Johnson Innovative Medicine, Spring House, PA*

MP 025 **Evaluation and Refinement of De Novo Sequencing for Antibody Variable Regions**; Joel Hatungimana[1]; Clint Vorauer[2]; Justin Sanders[1]; Melih Yilmaz[1]; Devanshi Desai[1]; William S. Noble[1]; Miklos Guttman[1]; *[1]University of Washington, Seattle, WA; [2]University of Washington - Seattle, WA, Seattle, WA*

MP 026 **Automated Online Sample Preparation and Multidimensional Liquid Chromatography Mass Spectrometry Platform for Intact, Reduced, and Bottom-Up Protein Characterization**; Eli Larson; *Merck & Co., Rahway, NJ*

MP 027 **Conjugation and higher order structure characterization of antibody drug conjugates (ADC) by native SEC-MS**; Mingjie Cui[1]; Trust Razunguzwa[1]; Chendi Niu[1]; Rodrigo Vargas Eguez[1]; Wei Xu[1]; *[1]AstraZeneca, Gaithersburg, MD*

MP 028 **Enhancing mAb Subunit Analysis with Advanced Proteoform Identification and Multiple Fragmentation Strategies**; Ken Durbin[1]; Guillaume Tremintin[2]; Matthew T Robey[1]; Ryan Fellers[1]; Joseph B Greer[1]; Jonathan R Krieger[2]; Mariangela Kosmopoulou[2]; Athanasios Smyrnakis[2]; Dimitris Papanastasiou[2]; *[1]Proteinaceous, Evanston, IL; [2]Bruker Daltonics GmbH & Co. KG, Billerica, MA*

MP 029 **A Comprehensive Characterization Method for Cysteine-related Product Quality Attributes in Antibody-based Therapeutics**; Theresa A. Gozzo[1]; Jianji Chen[2]; Rosalynn Molden[1]; *[1]Just Evotec Biologics, Redmond, WA; [2]Just_Evotec Biologics, Seattle, WA*

MP 030 **Utilizing ion-ion and ion-photon activation for the enhanced middle-down characterization of antibody-based therapeutics**; Linda B. Lieu[1]; Joshua D. Hinkle[2]; Jingjing Huang[2]; Rafael D. Melani[2]; John E. P. Syka[2]; Luca Fornelli[1, 3]; *[1]Department of Chemistry and Biochemistry, University of Oklahoma, Norman, Oklahoma; [2]ThermoFisher Scientific, San Jose, CA; [3]School of Biological Sciences, Norman, Oklahoma*

MP 031 **A Highly Efficient Immunocapture-LC/MS/MS Method for Quantitation of An Antibody Drug Conjugate (ADC) From Monkey Plasma**; Eric W. Ma[1]; Sami Naser[1]; William Mylott Jr. [1]; *[1]PPD, Richmond, VA*

MP 032 **Application of EAD/CID mixed fragmentation mode followed by various data acquisition and processing strategies for Host Cell Proteins analysis**; Tomasz Kasper Gozdziewicz[1]; Maciej Stopa[2]; Katarzyna Krupczyńska-Stopa[1]; *[1]LabExperts Ltd, Lodz, Poland; [2]Bioanalytic Sp. z o.o., Gdańsk, Poland*

MP 033 **de novo antibody sequencing and antibody repertoir study from an influenza vaccinee**; Weiwei Peng[1]; Dalton Merrill Tower[1]; Rien Leuvenink[2]; Douwe Schulte[2]; Joost Snijder[2]; George Georgiou[1]; *[1]The University of Texas at Austin, Austin,, TX; [2]Utrecht University, Utrecht, Netherlands*

MP 034 **Leveraging high performance mass spectrometry in the Development of CQAs as part of Antibody Drug Conjugate Control Strategy**; Jeff Patrick[1]; Bryan Thacker[1]; Jessica Weaver[1]; Shiqian Zhu[1]; Shashank Gorityala[1]; Likun Duan[1]; *[1]BioAgilytix, Durham, NC*

MP 035 **Resolving the human polyclonal antibody response with proteomics**; Zoe Turner[1]; Yasmine Rais[1]; Anthony Chiu[1]; Andrei Drabovich[1]; *[1]Department of Laboratory Medicine and Pathology, University of Alberta, Edmonton, AB*

MP 036 **Native RPLC-HRMS Method Development Approach for the Rapid Characterization of Antibody Drug Conjugates**; Matt Boag; *Phenomenex, Torrance, CA*

MP 037 **Evaluating process development strategies through a multi-attribute mass spectrometry approach to minimize disulfide bond-related modifications in monoclonal antibodies (mAbs)**; Ameya Parkar[1]; Rahul Jaiswal[1]; Tanvi Sawant[1]; Ratnesh Jain[1]; Prajkata Dandekar[1]; *[1]Institute of Chemical Technology, Mumbai, India*

ARTIFICIAL INTELLIGENCE IN MS INSTRUMENTATION AND APPLICATIONS I

038-060

MP 038 **SpectroVQ enables Efficient Information Compression and De-noising of Peptide Tandem Mass Spectrum using Deep Learning**; James Ho Wa Li[1]; Henry Lam[1]; *[1]Hong Kong University of Science and Technology, Hong Kong, Hong Kong*

MP 039 **Combining comprehensive search with peptide-based differential analysis to identify signal in DIA and DDA datasets missed by other approaches**; Dejan Stepec[1]; Maximilien Burq[1]; Bryan Crampton[1]; Rehan Chinoy[1]; Shivani Tiwary[1]; Peter Cimermancic[1]; *[1]Tesorai, MOUNTAIN VIEW, CA*

MP 040 **Automated hyperparameter tuning of MS database searching achieves robust peptide identification with improved accuracy and sensitivity**; Maximilien Burq[1]; Dejan Stepec[1]; Bryan Crampton[1]; Rehan Chinoy[1]; Shivani Tiwary[1]; Peter Cimermancic[1]; *[1]Tesorai, MOUNTAIN VIEW, CA*

MP 041 **Investigation of a Deep Learning-Assisted Workflow for the Analysis of Per- And Polyfluoroalkyl Substances in Environmental Matrices**; Ruoji Luo[1]; Tamas King[2]; Oleksandr Sosnovshchenko[3]; Charudatta Manwatkar[4]; Flavio Avila[5]; Edison Cerda[6]; Yvonne Koch[7]; *[1]Agilent Technologies, Inc., Santa Clara, CA; [2]Agilent Technologies, Inc., Hong Kong, China; [3]Agilent Technologies, Inc., --, Finland; [4]Agilent Technologies, Inc., Cedar Creek, TX; [5]Agilent Technologies, Santa Clara, CA; [6]Agilent Technologies, Inc., --, --; [7]Agilent Technologies, Inc., Waldbronn, Germany*

MP 042 **Chemometric Techniques for the Automated Batch Processing of GC-MS Data for Chemical Identification and Supervised Model Development**; Bob Schweitzer[1]; Spiros Manolakos[2]; Ashish Chaudhary[2]; *[1]Detect-ION, Tampa, FL; [2]Detect-Ion, Tampa, FL*

MP 043 **Automating Discovery-to-Targeted Proteomics: A High-Throughput Pipeline for Biomarker Assay Development**; Anirudh A Kashyap[1]; Morgan Fair[1]; Liang Zhao[1]; Raghothama Chaerkady[1]; Qing Wang[1]; *[1]Complete Omics Inc., Baltimore, MD*

MP 044 **LIGER: AI-Driven Lipidome-Gene Enrichment and Reaction Mapping for Advanced MRM-Based Lipidomics**; Connor H Beveridge[1]; Caitlin Randolph[2]; Gaurav Chopra[2, 3, 4, 5, 6]; *[1]Purdue, West Lafayette, IN; [2]Purdue Univeristy, West Lafayette, IN; [3]Purdue Institute for Drug Discovery, West Lafayette, IN; [4]Purdue Institute for Cancer Research, Purdue University, West Lafayette, IN; [5]Purdue Institute for Integrative Neuroscience, West Lafayette, IN; [6]Purdue Institute for Inflammation, Immunology, and Infectious Disease, West Lafayette, IN*

MP 045 **Harnessing Laser Desorption Mass Spectrometry and Machine Learning for the Detection of Extraterrestrial Microbes**; Ashley M Hanna[1]; Jacob M C Shaffer[2]; Jill A Mikucki[2]; Vedran Lekić[1]; *[1]University of Maryland, College Park, MD; [2]University of Tennessee, Knoxville, TN*

MP 046 **Deep learning-driven proteomics mapping to unveil Acute Myeloid Leukemia therapeutic sensitivity and guide precision treatment strategies**; Salvador Martínez-Bartolomé[1]; James T Sorrentino[1]; Mahan Abbasian[1]; Antonius Koller[1]; Christina Lamm[1]; Pilgrim Jackson[1]; *[1]YatiriBio LLC, San Diego, CA*

MP 047 **From drugs to PFAS – classification of mass spectra using a deep learning model**; Nitzan Tzanani[1]; Nir Cohen[1]; Shai Kendler, [1]; Lilach Yishai-Aviram[1]; *[1]IIBR, Ness Ziona, Israel*

MP 048 **Training a tandem mass spectrometry foundation model with de novo peptide sequencing**; Melih Yilmaz[1]; Justin Sanders[1]; Wout Bittremieux[2]; William E. Fondrie[3]; Sewoong Oh[1]; William Noble[1]; *[1]University of Washington, Seattle, WA; [2]University of Antwerp, Antwerpen, Belgium; [3]Talus Bioscience, Seattle, WA*

MP 049 **Transferable hypergraph-powered multimodality AI framework for predicting retention times of small molecules using HyperRT**; Fanzhou Kong[1, 2]; Oliver Fiehn[2, 3]; *[1]UC Davis West Coast Metabolomics Center, Davis, CA; [2]UC Davis, Davis, CA; [3]West Coast Metabolomics Center, University of California, DAVIS, CA*

MP 050 **Beyond Mass-Only Filtering: A Multitask Deep Learning Framework for Predicting Peptide Properties from Mass Spectrometry Data**; Bilal Shabbir[1]; Syed Talha Khalid[1]; Francisco Fernandez-Lima[2, 3]; Fahad Saeed[1]; *[1]School of Computing and Information Science, Florida International University, Miami, FL; [2]Department of Chemistry and Biochemistry, Florida International University, Miami, FL; [3]Institute of Environment, Florida International University, Miami, FL*

MP 051 **Decoding enzyme specificity through explainable artificial intelligence (XAI)**; Sabrina Khuntia[1]; Yu Gao[1]; *[1]University of Illinois at Chicago, Chicago, IL*

MP 052 **Machine Learning for classification of individual EVs based on highly sensitive multiplexed mass spectrometry measurements**; Muhammad Ramzan[1]; Francis E. Godfrey[2]; Anthony Giron[1]; Seonhwa Lee[3]; Alexender Revzin[3]; Dmitriy S. Verkhoturov[4]; Stanislav V. Verkhoturov[4]; Emile A. Schweikert[4]; Harmeet Malhi[3]; Michael J. Eller[1]; *[1]California State University, Northridge, Northridge, CA; [2]California State University Northridge, Northridge, CA; [3]Mayo Clinic, Rochester, MN; [4]Texas A&M University, College Station, TX*

MP 053 **Development of a Python-based GUI For Machine Learning of 2D MS/MS Data**; Edwin Gonzalez[1]; Casey Flynn[1]; Dalton Snyder[1]; Megan Guetzloff[1]; Robert Graham Cooks[2]; Mitch Wells[1]; *[1]Teledyne FLIR Detection, West Lafayette, IN; [2]Purdue Univeristy, West Lafayette, IN*

MP 054 **Harnessing proteomics and machine learning to systematically map protein expression regulons in microbial pathogens**; Ian Lewis; *University of Calgary, Calgary, AB*

MP 055 **Limited Sample Model (LSM) AI Automation and Enhanced Untargeted Drug Metabolite Analysis Using High-Resolution Mass Spectrometry (HRMS)**; Sanoj Silva[1]; Osanda Hemachandra[1]; Chamika Perera[1]; Doreen Chrishanthy[1]; Lalin Theverapperuma[1]; *[1]Expert Intelligence, Santa Clara, CA*

MP 056 **Improving PFAS Identification Using Limited Sample Model (LSM) and Generative AI for MS/MS Spectral Analysis**; Leiver Campeon[1]; Sebastian Gómez[1]; Pulasthi Ekanayake[1]; Osanda Hemachandra[1]; Mihira K Vithanage[1]; Sanoj Silva[1]; Lalin Theverapperuma[1]; *[1]Expert Intelligence, Santa Clara, CA*

MP 057 **Benchmarking Pretrained Graph Transformers vs. Ensembled Tree-Based Methods: A Case Study of Retention Time Prediction Accuracy and Training Data Size**; Yen Nhi Hoang[1]; Cailum MK Stienstra[1, 2]; Tao Huan[1]; *[1]University of British Columbia, Vancouver, BC; [2]University of Waterloo, Waterloo, ON*

MP 058 **Analysis of various fragment ion prediction algorithms for the structure elucidation of xenobiotic metabolites**; Corin Wagen[1]; Chris J Brown[2]; Arien Wagen[1]; Yannick Djoumbou-Feunang[3]; *[1]Rowan Scientific, Boston, Massachusetts; [2]Corteva Agrisciences, Indianapolis, IN; [3]Corteva Agriscience, Indianapolis, IN*

MP 059 **The Impact of Social Media and Technology on the Science Industry**; Amy Nguyen[1]; Jannette Avila[1]; *[1]Phenomenex, Torrance, CA*

MP 060 **Development of automated peaks classification using Convolutional Neural Networks (CNNs) on MALDI-TOF datasets**; SYED MUHAMMAD ALI FARHAN[1]; Yi-Sheng Wang[1]; *[1]Genomics Research Center, Academia Sinica, Taipei, Taiwan*

BIOMARKERS: DISCOVERY I
061-104

MP 061 **Spatial proteomics to discover aging-associated alterations in the renal tubulointerstitium**; Dong-Gi Mun[1]; Gunveen Sachdeva[1]; Benjamin Madden[1]; Andrew Rule[1]; Akhilesh Pandey[1]; *[1]Mayo Clinic, Rochester*

MP 062 **Assessment of Protein S-Nitrosylation in a ZSF1 Rat Model of Heart Failure with Preserved Ejection Fraction (HFpEF) using Orbitrap Astral**; Philip To[1]; Sophia Chung[1]; Sonja Hess[1]; *[1]AstraZeneca, Gaithersburg, MD*

MP 063 **Analyzing serum biomarkers in cardiac transthyretin amyloidosis: implications for diagnosis and future outcomes**; Joanna Waś[1]; Monika Gawor-Prokopczyk[2]; Agnieszka Sioma[2]; Rafał Szewczyk[3]; Aleksandra Pel[3]; Jolanta Krzysztoń-Russjan[1]; Magdalena Niedolistek[1]; Dorota Sokołowska[1]; Jacek Grzybowski[2]; Łukasz Mazurkiewicz[1]; *[1]Department of Medical Biology, National Institute of Cardiology, Warsaw, Poland; [2]Department of Cardiomyopathy, National Institute of Cardiology, Warsaw, Poland; [3]LabExperts sp z o.o., Gdansk, Poland*

MP 064 **Multi-Omics Analysis of Molecular and Metabolic Mechanisms Underlying Long-Term Exercise Adaptations in Elite Athletes**; Seo Yoondam[1]; Jiin Hwang[1]; Joohee Cho[1]; Mu Hyun Lee[1]; Hophil Min[1]; *[1]Korea Institute of Science and Technology, Seoul, South Korea*

MP 065 **Expanded Coverage of Protein Post Translational Modifications Through Use of Alternative Proteases**; Jeffrey C. Silva[1]; Barry M. Zee[1]; Mukesh Kumar[1]; Anthony P. Possemato[1]; Matthew P. Stokes[1]; *[1]Cell Signaling Technology, Danvers, MA*

MP 066 **Comparison of DNA Damage Profiles in Chromatin versus Purified Bovine DNA using LC-MS/MS and Click Chemistry**; Quynh-Trang Do[1]; Shu-Jung Hsu[1]; Thanh-Tuyen Thi Phan[1]; Shu-Hui Chen[1]; *[1]National Cheng Kung University, Tainan, Taiwan*

MP 067 **Affinity-based proteomics combined with mass spectrometry reveals biological insights into the tissue specificity of disease in 164 cancer cell lines**; Ryan Lamers[1]; Raffaella Giugliano[1]; Klev Diamanti[1]; Kirsty Wienand[2]; Andrew Tuttle[2]; Simone Zhang[3]; Francisca Vazquez[2]; Catarina Campbell[3]; *[1]Olink Proteomics, Waltham, MA; [2]Cancer Dependency Group, Broad Institute of MIT and Harvard, Cambridge, MA; [3]Cancer Data Science, Broad Institute of MIT and Harvard, Cambridge, MA*

MP 068 **Proteomic Differences of Raw and Extracellular Vesicle Enriched Bronchoalveolar Lavage Fluid from Healthy and Asthmatic Mice**; Zachary Hutchins[1]; Xuefang Jing[2]; Abu Eabrahim Siddique[2]; Andrea Adamcakova-Dodd[2]; Yinsheng Wang[1]; *[1]University of California, Riverside, Redlands, CA; [2]University of Iowa, Iowa City, IA*

MP 069 **A new approach to glycan biomarker discovery from liquid biopsies**; Ali Abikhodr[1]; Wissem Allouchi[1]; Ahmed Ben Faleh[1]; Jessica Medina[1]; Kamil Seghrouchni[1]; Stephan Warnke[1]; Leila Zuccalli[1]; Liudmila Voronina[2, 3]; Mihaela Žigman[2, 3]; Thomas R. Rizzo[1, 4]; *[1]Isospec Analytics SA, Renens, Switzerland; [2]Ludwig Maximilian University of Munich, Munich, Germany; [3]Max Planck Institute of Quantum Optics, Garching, Germany; [4]Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland*

MP 070 **Metabolomics and lipidomics in a murine model of radiation induced lung injury**; Evan Pannkuk[1]; Evagelia C Laiakis[1]; Guy Y Garty[2]; Igor Shuryak[2]; Kamendra Kumar[1]; Shubhankar Suman[1]; Shanaz A. Ghandhi[2]; Yuewen Tan[2]; Brian Ponnaiya[2]; Xuefeng Wu[2]; Sally A. Amundson[2]; David J Brenner[2]; Albert J Fornace Jr. [1]; *[1]Georgetown University, Washington, DC; [2]Columbia University, New York City, NY*

MP 071 **Metabolomics Profiling Reveals Distinct Stages of Diabetic Kidney Disease**; Xiang Tian[1]; Cristina Di Poto[1]; Erik L. Allman[1]; Sonja Hess[1]; Susanna Eketijall[2]; Marcus Henricsson[2]; Robert Unwin[3]; Pia Davidsson[2]; Stefano Bartesaghi[2]; Vikensh Selvarajah[3]; Marvin Sinsakul[1]; Michael C McCarthy[1]; Benjamin Challis[3]; Vijayalakshmi Varma[1]; *[1]AstraZeneca, Gaithersburg, MD; [2]AstraZeneca Pharmaceuticals LP, Gothenburg, Sweden; [3]AstraZeneca, Cambridge, United Kingdom*

MP 072 **Transforming Cancer Biomarker Discovery Through Maximum ID and High-Throughput Plasma Proteomics Workflows**; Sudipa Maity[1]; Jared Deyarmin[1]; Kevin Yang[1]; Stephanie Samra[1]; Amirmansoor Hakimi[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

MP 073 **LCMS-Based Strategy for Site-Specific Receptor Occupancy Characterization in Mouse Blood**; Pei Zhang[1]; Zehua Li[1]; Jing Huang[1]; Xiaoying Jin[1]; Lan Li[2]; *[1]WuXi AppTec (Suzhou), Suzhou, China; [2]WuXi AppTec, Shanghai, China*

MP 074 **Development of a Holistic Human Model for Organophosphate Chemical Warfare Agents**; Madison G Thornhill[1]; Emilio S. Rivera[1]; Jessica A. Salguero[1]; Chi Yen Tseng[1]; Joshua Breidenbach[1]; Tara Harvey[1]; Emilia Solomon[1]; Claire Sanders[2]; Brett Blackwell[1]; Ethan M. McBride[1]; Marc Alvarez[1]; Robert F. Williams[1]; Philip Mach[1]; Trevor Glaros[1]; *[1]Biochemistry and Biotechnology Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; [2]Microbial and Biome Science Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM*

MP 075 **High mobility group box proteins as potential new biomarkers for Alzheimer's disease diagnosis and prognosis**; Elaine Liu[1]; Jingqi Fan[1]; Clementina Mesaros[1]; Ian A. Alexander Blair[1]; *[1]University of Pennsylvania, Perelman School of Medicine, Philadelphia, PA*

MP 076 **Plasma phosphorylated HMGB2 as a Potential Biomarker for Parkinson's Disease**; Jingqi Fan[1]; Elaine Liu[1]; Clementina Mesaros[1]; Ian A. Alexander Blair[1]; *[1]University of Pennsylvania, Perelman School of Medicine, Philadelphia, PA*

MP 077 **Reconstruction of Dietary Information from Untargeted Metabolomics Data for Personalized Nutrition and Precision Medicine**; Harsha Gouda[1]; Julius Agongo[1]; Patricia Kelly[2]; Shipei Xing[1]; Wilhan Nunes[1]; Konstantinos Gkikas[3]; Caroline Kerbiriou[3]; Richard Russell[4]; Richard Hansen[5]; Maria Lima[3]; Nicholas Rattray[2]; Konstantinos Gerasimidis[3]; Pieter C. Dorrestein[1]; *[1]University of California San Diego, San Diego, CA; [2]University of Strathclyde, Glasgow, United Kingdom; [3]University of Glasgow, Glasgow, United Kingdom; [4]Royal Hospital for Children & Young People, Edinburgh, United Kingdom; [5]University of Dundee, Dundee, United Kingdom*

MP 078 **Comprehensive and High-Throughput Plasma Proteome Profiling for Biomarker Discovery using a modified Thermo Scientific™ Orbitrap™ Astral™ Mass Spectrometer**; Jared S Deyarmin[1]; Qingling Li[1]; Kevin Yang[1]; Taher Elgierari[2]; Ting Huang[2]; Taylor Page[2]; Amirmansoor Hakimi[1]; Stephanie Samra[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Seer Inc., Redwood City, California*

MP 079 **Discovery of Metabolomic Biomarkers Associated with Seed Vigor and Aging in Hybrid Rice**; Jun Liu[1]; Shijuan Yan[1]; Junting Jia[1]; Bingxian Chen[1]; Hua Fu[1]; Jiadong Gao[1]; Sheng Zhang[2]; *[1]Guangdong Academy of Agricultural Sciences, Guangzhou, China; [2]Cornell University, Ithaca, NY*

MP 080 **Plasma Metabolomic Signatures Linked to Arsenic Exposure in Industrially Affected Populations**; Mi Jeong Kim[1]; Ha Eun Song[1]; Hyo Yeong Lee[1]; Su Jung Kim[1]; Hyun Ju Yoo[1]; *[1]ASAN Medical center, SEOUL, South Korea*

MP 081 **Efficient Metabolic Fingerprinting of Follicular Fluid: A Novel Approach to Encode Ovarian Reserve and Fertility**

Potential; Jiao Wu[1]; Kun Qian[1]; *[1]Biomedical Engineering, SJTU, Shanghai, China*

MP 082 **Systematic assessment of optimal workflows for high-throughput plasma proteomics**; Ole Østergaard[1]; Anders Handrup Kverneland[1]; Mia Østergaard Johansen[2]; Luisa Marie Schmidt[1]; Christina Christoffersen[2, 3]; Ruth Frikke-Schmidt[2, 4]; Jesper Velgaard Olsen[1]; *[1]NNF CENTER FOR PROTEIN RESEARCH, Copenhagen, Denmark; [2]Department of Clinical Biochemistry, Copenhagen University Hospital, Bispebjerg and Frederiksberg Hospital, Copenhagen, Denmark; [3]Department of Biomedical Sciences, Faculty of Health and Medical Sciences, University of Copenhagen, Copenhagen, Denmark; [4]Department of Clinical Medicine, Faculty of Health and Medical Sciences, University of Copenhagen, Copenhagen, Denmark*

MP 083 **Serum metabolic patterns for the diagnosis and prognosis of ocular adnexal lymphoma**; Yida Huang[1]; Kun Qian[1]; *[1]Shanghai Jiao Tong University, Shanghai, China*

MP 084 **Goldmining in the Plasma Proteome: benchmark of different enrichment strategies for Extracellular Vesicles, platelet and cytokines and chemokines content**; Kevin Roger[1]; Ines Metatla[1]; Sara Ceccacci[1]; Cerina Chhuon[1]; Chiara Guerrera[1]; *[1]Necker Proteomics, Université Paris Cité - Structure Fédérative de Recherche Necker, INSERM US24/CNRS UAR3633, Paris, France*

MP 085 **A Proteomics Investigation of Human Sera from African American Donors with Invasive Ductal Carcinoma Breast Cancer and Matched Controls**; Angiolina Hukovic[1]; Logan Seymour[1]; Panashe Mutsengi[1]; Danielle Whitham[1]; Brian T. Pentecost[1]; Costel C. Darie[1]; *[1]Clarkson University, Potsdam, NY*

MP 086 **Proceed with Caution: The Risk of Trying to Derive Insights from Underpowered Proteomics Studies**; Oliver K Lindhorst[1]; Dylan Tabang[1]; Arthur Viodé[1]; Asher S Hansen[1]; Lise E Nigrovic[2]; Jonathan R Krieger[3]; Judith A Steen[4]; Hanno Steen[1]; *[1]Department of Pathology, Boston Children's Hospital & Harvard Medical School, Boston, MA; [2]Division of Emergency Medicine, Boston Children's Hospital, Boston, MA; [3]Bruker Ltd., Milton, ON; [4]F.M. Kirby Neurobiology Center, Boston Children's Hospital & Department of Neurology, Harvard Medical School, Boston, MA*

MP 087 **Proteomics Investigation of Human Breast Milk for Early Detection of Breast Cancer: A Mass Spectrometry Approach**; Aneeta Arshad[1]; Brian T. Pentecost[1]; Kathleen F. Arcaro[2]; Costel C. Darie[1]; *[1]Clarkson University, Potsdam, NY; [2]University of Massachusetts Amherst, Amherst, MA*

MP 088 **Proteomic Investigation of Sera from Women with Triple-Negative Breast Cancer and matched controls**; Niyogushima Nuru[1]; Danielle Whitham[1]; Isabelle Sullivan[1]; Norman Haaker[1]; Brian T. Pentecost[1]; Costel C. Darie[1]; *[1]Clarkson University, Potsdam, NY*

MP 089 **Exploration of glycated human plasma metabolites: Plausible biomarkers of diabetic complications**; Sancharini Das[1, 2]; Rashdajabeen Q Shaikh[3]; Arvind Kumar Chaurasiya[3]; Murali G Ashtamy[2]; Amreen B Sheikh[4]; Moneesha Fernandes[5]; Shalbha Tiwari[6]; Ambika G Unnikrishnan[6]; Mahesh J Kulkarni[7]; *[1]CSIR National Chemical Laboratory Pune India, Pune, India; [2]Biochemical Sciences Division, CSIRNational Chemical Laboratory, Pune 411008, India, Pune, India; [3]Biochemical Sciences Division, CSIR-National Chemical Laboratory, Pune 411008, India, Pune, India; [4]Biochemical Sciences Division, CSIRNational Chemical Laboratory, Pune 411008, India; Academy of Scientific and Innovative Research (AcSIR), Ghaziabad, UP 201002, India, Pune, India; [5]Academy of Scientific and Innovative Research (AcSIR), Ghaziabad, UP 201002, India; Organic Chemistry Division, CSIR-National Chemical Laboratory, Pune 411008, India, Pune, India; [6]Department of Diabetes and Endocrine Research, Chellaram Diabetes Institute, Pune 411021, India, Pune, India; [7]Biochemical Sciences Division, CSIRNational Chemical Laboratory, Pune 411008, India; Academy of Scientific and Innovative Research (AcSIR), Ghaziabad, UP 201002, India;, Pune, India*

MP 090 **Nanotrap® PEAK: A Versatile Product for Protein Enrichment From Multiple Sample Types**; Jared Obermeyer[1]; Natalie Smith[1]; Anurag Patnaik[1]; Rico Duncan[1]; *[1]Ceres Nanosciences, Manassas, VA*

MP 091 **Biomarker Discovery in Controlled Normobaric Reduced Oxygen Exposures**; Campbell B Mousseau[1, 2]; Alena R Veigl-Lunsford[1, 2]; Rhonda L Pitsch[2]; Sean W Harshman[2]; *[1]BlueHalo, Dayton, Ohio; [2]US Air Force Research Laboratory, WPAFB, OH*

MP 092 **Exploring Membrane Proteomes: A Comparative Analysis of Extracellular Vesicles Using Different Digestion Methods**; Reihaneh Safavisohi; *Seton Hall University, South Orange, NJ*

MP 093 **In-Depth Plasma Proteome Profiling for High-Throughput Biomarker Discovery Using PreOmics Sample Preparation Kits and Thermo Scientific™ Orbitrap™ Astral™ Mass Spectrometer**; Jared Deyarmin[1]; Qingling Li[1]; Jana Richter[2]; Stephanie Samra[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

MP 094 **Evaluation of Protein Depletion Strategies for Citrate Plasma in Mass Spectrometry-Based Proteomics**; Shreya Chand[1]; Bich Nguyen[1]; Douglas Kirsher[1]; Sara Ahadi[1]; *[1]Alkahest, Inc., San Carlos, CA*

MP 095 **Sequential Method for Analysis of CTCs and Exosomes from the Same Sample of Patient Blood**; Jianhui Zhu[1]; Zhijing Tan[1]; Jie Zhang[1]; Mingrui An[1]; David M. Lubman[1]; *[1]University of Michigan, Ann Arbor, MI*

MP 096 **LC-MS Workflows for Diverse Omics Analysis of Plasma Samples in a Mini Cancer Cohort Using the Orbitrap Astral Mass Spectrometer**; Kevin Yang[1]; Julian Saba[2]; Rahul Deshpande[1]; Brittany Lee[1]; Khatereh Motamedchaboki[1]; Susan Bird[1]; Stephanie N. Samra[1]; Amirmansoor Hakimi[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, San Jose, California*

MP 097 **Identification of prognostic biomarkers in diffuse large B-Cell lymphoma through an untargeted metabolomics approach**; Denise Marradi[1]; Shahzaib Khoso[1]; Elettra Barberis[2]; Riccardo Moia[1]; Riccardo Dondolin[1]; Gianluca Gaidano[1]; Marcello Manfredi[1]; *[1]University of Piemonte Orientale, Novara, Italy; [2]University of Piemonte Orientale, Alessandria, Italy*

MP 098 **Using molecular information acquired with direct mass spectrometry to detect endometriosis in patient tissue biopsies**; Ruth Costa[1]; Emily Ma[1]; Monica Lin[1]; Brooke Lasher[2]; Virginia Chen[2]; Jennifer Travieso[2]; Christina Salazar[2]; Suzanne Ledet[3]; Michael Breen[3]; Livia S. Eberlin[1]; *[1]Baylor College of Medicine, Houston, TX; [2]University of Texas - Austin, Austin, TX; [3]Ascension Health, Waco, Texas*

MP 099 **Production of antimicrobial peptides is associated with the reduction of severe kidney infections in human patients**; Hannah Voß[1]; Stephanie Schaefer-Tautges[2]; Lars Borgads[2]; Florian Wagenlehner[3]; Lisa Schwarz[3]; Daniel Robert Engel[4]; Olga Shevchuck[1]; *[1]Group of Immunoproteomics,Department of Immunodynamics, University Clinic Essen, Essen, Germany; [2]Group of Immunoproteomics,Department of Immunodynamics, University Clinic Essen, Essen, Germany; [3]Klinik und Poliklinik für Urologie, Kinderurologie und Andrologie, University Clinic Giessen, Giessen, Germany; [4]Department of Immunodynamics, University Clinic Essen, Essen, Germany*

MP 100 **Quantification of Protein Recovery Using Nanotrap® Protein Enrichment Affinity Kits (PEAK)**; Rico Duncan[1]; Lauren Saunders[1]; Natalie Smith[1]; Ben Lepene[1]; *[1]Ceres Nanosciences, Manassas, VA*

MP 101 **Nanotrap® PEAK: A Protein Enrichment Kit Compatible with Multiple Protein Digestion and Clean-Up Methods**; Anurag Patnaik[1]; Monika Dzieciatkowska[2]; Natalie Smith[1]; Jared Obermeyer[1]; Rico Duncan[1]; *[1]Ceres Nanosciences,* *Manassas, VA; [2]Department of Biochemistry and Molecular Genetics, University of Colorado Denver – Anschutz Medical Campus, CO, USA, Denver, Colorado*

MP 102 **Discovery of biomarkers of TMAO that induce immunosenescence using a proteomic and metabolomic approach**; Manal Alsulami[1]; Hayat Shaibah[1]; Abdulelah Altolayyan[1]; Tlili Barhoumi[1]; Bandar Alghanem[1]; *[1]King Abdullah International Medical Research Center, Riyadh, Saudi Arabia*

MP 103 **Metabolomics profiles delineate exposure to Zika and Dengue flaviviruses in human induced pluripotent stem cells (hiPSCs)**; Khyati Y Mehta[1]; Tahira Fatima[2]; Djawed Bennouna[1]; Adam Tisch[1]; Aaron Scholl[2]; Bingjie Li[2]; Sandip De[2]; Ewy Mathe[1]; *[1]NCATS, Rockville, MD; [2]US Food and Drug Administration, Silver Spring, MD*

MP 104 **Clinical functional proteomic exploration of intercellular signaling in pancreatic cancer**; Ruijun Tian; *Southern University of Science and Technology, Shenzhen, China*

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MP 105 **Targeted metabolic analysis of head and neck squamous cell carcinoma via multiple reaction monitoring desorption electrospray ionization mass spectrometry imaging**; Gabriel Stefan Horkovics-Kovats[1]; István Pap[1]; Katja Dettmer-Wilde[2]; Peter Oefner[2]; Virág Sági-Kiss[3]; Yuchen Xiang[3]; Ines Ugele[4]; Kathrin Renner[4]; Zoltan Takats[1]; *[1]University of Regensburg, Department of Immune Medicine Multimodal Imaging of Intracellular Communication, Regensburg, Germany; [2]University of Regensburg, Department of Functional Genomics, Regensburg, Germany; [3]Imperial College London, Division of Systems Medicine, London, United Kingdom; [4]University Hospital Regensburg, Department of Otorhinolaryngology, Regensburg, Germany*

MP 106 **Ceramide-1-phosphate/CERK are regulators of ETMR growth and offer potential as a new therapeutic target**; Allison Maas[1]; Evangelos Liapis[1]; Derek Hanson[1]; Claire Louise Carter[1]; *[1]Hackensack Meridian Center for Discovery and Innovation, Nutley, NJ*

MP 107 **Proteomic Analyses of Expressed Prostatic Secretions and post-DRE Urine from Prostate Cancer Patients**; Shimin Chen[1]; Amanda Khoo[2]; Andrew Macklin[2]; Joseph Otto[1]; Vanessa L. Correll[1]; Vladimir Ignatchenko[2]; Yunee Kim[3]; Annie Ha[3]; Matthew Waas[2]; Shahbaz Khan[2]; Brian P. Main[1]; Dean A. Troyer[1]; Raymond S Lance[4]; Danny Vesprini[5]; Stanley K Liu[5]; Paul C. Boutros[6]; Thomas Kislinger[2, 3]; Oliver John Semmes[1]; Julius O Nyalwidhe[1]; *[1]Leroy T. Canoles Jr. Cancer Research Center, Eastern Virginia Medical School, Norfolk, VA; [2]Princess Margaret Cancer Centre, Toronto, ON; [3]University of Toronto, Toronto, ON; [4]Spokane Urology, Spokane, WA; [5]Sunnybrook Health Sciences Centre, Toronto, ON; [6]University of California Los Angeles, Los Angeles, CA*

MP 108 **Proteogenomics uncovers resistance mechanisms and identifies biomarkers for improving immune checkpoint inhibitor treatment of metastatic melanoma**; Kourosh Abdollahi[1]; Shrabanti Chowdhury[2]; Jacob J. Kennedy[1]; Richard G. Ivey[1]; Francesca Petralia[3]; Jeffrey R. Whiteaker[1]; Weiping Ma[2]; Azra Krek[2]; Marcin Cieslik[4]; Zachary T. Herbert[5]; Ata S. Moshiri[6]; Keith Flaherty[7]; Genevieve Boland[8]; Aleigha Lawless[7]; Tatyana Sharova[8]; Tara C. Mitchell[9]; Giorgos C. C. Karakousis[10]; Ahron J. Flowers[9]; Jeffrey E. Gershenwald[11]; Victor G. Prieto[11]; Alex Lazar[11]; Julie M Simon[11]; Jared C. Malke[11]; Khalida M Wani[11]; Richard A. Scolyer[12]; Georgina Long[12]; Douglas B Johnson[13]; Ruth Halaban[14]; Marcus Bosenberg[14]; Antonella Bacchiocchi[15]; Pei Wang[2]; Diwakar Davar[16]; Amanda G Paulovich[1]; *[1]Fred Hutchinson Cancer Center, Seattle, WA; [2]Icahn School of Medicine at Mount Sinai, New York City, NY; [3]Department of Genetics and Genomic Sciences, Icahn School of Medicine at Mount Sinai, New York City, NY; [4]University of Michigan, Ann Arbor, MI; [5]Molecular Biology Core Facilities, Dana-Farber Cancer Institute, Boston, MA; [6]The Ronald O. Perelman Department of Dermatology, NYU Grossman School of Medicine, New York City, NY; [7]Massachusetts General Hospital Cancer Center, Boston, MA; [8]Massachusetts General Hospital Surgical Oncology, Boston, MA; [9]Department of Medicine, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA, USA; Abramson Cancer Center, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA; [10]Department of Surgery, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA, USA; Abramson Cancer Center, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA; [11]The University of Texas MD Anderson Cancer Center, Houston, Texas; [12]Melanoma Institute Australia, The University of Sydney, Sydney, Australia; [13]Division of Hematology/Oncology, Department of Medicine, Vanderbilt University Medical Center, Nashville, TN; [14]Department of Dermatology, Yale University, New Haven, CT; [15]Yale University School of Medicine, New Haven, CT; [16]UPMC Hillman Cancer Center, Pittsburgh, PA*

MP 109 **Label-Free Proteomic Analysis of Ovarian Cancer 2D Cell Cultures and 3D Spheroids**; Nicole E Platzer[1]; Arbil Lopez[2]; Amanda B. Hummon[1, 2]; *[1]The Ohio State University, Columbus, OH; [2]The Ohio State University Department of Chemistry and Biochemistry, Columbus, OH*

MP 110 **Multi-omics analysis to investigate BRAF Inhibitor Resistance in Melanoma models**; Danny K Qiu[1]; YUE DOU[2]; Maja Wierzbinska[2]; Vivien Li[1]; Tian Zhang[2]; *[1]University of Virginia, Charlottesville, VA; [2]University of Virginia SOM, Charlottesville, VA*

MP 111 **MALDI-Mass Spectrometry Imaging and Spatial Transcriptomics unveil lipid biomarkers associated to intratumor heterogeneity in human colon cancer**; Karim Pérez-Romero[1]; Ramón María Rodríguez[1]; Cristina Huergo[2]; Albert Maimó-Barceló[1]; Teresa Ximelis[1]; José Andrés Fernández[2]; Gwendolyn Barceló-Coblijn[1]; *[1]Health Reserch Institute of the Balearic Islands, Palma de Mallorca, Spain; [2]University of the Basque Country, Leioa, Spain*

MP 112 **Method development for the denaturation, digestion and analysis of pembrolizumab by liquid chromatography mass spectrometry (LC-MS/MS)**; Michael Long[1]; Wen Tan Lu[1]; Kideok Jin[1]; F. Marcel Musteata[1]; *[1]Albany College of Pharmacy, Albany, NY*

MP 113 **Investigation of a novel mechanism of oxaliplatin resistance via inductively coupled plasma mass spectrometry (ICP-MS)**; Connor P Jewell[1]; Nisha Pawar[1]; Michael M. Gottesman[1]; Lisa M. Jenkins[1]; *[1]Laboratory of Cell Biology, Center for Cancer Research, National Cancer Institute, Bethesda, MD*

MP 114 **Investigation of the Targets of Zinc-Finger Inhibitors for Development of Novel Chemotherapeutics**; Tapan K Maity[1]; Connor P Jewell[2]; Massimiliano Bissa[2]; Genoveffa Franchini[2]; Daniel H. Appella[1]; Lisa Jenkins[1]; *[1]NIH, Bethesda, MD; [2]NIH, BETHESDA, MD*

MP 115 **Examining Post-Translational Modification Alterations in SDH-Deficiency**; Adam G Chatoff[1, 2]; Nathaniel W. Snyder[1]; Lori Rink[2]; *[1]Department of Cardiovascular Sciences Lewis Katz School of Medicine, Temple University, Philadelphia, PA; [2]Cancer Signaling and Microenvironment Program, Fox Chase Cancer Center, Philadelphia, PA*

MP 116 **Metabolic characterization of hepatocellular carcinoma cells using a novel enhanced dynamic range MS mode reveals potential key metabolic pathways**; Demi Rijlaarsdam[1]; Michał Kaczmarek[2]; Christian Klaas[2]; Jung-Chin Chang[1]; Esther Zaal[1]; Bernd Helms[1]; Celia Berkers[1]; *[1]Utrecht University, Department of Biomolecular Health Sciences, Utrecht, Netherlands; [2]Thermo Fisher Scientific, Bremen, Germany*

MP 117 **Robotic Laser-Assisted Mass Spectrometry for Surgical Treatment of Cervical Lesions**; Jinshi Zhao[1]; Amelia Fraser-Dale[2]; Galani Apostolia[2, 3]; István Pap[4]; Deirdre Lyons[3]; Daniel Simon[2, 4]; Stefania Maneta Stavrakaki[2]; Maria Paraskevaidi[2]; Maria Kyrgiou[2, 3]; Zoltan Takats[2, 4]; Burak

Temelkuran[2]; *[1]Imperial College London, London, United Kingdom; [2]Imperial College London, London, United Kingdom; [3]Imperial College Healthcare NHS Trust, London, United Kingdom; [4]University of Regensburg, Regensburg, Germany*

MP 118 **Metabolic signatures predict ONC201 efficacy in DMG patients**; Peter Sajjakulnukit[1]; Sunjong Ji[1]; Benison Lau[1]; Li Zhang[1]; Carl Koschmann[1]; Costas Lyssiotis[1]; *[1]University of Michigan, Ann Arbor, MI*

MP 119 **Spatial proteomics reveals alterations in colon tumors associated with mismatch repair status**; Firdous A Bhat[1]; Amy J French[1]; Gunveen Sachdeva[1]; Shilpa Venkataraman[2]; Lisa A. Boardman[3]; Akhilesh Pandey[1]; Richard K. Kandasamy[1, 4]; *[1]Department of Laboratory Medicine and Pathology, Mayo Clinic, Rochester, MN; [2]Beth Israel Deaconess Medical Center, Harvard Medical School, Boston, MA; [3]Division of Gastroenterology and Hepatology, Mayo Clinic, Rochester, MN; [4]Department of Immunology, Mayo Clinic, Rochester, MN*

MP 120 **Real-Time Mass Spectrometry for Head and Neck Cancer Surgery: Bringing Metabolomics into the Operating Theatre**; Amelia Fraser-Dale[1]; Jinshi Zhao[1]; Jasmin Werner[1]; Apostolia Galani[1, 2]; István Pap[3]; Lauren Ford[1]; Jonathan Bernstein[2]; Zaid Awad[2, 4]; Vinidh Paleri[5, 6]; Zoltan Takats[1, 3]; Burak Temelkuran[1]; *[1]Imperial College London, London, United Kingdom; [2]Imperial College Healthcare NHS Trust, London, United Kingdom; [3]University of Regensburg, Regensburg, Germany; [4]Imperial college london, London, United Kingdom; [5]The Royal Marsden NHS Foundation Trust, London, United Kingdom; [6]The Institute of Cancer Research, London, United Kingdom*

MP 121 **Investigation of per- and poly-fluoroalkyl substances (PFAS) Levels in Cancerous Tissues of Firefighters**; Kushal Biswas[1]; Dhimiter Bello[2]; Anila Bello[2]; Christine Lau[3]; Chani Sahabandu Hewa Sahabanduge[2]; Pengyuan Liu[1]; Jennifer J Schlezinger[4]; Vershalee Shukla[3]; *[1]University of Massachusetts Lowell, Lowell, MA; [2]University of Massachusetts, Lowell, Lowell, MA; [3]Vincere Cancer Center, Phoenix, Arizona; [4]Boston University, Boston, MA*

MP 122 **Multidimensional proteomic interrogation of LCMV-induced T cell exhaustion identifies targets for in vivo genetic screens**; Christian M Beusch[1]; Abdelhameed S Dawood[1]; Ahmet Ozdilek[1]; Sarah Welbourne[1]; Carly Roman[1]; Mohamed S Abdel-Hakeem[1]; David Ezra Gordon[1]; *[1]Emory University, Atlanta*

MP 123 **Dissecting mammary epithelial phenotypic heterogeneity in high-risk women with a droplet-based low-input proteomic platform**; Matthew Waas[1]; Pirashaanthy Tharmapalan[2]; Bowen Zhang[1]; Curtis W McCloskey[1]; Paul D Waterhouse[1]; Rama Khokha[1]; Thomas Kislinger[1]; *[1]Princess Margaret Cancer Centre, Toronto, ON; [2]Princess Margaret Cancer Center, Toronto, ON*

MP 124 **Mass Spectrometry-Based Proteomic Investigation of Patient-Derived Tumoroids Using the Orbitrap Astral Mass Spectrometer Informs Precision Oncology and Drug Discovery**; Dominique Figueroa[1]; Kevin Yen-Yu Yang[2]; Colin Paul[3]; Pradip Shahi Thakuri[3]; Anthony Chatman[3]; Brett Larsen[4]; Julian Saba[2]; Tonya Pekar Hart[4]; Amirmansoor Hakimi[4]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, 355 River Oaks Pkwy, San Jose, California; [3]Thermo Fisher Scientific, Frederick, MD; [4]Thermo Fisher Scientific, San Jose, California*

MP 125 **Decoding the role of Histone H2AX in Glioma Stem Cells**; Sophia K Wu[1]; Chunhua Han[2]; Qi-En Wang[3]; *[1]The Columbus Academy, Gahanna, OH; [2]Department of Radiation Oncology, Comprehensive Cancer Center, The Ohio State University,, Columbus,, OH; [3]Department of Radiation Oncology, Comprehensive Cancer Center, The Ohio State University, Columbus, OH*

MP 126 **Proteomics of Breast Cancer Cell Lines Treated with Grape Extracts: A Potential Study for Biomarkers**; Keyura Katam[1]; Virginia Gottschalk[1]; Lekan Latinwo[1]; *[1]Florida A&M University, Tallahassee, FL*

MP 127 **Exercise dependent secretomics: a new platform for cancer therapeutics**; Amanda L Smythers[1, 2]; Joao A. Paulo[1]; Matthew Gilbert[2]; Ariana Vargas-Castillo[1, 2]; Katherine Blackmore[1, 2]; Edward Chouchani[1, 2]; Steven P Gygi[1]; Bruce Spiegelman[1, 2]; *[1]Harvard Medical School, Boston, Massachusetts; [2]Dana-Farber Cancer Institute, Boston, Massachusetts*

MP 128 **NK cell/cancer cell interactions in the tumor microenvironment**; Iulia M. Lazar[1]; Pratistha Sarkar[1]; *[1]Virginia Polytechnic Institute & State University, Blacksburg, VA*

MP 129 **Comprehensive analysis of proteome turnover dynamics during T cell exhaustion**; Sydnye L Shuttleworth[1]; Michael A Bauer[1]; Jessica L Kelliher[1]; Aaron J Storey[2]; Nicole E Scharping[3]; Jacob L Edmondson[1]; Lora J Rogers[1]; Anna L Bolding[4]; Daniel Fil[1]; Dennis W Province[1]; Rick D Edmondson[1]; Stephanie G Byrum[5]; Sam G Mackintosh[1]; Alan J Tackett[1]; Ananda W Goldrath[6]; Brian Koss[1]; *[1]University of Arkansas for Medical Sciences, Little Rock, AR; [2]Arkana Laboratories, Little Rock, AR; [3]University of California San Diego, San Diego, CA; [4]University of Arkansas, Fayetteville, AR; [5]St Jude Children's Research Hospital, Memphis, TN; [6]Allen Institute, Seattle, Washington*

MP 130 **PTEN/AKT Isoform-Specific Regulation of Lipid Peroxidation in Liver Disease Progression**; Dante Dikeman[1]; Mario M Alba[1, 2]; Qi Tang[1]; Ielyzaveta Slarve[1]; Aditya Naik[1]; Yushan Wang[1]; Guo Zhang[1]; Taojian Tu[1]; Zixin Zong[1]; Ebony Flowers[1]; Lina He[1]; Lucy Wang[3]; Whitaker Cohn[1, 3]; Isaac Asante[1]; Julian Whitelegge[3]; Bangyan Stiles[1]; Stan Louie[1]; *[1]University of Southern California, Los Angles, CA; [2]Cedars Sinai Medical Center, Los Angeles, CA; [3]UCLA, Los Angeles, CA*

MP 131 **Mass Spectrometry-Based Approach for Identifying Protein-Aptamer Complexes**; Anna Drabik[1]; Joanna Ner-Kluza[1]; Kim Juseong[2]; *[1]Department of Analytical Chemistry and Biochemistry, AGH University, Krakow, Poland; [2]Division of Artificial Intelligence, Pusan National University, Busan, Republic of Korea, Busan, South Korea*

MP 132 **Unraveling the Quantitative Proteomic Signature of Anaplastic Thyroid Cancer in Contrast to Well-Differentiated Thyroid Cancer**; Gyuri Park[1, 2, 3]; Yeonju Kyoung[1]; Hong-Beom Park[2, 3, 4]; Sinae Lee[2, 3, 5]; Hyeon Chang Lee[1, 2, 3]; Eunseo Kim[2, 3, 4]; Minhyeok Kang[1, 2, 3]; Soeun Yun[2, 3, 4]; Jin Lee[2, 3, 4]; Yoo Hyung Kim[6]; Young Joo Park[1, 6, 7]; Dohyun Han[2, 3, 8]; *[1]Molecular Medicine and Biopharmaceutical Sciences, WCU Graduate School of Convergence Science and Technology Seoul National University, Seoul, South Korea; [2]Proteomics Core Facility, Biomedical Research Institute, Seoul National University Hospital, Seoul, South Korea; [3]Department of transdisciplinary medicine, Seoul National University Hospital, Seoul, South Korea; [4]Department of Biomedical Science, College of Medicine, Seoul National University, Seoul, South Korea; [5]Cancer Research Institute, Seoul National University college of medicine, Seoul, South Korea; [6]Department of Internal Medicine, Seoul National University College of Medicine, Seoul, South Korea; [7]Genomic Medicine Institute (GMI), Medical Research Center, Seoul National University, Seoul, South Korea; [8]Department of Medicine, Seoul National University College of Medicine, Seoul, South Korea*

MP 133 **Exploring Metabolic Changes in Glioblastoma Cells Induced by AI-Selected Ciclopirox Through Metabolomics**; Djawed Bennouna[1]; Adam Tisch[1]; Zeenat Shyr[1]; Kathleen McDaniel[1]; Catherine Chen[1]; Qian Zhu[1]; Wei Zheng[1]; Ewy A. Mathé[1]; *[1]NIH NCATS, Rockville, MD*

MP 134 **Global phospho-proteomic analysis of cancer tissues from lung cancer patients undergoing osimertinib/local ablative therapy**; Tapan Maity[1]; Xu Zhang[1]; Udayan Guha[1]; Lisa Jenkins[1]; *[1]National Cancer Institute, Bethesda, MD*

MP 135 **Elucidation of Mg2+induced size and charge heterogeneity in monoclonal antibody therapeutics**;

Anurag Singh Rathore[1]; KUNAL KRISHNA[1]; Vadiraja Bhat[2]; Sunil Kumar[1]; Himanshu Malani[1]; *[1]IIT Delhi, Delhi, India; [2]Agilent Technologies, BENGALURU, India*

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MP 136 **High-Throughput Analysis of Testosterone and DHEA in Human Serum by LDTD-MS/MS: Towards Increased Diagnostic Accuracy**; Pierre Picard[1]; Mégane Moreau[1]; Serge Auger[1]; Sarah Demers[1]; Jonathan Rochon[1]; Jean Lacoursière[1]; *[1]Phytronix Technologies, Inc., Quebec, QC*

MP 137 **Miniature Mass Spectrometer-based Point-of-care Assay for valproate sodium monitoring in glioma patients**; Xinqi Fang[1]; Junhan Wu[2]; Yuan Hong[2]; Jiexun Bu[3]; Wenpeng Zhang[4]; Zheng Ouyang[4]; Wei Hua[1]; Ying Mao[1]; *[1]Department of Neurosurgery, Huashan Hospital, Fudan University, Shanghai, China; [2]PURSPEC Technology (China) Ltd., Suzhou, China; [3]PURSPEC Technology (Beijing) Ltd., Beijing, China; [4]Tsinghua University, Beijing, China*

MP 138 **Direct and simultaneous identification of multiple beta-lactamases using A-MALDI**; Je-Hyun Baek[1]; Dong Huey Cheon[1]; Heejung Jang[1]; Saeyoung Lee[1]; Yoon Kyung Choi[1]; Won Suk Yang[1]; *[1]Seegene Medical Foundation, Seungdong-gu, South Korea*

MP 139 **Integrated TIMS-PASEF- platform for global lipidome and glycosphingo-lipidome investigation in Parkinson's Disease**; Dhanwin Baker[1]; Huong Giang Vo[1]; Gabriel Gonzalez Escamilla[2]; Sergiu Groppa[2]; Laura Bindila[1]; *[1]University Medical Center of Mainz, Mainz, Germany; [2]Universitatsklinikum des Saarlandes, Homburg, Germany*

MP 140 **Plasmonic alloys enhanced metabolic fingerprints for diagnosis of COPD and exacerbations**; Haiyang Su; *Shanghai Jiao Tong University, Shanghai, China*

MP 141 **Advancing Biomarker Discovery: Characterization of the P2 Technology for Plasma Samples for Pharma and Biobank, use and application to NSCLC**; Arthur Viodé[1]; Sandra Schär[1]; Polina Shichkova[1]; Tobias Treiber[1]; Christopher Below[1]; Angelica Rigutto[2]; Alessandra Curioni-Fontecedro[2, 3]; Yuehan Feng[1]; Lukas Reiter[1]; Roland Bruderer[1]; *[1]Biognosys AG, Schlieren, Switzerland; [2]Faculty of Science and Medicine, University of Fribourg, Fribourg, Switzerland; [3]Clinic of Oncology, HFR Hospital Fribourg, Fribourg, Switzerland*

MP 142 **Sample preparation advancements for clinical tissue specimen for immunopeptidomics**; Arthur Viodé[1]; Yuehan Feng[1]; Anamarija Pfeiffer[1]; Lukas Reiter[1]; Roland Bruderer[1]; *[1]Biognosys AG, Schlieren, Switzerland*

MP 143 **Exploring Different HPLC Column Chemistries for Optimal Separation of 17 Bile Acids by LC-MS/MS**; Haley Berkland; *Restek Corporation, Bellefonte, PA*

MP 144 **E2, Phone Home: Estradiol-ing in Accuracy and Efficiency with the Cobas i 601 analyzer**; Meghan Bradley[1]; Matthew R Chappell[1]; Matthew L Crawford[1]; Russell P Grant[1]; Philippe Metz[2]; Sven Groesgen[2]; *[1]LabCorp, Burlington, NC; [2]Roche Diagnostic GmbH, Mannheim, Germany*

MP 145 **Magnetic Bead-Based Automated Sample Preprocessing for LC-MS/MS-Based Therapeutic Drug Monitoring**; Pengyun Liu[1]; Zhouyang Kang[1]; Wenlie Huang[1]; Yikun Li[1]; Ziqing Kong[1]; Weijia Wu[1, 2]; Huafen Liu[1]; *[1]Calibra Scientific, Inc., Hangzhou, China; [2]3P BioSolutions Inc., Woodbridge, VA*

MP 146 **I Still Haven't Found ... the Ion Ratio I'm Looking For**; Christopher M. Shuford[1]; Stacy Dee[1]; Scott Wright[1]; Lyelle Davis[1]; Russell P Grant[1]; *[1]Laboratory Corporation of America, Burlington, NC*

MP 147 **The Nine Lives of a PCATs LC-MS/MS Assay Validation**; Stacy Dee[1]; Lyelle Davis[1]; Christopher M. Shuford[1]; Russell P Grant[1]; *[1]Laboratory Corporation of America, Burlington, NC*

MP 148 **Strata™SE – An Enhanced Supported Liquid Extraction (SLE) for Efficient Cleanup of LLOD Steroid Analytes in Serum**; Rajashree Chakravarti[1]; Shahana W Huq[1]; Stephanie J. Marin[1]; *[1]Phenomenex, Torrance, CA*

MP 149 **Sample Preparation for the Determination of an Extended Panel of Per- and Polyfluoroalkyl Substances (PFAS) from Human Serum using UHPLC-MS/MS**; Adam James Senior[1]; Kyle Bevan[1]; Steve Plant[1]; Helen Lodder[1]; Lee Williams[1]; Geoff M Davies[1]; Alan Edgington[1]; Charlotte Hayes[1]; Zainab Khan[1]; Lucy Richards[1]; Russell Parry[1]; Claire Desbrow[1]; Dan Menasco[1]; *[1]Biotage GB Limited, Cardiff, United Kingdom*

MP 150 **Resolving Interferences in 3α-Androstanediol Glucuronide Quantification: The Essential Role of Chromatography in Clinical Mass Spectrometry**; André Filipe Rodrigues De Oliveira[1]; Andréa Tedesco Faccio[1]; Breno Pereira Paulo[1]; Caroline Lacerra De Souza[1]; Guilherme Goncalves Okai[1]; Luciana Godoy Viana[1]; Luiz Carlos Fialho[1]; Rodrigo Andrade Schuch[1]; Karina Helena Morais Cardozo[1]; Valdemir Melechco Carvalho[1]; *[1]Fleury Group, São Paulo, Brazil*

MP 151 **Direct Analysis of Ascorbic Acid in Plasma Using Solvent-Free DART-MS/MS: A Reliable and High-Throughput Alternative to HPLC**; Breno Pereira Paulo[1]; Luiz Carlos Fialho[1]; Andre Filipe Rodrigues de Oliveira[1]; Andréa Tedesco Faccio[1]; Caroline Lacerra de Souza[1]; Guilherme Goncalves Okai[1]; Luciana Godoy Viana[1]; Rodrigo Andrade Schuch[1]; Valdemir Melechco Carvalho[1]; Karina Helena Morais Cardozo[1]; *[1]Fleury Group, São Paulo, Brazil*

MP 152 **Applying native multiomics to the study of hepatocarcinoma and rectal cancer signatures from tumors using the MSPen**; Raul Villacob[1]; Mary Hutchinson[1]; Charlie Wolfe[1]; Faith Jackobs[1]; Trevor Godfrey[1]; Atif Iqbal[1]; Livia S. Eberlin[1]; *[1]Baylor College of Medicine, Houston, TX*

MP 153 **Don't Let Your Ions Drift Away: Controlling Thermal Drift in Quantitative LC-SRM Measures**; Erin M Lewis[1]; Matthew L Crawford[2]; Christopher M. Shuford[2]; Stacy Dee[2]; Russell P Grant[2]; *[1]Labcorp, Burlington, NC; [2]LabCorp, Burlington, NC*

MP 154 **A multi-site evaluation of the performance of the MasSpec Pen for surgical margin analysis during breast cancer surgeries**; Keziah E. Liebenberg[1]; Ruth A.P. Costa[1]; Sarah Bench[1]; Emily X. Ma[1]; Mary L. Hutchinson[1]; Faith Jackobs[1]; Jacob I. Mardick[1]; Eric J. Silberfein[1]; Cary Hsu[1]; Alastair Thompson[1]; Stacy A. Carter[1]; Elizabeth Bonefas[1]; Chandandeep Nagi[1]; Jing Wang[1]; James W. Suliburk[1]; Livia S. Eberlin[1]; *[1]Baylor College of Medicine, Houston, TX*

MP 155 **Glycoproteomics for investigating congenital disorders of glycosylation: from disease biology to biomarkers for diagnosis and therapeutic monitoring**; Kishore Garapati[1]; Rohit Budhraja[1]; Neha Joshi[1]; Anu Jain[1]; Gunveen Sachdeva[1, 2, 3]; Jinyong Kim[1]; Raghavendra Pasupuleti[1]; Dowoon Nam[1]; Sandip Chavan[1]; Saniha Sabu[1, 2, 3]; Silvia Radenkovic[1, 4]; Anna N. Ligezka[1]; Kyriakie Sarafoglou[5]; Mayank Saraswat[1, 6]; Matthew J. Schultz[1]; Queenie K. G. Tan[1]; Gaurav K. Varshney[7]; Tamas Kozicz[8]; Andrew C. Edmondson[9]; Hudson H. Freeze[6]; Eva Morava[8]; Akhilesh Pandey[1]; *[1]Mayo Clinic, Rochester, MN; [2]Manipal Academy of Higher Education, Manipal, India; [3]Institute of Bioinformatics, Bangalore, India; [4]Utrecht University, Utrecht, Netherlands; [5]University of Minnesota, Minnneapolis, MN; [6]Sanford Burnham Prebys Medical Discovery Institute, La Jolla, CA; [7]Oklahoma Medical Research Foundation, Oklahoma City, OK; [8]Icahn School of Medicine at Mount Sinai, New York City, NY; [9]Children's Hospital of Philadelphia, Philadelphia, Pennsylvania, United States, Philadelphia, PA*

MP 156 **An Antibody Cocktail-based Immunoaffinity-LC-MS method enabled Ultra-sensitive and Accurate Multiplexed Quantification of Circulating Proinsulin Proteoforms**; Qingqing Shen[1]; Wang Cao[2]; Chao Xue[1]; Wei-jun Qian[3]; Tai-Tu Lin[3]; Jun Qu[1]; *[1]University at Buffalo, Buffalo, NY; [2]University at buffalo, buffalo; [3]Pacific Northwest National Laboratory, Richland, Washington*

MP 157 **Characteristics of Triple Quadrupole Tandem Mass Spectrometer for Solving Essential Problems in Medical Practice**; Andreas Tsakalof[1]; Alexey A. Sysoev[2]; Kira V. Vyatkina[3, 4, 5]; Alexander A. Eganov[3]; Nikolay N. Eroshchenko[3]; Alexey N. Kiryushin[2, 3]; Alexey Yu. Adamov[2]; Elena Yu. Danilova[3]; Alexander E. Nosyrev[3]; *[1]University of Thessaly, Biopolis, Larissa, Greece; [2]National Research Nuclear University MEPHI, Moscow, Russia; [3]Sechenov University, Moscow, Russian Federation; [4]Saint Petersburg State University, St Petersburg, Russia; [5]Saint Petersburg Electrotechnical University "Leti", St Petersburg, Russia*

MP 158 **GC-MS Profiling of Gut Microbiota-Derived SCFAs in PCOS: Diagnostic and Therapeutic Implications**; Evgenii Kukaev[1]; Ekaterina Kirillova[1]; Alisa Tokareva[1]; Elena Rimskaya[1]; Nataliia Starodubtseva[1]; Galina Chernukha[1]; Tatiana Priputnevich[1]; Vladimir Frankevich[1]; Gennady Sukhikh[1]; *[1]Kulakov National Medical Research Center for Obstetrics, Gynecology and Perinatology, Moscow, Russia*

MP 159 **Quantitation of Deep-Lung Fluid Exhaled Breath Particles by LC-MS and NMR**; Peter J Walter[1]; Ad Bax[1]; Tayeb Kakeshpour[1]; *[1]NIH, Bethesda, MD*

MP 160 **Development of a Simple and Sensitive Liquid Chromatography-Tandem Mass Spectrometry (LC-MS/MS) Method for Clinical Analysis of Liraglutide in Plasma**; Hongyi Cai[1]; Peter J Walter[1]; Stephanie Chung[1]; *[1]NIH, Bethesda, MD*

MP 161 **LC-MS/MS with Polarity Switching for Newborn Screening of Over 60 Biomarkers in Under 2-min**; Samantha L Isenberg[1]; C. Austin Pickens[1]; Daquille Peppers[1]; Carla Cuthbert[1]; Rachel Lee[1]; Konstantinos Petritis[1]; *[1]Centers for Disease Control and Prevention, Atlanta, GA*

MP 162 **Restoration of Antibiotic-Impacted Microbiome in Human Babies: Pilot Metabolomic & Metagenomic Study on the Efficacy of Autologous Fecal Microbiota Transplantation**; Shashikant S. Kotwal[1, 2]; Haipeng Sun[3]; Anna Dulencin[3]; Maria Gloria Dominguez-Bello[3]; Qingli Wu[1, 2]; James E. Simon[1, 2]; *[1]Department of Plant Biology, Rutgers, The State University of New Jersey, New Brunswick, New Jersey; [2]New Use Agriculture & Natural Products Program, New Brunswick, New Jersey; [3]Department of Biochemistry and Microbiology, Rutgers, The State University of New Jersey, New Brunswick, New Jersey*

MP 163 **Semi-automatic LC-MS/MS method for measurement of 3-methoxytyramine, Metanephrine and Normetanephrine in plasma**; Ning Pan Bernhardt[1]; Caroline Nottingham[1]; *[1]National Institute of Health, Bethesda, MD*

COVALENT LABELING AND CHEMICAL CROSSLINKING
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MP 164 **Comparing protein dynamics of NO synthase proteins by quantitative crosslinking mass spectrometry**; Ting Jiang[1]; Changjian Feng[1]; *[1]UNM College of Pharmacy, Albuquerque, NM*

MP 165 **High-Throughput Screening of Amyloid Inhibitors via Covalent Labeling Mass Spectrometry**; Kanitin Khamnong[1]; Richard W Vachet[1]; *[1]Department of Chemistry, University of Massachusetts Amherst, Amherst, MA*

MP 166 **Establishing a Click-compatible Cross-linking Chemoproteomics Platform**; Joelle Darrouj[1]; Miranda Villanueva[1]; Keriann Backus[1]; *[1]University of California, Los Angeles, Los Angeles, CA*

MP 167 **XLeu: A Novel Cleavable Crosslinker with Quantitative Isobaric Tag Labeling**; Zexin Zhu[1]; Wei Li[1]; Charlotte Anne Douglas[2]; Zicong Wang[1]; Lingjun Li[1]; *[1]University of Wisconsin-Madison School of Pharmacy, Madison, WI; [2]University of Wisconsin-Madison, College of Letters and Science, Madison, Wisconsin*

MP 168 **Evaluating Antigen-Antibody Interactions: A Comparative Study of Higher-Order Structural MS Methods**; Yiran Ma[1]; Kristin Hughes[1]; Deepa Balasubramaniam[1]; *[1]Eli Lilly, San Diego, CA*

MP 169 **Innovative data-independentacquisition(DIA) workflows for protein–nucleic acid interaction**; Yi He[1]; Sergei Moshkovskii[2, 3]; Olexandr Dybkov[2]; Arslan Siraj[4]; Timo Sachsenberg[4, 5]; Oliver Kohlbacher[4, 5, 6]; Robert Justin Grams[7]; Ku-Lung Hsu[7]; Henning Urlaub[2, 3]; Rosa Viner[8]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Bioanalytical Mass Spectrometry Group, Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany; [3]Bioanalytics Group, Institute of Clinical Chemistry, University Medical Center Göttingen, Göttingen, Germany; [4]Institute of Bioinformatics and Medical Informatics, University of Tübingen, Tübingen, Germany; [5]Applied Bioinformatics, Dept. of Computer Science, University of Tübingen, Tübingen, Germany; [6]Institute of Translational Bioinformatics, University Hospital Tübingen, Tübingen, Germany; [7]Department of Chemistry, University of Texas at Austin, Austin, TX; [8]ThermoFisher Scientific, San Jose, CA*

MP 170 **Revealing Glycan mediated protein-protein interactions in human liver cells through a Quantitative Cross-Linking Mass Spectrometry**; Riya Gogte[1]; Michael Russelle S Alvarez[2]; Sheryl Joyce G. Alvarez[2]; Siyu Chen[2]; Yixuan Xie[2]; Shivraj Gill[1]; Tristan Seales[2]; Kayla Pakulski[2]; Carlito B. Lebrilla[2]; *[1]University of California, Davis, Davis, CA; [2]University of California Davis, Davis, CA*

MP 171 **Investigating Interactions of Synaptic Proteins in Neuron-like SH-SY5Y Cells Utilizing Proximity Labelling**; Gihyun Sung[1]; Carla Schmidt[1]; *[1]Johannes Gutenberg University Mainz, Mainz, Germany*

MP 172 **Using photoactivatable probes and MS to determine the location of polyisoprenoid tails in the hydrophobic pocket of UppS**; Alaina Rosen[1]; Brian T. Cooper[1]; Jerry Troutman[1]; *[1]University of North Carolina at Charlotte, Charlotte, NC*

MP 173 **Structural Study of Neural Cadherin Dimerization**; Anter A Shami[1]; Sandeep K Misra[1]; Addison E. Roush[1]; Samantha Davila[1]; Shana V. Stoddard[2]; Joshua S. Sharp[1]; Susan Pedigo[1]; *[1]The University of Mississippi, University, MS; [2]Rhodes College, Memphis, TN*

MP 174 **Assessment of Protein Conformation via Diazirine-Promoted Oxidation (DPO)**; Supadach Prertprawnon[1]; Salem R. Neufeld[1]; Nicholas B. Borotto[1]; *[1]University of Nevada, Reno, Reno, NV*

MP 175 **Inline Liquid Chromatography-Flash Oxidation for Structural Analysis of Dynamic Protein-Ligand Interactions**; Ajay Sharma[1]; Suman Choudhary[1]; Sandeep K Misra[1]; Anter A Shami[1]; Joshua S. Sharp[1]; *[1]University of Mississippi, University, MS*

MP 176 **Diethylpyrocarbonate - based covalent labeling of the Tau and Low-Density Lipoprotein Receptor-Related Protein 1 complex in vitro and in cells**; Vanessa L. Stahl[1]; Wen-Chuan Chou[1]; Jennifer N. Rauch[1]; Richard W. Vachet[1]; *[1]UMass Amherst, Amherst, MA*

MP 177 **Inline HIC LC–HRPF for Structural Analysis of Heteromeric Protein Complexes**; Godson I. Orachor[1]; Ajay Sharma[1]; Sandeep K Misra[1]; Joshua S. Sharp[1]; *[1]University of Mississippi, University, MS*

MP 178 **Novel mass spec-cleavable protein crosslinking agents that detect direct residue-residue contacts in vivo**; Bjorn-Erik Wulff[1]; Joshua E. Elias[2]; Pehr A.B. Harbury[1]; *[1]Stanford University, Stanford, CA; [2]Chan Zuckerberg BioHub, Stanford, CA*

MP 179 **Assessment of Protein Conformation with Online Ozone Labeling and Mass Spectrometry**; Keshari Kunwor[1]; Nicholas B. Borotto[2]; *[1]University of Nevada, Reno, Nevada; [2]University of Nevada, Reno, Reno, Nevada*

MP 180 **In-cell Drug Screening and Structural Insights for Integral Membrane Proteins by footprinting**; Jie Sun[1]; Mixiaerti Saimi[2]; Don Rempel[3]; Mengqi Chai[3]; Weikai Li[2]; Michael L Gross[3]; *[1]University of Tennessee Knoxville, Knoxville, TN; [2]Washington University School of Medicine, St. Louis, MO; [3]Washington University in St. Louis, University City, MO*

MP 181 **Enhancing Hydroxyl Radical Protein Footprinting Resolution Using Multiplex Trifluoromethyl and Hydroxyl Chemistry on Larger Protein Systems**; JOSHUA Joloba LUTAAKOME[1]; Rohit Jain[1]; Erik R. Farquhar[1]; Mark R Chance[1]; Janna Kiselar[1]; *[1]Case Western Reserve University, Cleveland, OH*

MP 182 **Identifying a drug binding site in MukB protein using cross-linking mass spectrometry**; Thilini Peramuna[1]; Hang Zhao[1]; Nagib Ahsan[1]; Valentin V Rybenkov[1]; *[1]University of Oklahoma, Norman, OK*

MP 183 **Mass Spectrometry and Computational Elucidation of Selective Labeling of DJ-1 Active Site by Conjugate of α-Methylene-β-Lactone and Dopamine**; Robert Jervine V Ortega[1]; Abraham Mahjoob[1]; José Gascón[1]; Xudong Yao[1]; *[1]University of Connecticut - Storrs, Storrs Mansfield, CT*

MP 184 **Legumain: Extending the Crosslinking-MS toolbox by an protease with orthogonal cleavage specificity**; Luca Riermeier[1, 2]; Alexander Leitner[1]; *[1]ETH Zurich, Zurich, Switzerland; [2]Life Science Zurich Graduate School, Zurich, Switzerland*

MP 185 **Benchmarking in-cellCrosslinking Mass Spectrometry Against Cell Fixed vs Non-Fixed Cells for the Investigation of in-situ Protein-Protein Interactions**; Kish Adoni[1]; Fanindra Deshmukh[1]; Konstantinos Thalassinos[1]; *[1]University College London, London, United Kingdom*

MP 186 **Development of Photoactivatable Lysine Reactive Crosslinking Reagents**; Adam Cahill[1]; Martin Walko[1]; Nikil Kapur[1]; Benjamin Fenton[1]; Keith Livingstone[1]; Megan Wright[1]; Antonio N. Calabrese[1]; *[1]University of Leeds, Leeds, United Kingdom*

MP 187 **Engineered Affinity Binders for Crosslinking Mass Spectrometry**; Yan Yan[1]; Ying Zhang[1]; Bret Redwine[1]; Jose Emmanuel Javier[1]; Paulo Leal[1]; Jay Unruh[1]; Laurence Florens[1]; Kausik Si[1]; *[1]Stowers Institute for Medical Research, Kansas City, MO*

MP 188 **Discovery of covalent c-Myc mRNA-binding small molecules using chemical probing, PAL-MaP, and mass spectrometry techniques**; Peter T Rye[1]; Somayeh Talebzadeh[1]; Terryl Fritz[1]; MaryRose Steed[1]; Can C Ozbal[1]; Krista Marran[2]; Brittani Patterson[2]; Caleb Sutherland[2]; Ramamurty VS Changalvala[2]; James Lanter[2]; Katherine Deigan Warner[2]; Matthew Friedersdorf[2]; Matthew J Smola[2]; *[1]Momentum Biotechnologies, Billerica, MA; [2]Ribometrix, Durham, NC*

MP 189 **MS-cleavable Cross-linking analysis on modified Orbitrap Astral mass spectrometer**; Yi He[1]; Tabiwang N. Arrey[2]; Eugen Damoc[2]; Erum Raja[3]; Leigh Foster[3]; Ryan Bomgarden[3]; Rosa Viner[1]; Thomas Moehring[2]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [3]Thermo Fisher Scientific, Rockford, IL*

MP 190 **Hydroxyl Radical Protein Footprinting Combined with Affinity Purification Mass Spectrometry Provides Insight into Protein-Protein Interactions and their Structural Organization**; Tyler C Cropley[1]; Amanda J Keplinger[2]; Alexander J Ruthenburg[2]; Beatrix Ueberheide[1]; Amoldeep S Kainth[2]; *[1]NYU Langone Medical Center, New york, NY; [2]University of Chicago, Chicago, IL*

MP 191 **Accessing deeper in-gel cross-linking with in vivoformaldehyde fixation and sequential reactions reveals intermolecular cross-links for modeling the primed epichaperome.**; Luke A Botticelli[1]; Kathleen Madison Feener[1]; Seth McNutt[1]; Feixia Chu[1]; *[1]University of New Hampshire, Durham, NH*

MP 192 **Simultaneous use of Multiple Covalent Labeling Reagents to Making Protein Folding Stability Measurements on the Proteomic Scale**; Jhih-Hao Ho[1]; Yueqi Chen[1]; Michael C. Fitzgerald[1]; *[1]Duke University, Durham, NC*

MP 193 **Enhanced Protein Footprinting with Single Amino Acid Resolution: Integrating AutoFox, Ion Mobility Q-TOF, and ECD Fragmentation for Multi-Tier Structural Proteomics**; Emily Chea[1]; Mike Hare[2]; Yury V. Vasilev[2]; Scot Weinberger[1]; *[1]GenNext Technologies, Half Moon Bay, CA; [2]Agilent, Corvallis, OR*

MP 194 **Probing Binding Interfaces in Viral and Allergenic Protein complexes Using Chemical Crosslinking and Mass Spectrometry**; William LaFon[1]; Akash Talukder[1]; Saiful Chowdhury[1]; *[1]University of Texas at Arlington, Arlington, TX*

MP 195 **Development of a Novel Mass-Spectrometry-based Platform for Examining Higher Order Structure of RNA**; Sanjeev Kumar[1]; Hsin-Chieh (Natashia) Yang[1]; Don L. Rempel[1]; Henry Rohrs[1]; Leah Hanliu Wang[2]; Brian Gau[2]; Michael L. Gross[1]; *[1]Department of Chemistry, Washington University, St. Louis, MO; [2]Bioptherapeutics Pharm. Sci., Pfizer Inc., St. Louis, MO*

MP 196 **Integrating Multiplexed Quantitation with Co-Fractionation Cross-linking Mass Spectrometry to Define Endogenous Protein Complexes**; Sean Tang[1]; Clinton Yu[1]; Fenglong Jiao[1]; Lan Huang[1]; *[1]University of California, Irvine, Irvine*

MP 197 **Characterization of Amyloid Beta 1-42 Aggregation with Mass Spectrometry-based Footprinting**; Xinzhu Li[1]; Nolan McLaughlin[1]; Michael L Gross[1]; *[1]Washington University in St. Louis, University City, MO*

MP 198 **Developing a Multimeric Trioxane-based MS-cleavable Cross-linker for Improving the Depth of PPI Profiling and Structural Modeling**; Clinton Yu[1]; Xiaorong Wang[1]; Eric Novitsky[1]; Sree Ganesh Balasubramani[2]; Paul Morenkov[1]; Scott Rychnovsky[1]; Ignacia Echeverria[2]; Lan Huang[1]; *[1]University of California, Irvine, Irvine, CA; [2]University of California San Francisco, San Francisco, CA*

MP 199 **An SEC-UV-nMS platform for optimizing XL-MS analysis of heterogeneous mixtures of protein-protein interactions**; Nicole D. Wagner[1]; Xinyi (Cynthia) Kuang[1]; David Price[2]; Leonard Ma[2]; Gaya K. Amarasinghe[2]; Daisy W. Leung[2]; Michael L Gross[1]; *[1]Washington University in St. Louis, St. Louis, MO; [2]Washington University School of Medicine, St. Louis, MO*

MP 200 **High-Resolution Proteomic Interaction Mapping Using a Dityrosine Crosslinking Platform**; Trenton M Peters-Clarke[1]; Johnathan C Maza[1]; Paul Burroughs[1]; Yifei Chen[1]; Kevin Leung[1]; Jim Wells[1]; *[1]University of California, San Francisco, San Francisco, CA*

MP 201 **A Glycosidic-Bond-Based Mass-Spectrometry-Cleavable Cross-linker Enables In vivo Cross-linking for Protein Complex Analysis**; Jing Chen[1]; Qun Zhao[1]; Hang Gao[1]; Yukui Zhang[1]; Lihua Zhang[1]; *[1]Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China*

MP 202 **Elucidating the Salmonella interactome by crosslinking mass spectrometry**; Anthony Ciancone; *NIH/NCI, Frederick, MD*

MP 203 **Development of DIA workflow for Multiplex Hydroxyl Radical Protein Footprinting**; Carolina Rojas Ramirez[1]; Rohit Jain[2]; Nicolas Hartel[3]; Fengchao Yu[1]; Janna Kiselar[2]; Mark R Chance[2]; Alexey Nesvizhskii[1]; Rosa Viner[3]; *[1]University of Michigan, Ann Arbor, Michigan; [2]Case Western Reserve University, Cleveland, Ohio; [3]Thermo Fisher Scientific, San Jose, CA*

DRUG DISCOVERY: QUALITATIVE AND QUANTITATIVE ANALYSIS I

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MP 204 **High-throughput PROTAC compound screening workflow for targeted protein degradation on an Orbitrap Astral mass spectrometer with accurate label-free quantitation**; Kevin Yang[1]; Brett Larsen[1]; Amirmansoor Hakimi[1]; Tonya Pekar Hart[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

MP 205 **Benchmarking Proteomic Methods for Effective Covalent Drug Target Profiling Studies**; Mario Leutert[1]; Ludwig Bauer[1]; Christoph Paschen[1]; Marcus Bantscheff[1]; *[1]Roche Pharma Research and Early Development (pRED), 360Labs, Basel, Switzerland*

MP 206 **PRISM: a universal proteomics pipeline for drug discovery research**; Johannes Krumm[1]; Michael Zollo[1]; Raffaela Berger[1]; Gözde Kibar[1]; Philipp Weber[1]; Barbara Schnitzer[1]; Christin Zasada[1]; Hannes Hahne[1]; *[1]OmicScouts GmbH, Freising, Germany*

MP 207 **Novel peptide optimization strategy for the selection of membrane protein ligands using direct cell culture LC-MS analysis**; Ian Gering[1]; Janine Kutzsche[1]; Dieter Willbold[1]; *[1]Forschungszentrum Jülich GmbH, Jülich, Germany*

MP 208 **Development of a Multi-omics Platform to Generate Cellular Phenotypic Compound 'Signatures'**; Tao Wang; *GSK, Collegeville, PA*

MP 209 **Pharmacokinetic ADC quantitation and DAR determination by intact protein LC-MS for large-scale preclinical in vivo stability screening**; Wonhyeuk Jung[1]; Jaqueline Picache[1]; Jake A. Melby[1]; Iliana Levesque[1]; John Kellie[1]; *[1]AstraZeneca, Gaithersburg, Maryland*

MP 210 **State-of-the-art Intact and Reduced LC-MS Platform for a Diverse Oncology and Biopharmaceutical Pipeline: In-life Quantitation, Characterization, and Pharmacokinetic Support**; Jake A. Melby[1]; Jaqueline Picache[1]; Wonhyeuk Jung[1]; John Kellie[1]; *[1]AstraZeneca, Gaithersburg, MD*

MP 211 **Quantification of an Investigational New Anticancer Drug SHetA2 in Single Spheroids Derived from Patients with Ovarian Cancer**; Amit Singh; *University of Oklahoma, Norman, OK*

MP 212 **Proteomics Enabled Mechanistic Characterization of KT-333, a Potent and Selective Heterobifunctional STAT3 Degrader**; Yatao Shi[1]; Christopher Browne[1]; Karen Yuan[1]; Sarah Martinez[1]; Lijing Su[1]; Yogesh Chutake[1]; Vaishali Dixit[1]; Xue Fei[1]; Caroline Daigle[1]; Kiran Mahasenan[1]; Anand Ramanathan[1]; Alyssa Fasciano[1]; Michele Mayo[1]; Rahul Karnik[1]; Eric Kuhn[1]; Susanne Breitkopf[1]; Joyoti Dey[1]; Haojing Rong[1]; Xin Huang[1]; Phillip CC Liu[1]; Richard Miller[1]; Bin Yang[1]; Dirk M Walther[1]; Kirti Sharma[1]; *[1]Kymera Therapeutics, Watertown, MA*

MP 213 **SenoCETSA software identifies potential targets of senolytics from MS-CETSA data**; Tomas Pierce[1]; Quinn Strassheim[1]; Amit Dey[1]; Delaney Rutherford[1, 2]; Reema Banarjee[1]; Dimitrios Tsitsipatis[1]; Bradley Olinger[1]; Ruin Moaddel[1]; Myriam Gorospe[1]; Nathan Basisty[1]; *[1]National Institute on Aging, Baltimore, MD; [2]University of Michigan, Ann Arbor, Michigan*

MP 214 **Optimizing a cell-based model for High-Throughput assessment of energy metabolism using Echo-MS**; Jon Shrimp[1]; Nate Hoxie[1]; Matthew Hall[1]; Stephan Siebel[2]; Richard G Kibbey[2]; John Janiszewski[3]; Chang Liu[4]; Thomas R. Covey[4]; *[1]National Center for Advancing Translational Sciences (NCATS), Rockville, MD; [2]Yale University, New Haven, CT; [3]J2.Bioanalytical, Westerly, RI; [4]SCIEX, Concord, ontario*

MP 215 **Monitoring protein conjugation reaction kinetics to support process development using an online buffer exchange-native mass spectrometry method**; Josue Baeza[1]; Brent Kochert[1]; Christine Thomas[1]; Janelle Lukens[1]; Lee Klein[1]; *[1]Merck & Co., Inc., West Point, PA*

MP 216 **Enabling High-Throughput Protein-Drug Screening with Ultra-Fast Deconvolution**; Matthew T Robey[1]; Aisha-Ben Younis[2]; Tatiana Silva[2]; Idlir Liko[2]; Kleitos Sokratous[2]; Kenneth R Durbin[1]; *[1]Proteinaceous, Evanston, IL; [2]OMass Therapeutics, Oxford, United Kingdom*

MP 217 **Leveraging Adaptive RT on Orbitrap Ascend MultiOmics Tribrid Mass Spectrometer for Improved Sensitivity and Throughput in Targeted and Hybrid Workflows**; Jingjing Huang[1]; Qingling Li[1]; Philip Remes[1]; Xiao Wang[1]; Graeme McAlister[1]; Rafael Melani[1]; *[1]Thermo Fisher Scientific, San Jose, California*

MP 218 **Accelerating the Discovery and Development of Covalent Drugs Using Mass Spectrometry-based Chemoproteomic Assays**; William LaMarr[1]; David Garby[1]; Jeremiah Bowers[1]; Lisa Boatner[1]; Somayeh Talebzadeh[1]; Aaron Wolfe[2]; Sekar Ramachandran[3]; Peter Rye[1]; *[1]Momentum Biotechnologies, Inc., Billerica, MA; [2]ICHOR Life Sciences, Inc., Syracuse, NY; [3]ICHOR Life Sciences, Inc., Syracuse, New York*

MP 219 **Advanced Mass Spectrometry Strategies for Deciphering the Complex Composition of an Unknown Chinese Patent Medicine**; Fu Shuna[1]; Wu Huakai[2]; *[1]Agilent Technologies, Inc., Guangzhou, China; [2]Zhangzhou Pientzehuang Pharmaceutical Co., Ltd., Fujian, China*

MP 220 **Leveraging proteomics to advance targeted protein degraders from hit identification through development candidate selection**; Sarah Bollinger Martinez[1]; Charles L Howarth[1]; Yi-Ting Wang[1]; Yatao Shi[1]; Min Yuan[1]; Ginny Massa[1]; Rujuta Kshirsagar[1]; Christopher Brown[1]; Dirk M Walther[1]; Susanne Breitkopf[1]; Eric Kuhn[1]; Kirti Sharma[1]; *[1]Kymera Therapeutics, Inc, Watertown, MA*

MP 221 **Automating an end to end adaptive workflow for uScale purification via multiple separation techniques to enable quicker hit to lead**; Neal Liddle[1]; Hui Zhang[2]; *[1]Sciex, San Diego, CA; [2]Iambic Therapeutics, San Diego, CA*

MP 222 **Applying immunoprecipitation of drug-protein complexes for LC-MS/MS bioanalysis**; Li Sun[1]; Habib Sistani[1]; Ming Wang[1]; Cynthia Chavez-Eng[1]; Shivangi Awasthi[1]; Wolfgang Seghezzi[1]; Brad Roadcap[1]; Faye Vazvaei-Smith[1]; *[1]Merck & Co., Rahway, NJ*

MP 223 **Simultaneous Quantitation and Discovery (SQUAD) workflow using multiple fragmentation techniques for quantitation and characterization of trace level nitrosamines in medicines**; Sunandini Yedla[1]; Brandon Bills[1]; Rahul R. Deshpande[1]; Bashar Amer[1]; Vlad Zabrouskov[1]; Susan S Bird[1]; Min Du[1]; *[1]Thermo Fisher Scientific, San Jose, California*

MP 224 **Evaluating and optimizing transcription factor targets for a high-throughput mass spectrometry-based drug discovery platform**; Daniele Canzani[1]; Julia Robbins[1]; Andrea Gutierrez[1]; Brian McEllin[1]; Kyle Siebenthall[1]; Gaelle Mercenne[1]; Alexander J. Federation[1]; Lindsay K Pino[1]; *[1]Talus Bioscience, Seattle, WA*

MP 225 **Profiling anthracycline toxicity and mechanisms in pediatric tumors using high-throughput proteomics**; Julia E Robbins[1]; Gabriel E Boyle[2]; Andrea Gutierrez[1]; Sebastian J. Paez[1]; Daniele Canzani[1]; Jay F. Sarthy[2]; Lindsay K Pino[1]; Alexander J. Federation[1]; *[1]Talus Bioscience, Seattle, WA; [2]Ben Towne Center for Childhood Cancer Research, Seattle, WA*

MP 226 **Pre-clinical Characterization of Orally Bioavailable CNS-Penetrant Degraders for the Treatment of Multiple Sclerosis**; Bekim Bajrami; *Biogen, Cambridge, MA*

MP 227 **Re-Evaluate the Whole Blood Stability in Regulated Bioanalysis to Support Pre-clinical and Clinical Studies**; Song Zhao[1]; Yashpal Singh Chhonker[1]; Raul Morales-Hurtado[1]; Xiaonan Tang[1]; Harry Zhao[1]; *[1]Frontage Laboratories, Inc - Exton, PA, Malvern, PA*

MP 228 **Integrated Mass Spectrometry Platform for Biologic Drug Discovery and Lead Optimization**; Lei Guo; *WuXi Biologics, Shanghai, China*

MP 229 **Sensitive Quantitation of Glucagon-like peptide-1 (GLP-1) Analog Tirzepatide in Plasma Using Automated LC-MS/MS workflow**; Xi Qiu[1]; Steve Murphy[2]; David Wong[2]; *[1]Agilent Technologies, Wilmington, DE; [2]Agilent Technologies, Santa Clara, CA*

MP 230 **Small-footprint Capillary UHPLC/MS technology significantly reducing consumption of PFAS containing modifiers for Fast and High Resolution separation of Synthetic Oligonucleotides**; Greg Ward[1]; Patrick M Batoon[2]; *[1]Axcend, Provo; [2]Agilent Technologies Inc, Santa Clara, CA*

MP 231 **The cyanine dye Cy3 demonstrates a highly potent, but glycerol-dependent, in vitro activity towards Mycobacterium tuberculosis**; David Podlesainski[1]; Violetta Krisilia[2]; Tim Richter[3]; Emmanuel T. Adeniyi[2]; Farnusch Kaschani[3]; Rainer Kalscheuer[2]; Markus Kaiser[3]; *[1]University Duisburg-Essen, Essen, Germany; [2]Heinrich Heine*

University, Düsseldorf, Germany; [3]University Duisburg-Essen, Essen, Germany

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MP 232 **Identification of histone lactylation readers by combining photoaffinity probe with mass spectrometry**; Kai Zhang; *Tianjin Medical University, Tianjin, China*

MP 233 **Cleavage of histone H2A during stem cell differentiation by cathepsin L destabilizes nucleosomes to counteract gene activation**; Mariel Coradin[1]; Francisca NDL Vitorino[2]; Richard M. Searfoss[2]; Benjamin A Garcia[2]; *[1]University of Pennsylvania, Perelman School of Medicine, Philadelphia, PA; [2]Washington University School of Medicine, St. Louis, MO*

MP 234 **Characterization of Low-Abundance Histone Post-Translational Modifications in Alzheimer's Disease by LC-MS/MS**; Sarah A Sahioun[1]; Vishal Sandilya[1]; Cristian D. Gutierrez-Reyes[1]; Joy O Solomon[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX*

MP 235 **Screening Histone PTM changes associated with drug treatment using nLC-TIMS-ddaPASEF-ToF MS/MS**; Moshfiqur Rahman[1]; Md Shofiul Alam[1]; Cassandra N. Fuller[1]; Lilian Valadares Tose[1]; Manuel Alejandro Barbieri[1]; Francisco A. Fernandez Lima[1]; *[1]Florida International University, Miami, FL*

MP 236 **Top-down and bottom-up proteomics to study the molecular functions of protein deacetylase SIRT6**; Kevin M Buck[1]; Sherry Bakhtiar[2]; Vyacheslav I. Kuznetsov[2]; John Denu[2]; *[1]University of Wisconsin-Madison, Madison, WI; [2]Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI*

MP 237 **Understanding the crosstalk of silencing and active modifications on histone H3 using quantitative mass spectrometry**; Alina A Garcia[1]; Francisca NDL Vitorino[1]; Benjamin A Garcia[2]; *[1]Washington University School of Medicine, St. Louis, MO; [2]Washington University in St. Louis, St. Louis, Missouri*

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MP 238 **Chilling Truth: Unveiling the Effects of Storage Temperature on the Metabolomic Profiles of Food**; Macy J. Gruszczynski[1]; Jacqueline M. Chaparro[1]; Margaret L. Read[1]; Melanie T. Odenkirk[1]; Nathan Montgomery[1]; Corey D. Broeckling[1]; Chi-Ming Chien[2]; Tracy Shafizadeh[2]; Steve Watkins[2]; Jessica E. Prenni[1]; *[1]Colorado State University, Fort Collins, CO; [2]Verso Biosciences, Inc., Davis, CA*

MP 239 **Optimizing Methods for Extracting and Quantifying Per- and Polyfluoroalkyl Substances (PFAS) in Different Types of Beer Throughout the World**; Ashlee T. Falls[1]; Kara M. Joseph[1]; Erin S. Baker[1]; *[1]University of North Carolina - Chapel Hill, Chapel Hill, NC*

MP 240 **Fully Automated Sensitive Quantitation of PFAS in Seafood for Regulatory Screening Using Triple Quadrupole LC/MS**; Aimei Zou[1]; Gwen Sin Yee Lim[2]; M. Lorna De Leoz[3]; *[1]Agilent Technologies Singapore, Singapore, Singapore; [2]CTC Analytics AG, Zwingen, Switzerland; [3]Agilent Technologies, Santa Clara, CA*

MP 241 **GC-Ion Mobility-HRMS as a Powerful Alternative to Magnetic Sector MS for a Comprehensive Quantitation of Dioxins and Multiple POP Classes**; Arnd Ingendoh[1]; Miguel Angel Perez[2]; Hugo Muller[3]; Gauthier Eppe[3]; *[1]Bruker Daltonics, Bremen, Germany; [2]Bruker Espanola, Madrid, Spain; [3]University Liege, Liege, Belgium*

MP 242 **Evaluation of improved ESI probe in pesticide analysis using triple quadrupole LC-MS**; Takanari Hattori[1]; Hiroki Miyashiro[1]; Kazunari Yamaguchi[1]; Natsuyo Asano[1]; Keisuke Iso[1]; Yuka Fujito[1]; *[1]Shimadzu, Kyoto, Japan*

MP 243 **Colorful Confections: Analyzing Artificial Food Dyes in Sports Drinks, Gelatins, and Gummies**; Gordon T. Fujimoto[1]; Lindsay E. Hatch[1]; Sarah E. Dowd[1]; Nicholas Ellor[1]; *[1]Waters, Milford, MA*

MP 244 **Unmatched Robustness for Analysis of Per- and Poly-fluoroalkyl Substances in Difficult Food Matrices Using QSight 500 LC-MS/MS System**; Jingcun Wu[1]; Jamie Foss[2]; Vlad Kardelis[1]; Gavin Fischer[1]; *[1]PerkinElmer Inc., Woodbridge, ON; [2]PerkinElmer Inc., Shelton, CT*

MP 245 **Trace metals analysis in baby food using triple quadrupole inductively coupled plasma mass spectrometry (TQ-ICP-MS)**; Adam Ladak[1]; Andy Fornadel[2]; Daniel Kutscher[3]; Sukanya Sengupta[3]; Laurent Naels[4]; Doug Sears[5]; Gwyneth Trojan[5]; *[1]Thermo Scientific, Macclesfield, United Kingdom; [2]Thermo Scientific, Bannockburn, IL; [3]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [4]Thermo Fisher Scientific, Countaboeuf, France; [5]Thermo Fisher Scientific, San Jose, CA*

MP 246 **Analysis of Per- and Polyfluoroalkyl Substances (PFAS) in Drinking Water and Milk using LC-MS/MS coupled with Online-SPE Interface**; MAHO TANAKA[1]; Nozomi Maeshima[1]; Dominika Gruszecka[2]; Ruth Marfi-Vega[2]; Yuka Fujito[3]; Manami Kobayashi[1]; *[1]Shimadzu corporation, Kawasaki, Japan; [2]Shimadzu Scientific Instruments, Columbia, MD; [3]Shimadzu Corporation, Kyoto, Japan*

MP 247 **Improvements in robustness of signal response in multiresidue pesticide analysis offered by a new novel slotted bandpass ion guide**; David Gould[1]; Peter Hancock[1]; Stuart J Adams[1]; Cristian Cojocariu[1]; Mark Roberts[1]; *[1]Waters Corporation, Wilmslow, United Kingdom*

MP 248 **Performance evaluation of GC-MS/MS for Dioxin analysis with amendments to EU Regulations 644/2017 and 771/2017 for food and feed**; Adam Ladak[1]; Andy Fornadel[2]; Alexander Schaechtele[3]; Kerstin Krätschmer[4]; Nick Warner[5]; Amit Gujar[6]; Jason Cole[6]; Xin Zheng[6]; Mark Belmont[2]; Matthew Menesini[6]; *[1]Thermo Scientific, Macclesfield, United Kingdom; [2]Thermo Scientific, Bannockburn, IL; [3]European Union Reference Laboratory (EURL) for Halogenated POPs in Feed and Food, Freiburg, Germany; [4]Wageningen Food Safety Research, Part of Wageningen University & Research,, Wageningen, Netherlands; [5]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [6]Thermo Fisher Scientific, San Jose, CA*

MP 249 **High-Throughput Screening for Polyfluoroalkyl Substances in Complex Samples Using Solid-Phase Microextraction Probe Coupled to Mass Spectrometry**; Wei Zhou[1]; Yaping Li[1]; Janusz Pawliszyn[1]; *[1]University of Waterloo, Waterloo, ON*

MP 250 **Sip Happens: The Smoky Truth Behind Your Brew**; Maria Tolstyakova[1]; Gyuri Vas[2]; Emre Seyyal[2]; *[1]Intertek Pharmaceuticals, Whitehouse, NJ; [2]Intertek Pharmaceuticals, Whitehouse, New Jersey*

MP 251 **The Superior Advantages of Microflow LC-MS/MS in Pesticide Residue Analysis for Food Safety**; Florencia Jesús[1]; Víctor Cutillas[1]; Carmen Ferrer[1]; María Jesús Martínez-Bueno[1]; Amadeo Rodríguez Fernández-Alba[1]; *[1]UNIVERSITY OF ALMERIA, Almeria, Spain*

MP 252 **Novel Triple Quad Approaches for Sensitive Quantification of 1000 Compounds in Single Runs**; Christopher Elicone[1]; Arnd Ingendoh[2]; Juan Gomez[3]; Miguel Angel Perez[3]; *[1]Bruker Scientific, Billerica, MA; [2]Bruker Daltonics, Bremen, Germany; [3]Bruker Espanola, Madrid, Spain*

MP 253 **The Quantification of Thiophenols in Wine Using Liquid Chromatography Mass Spectrometry**; Liping Yang[1]; Tracy Onufer[1]; Jaewoo Choi[1]; Elizabeth Tomasino[1]; Jan F. Stevens[1]; Claudia S. Maier[1]; *[1]Oregon State University, Corvallis, OR*

MP 254 **Analysis of Cereulide in Food Using Triple Quadrupole Mass Spectrometer**; Saho Yoshioka[1]; Nozomi Maeshima[1]; Mattia Casanova[2]; Dominika Gruszecka[3]; Ruth Marfil-Vega[3]; Ryo Yamaguchi[1]; Yuka Fujito[4]; Manami Kobayashi[1]; *[1]SHIMADZU Corporation, Kawasaki, Japan; [2]Shimadzu Italia S.r.l., Milano, Italy; [3]Shimadzu Scientific Instruments, Columbia, MD; [4]Shimadzu Corporation, Kyoto, Japan*

MP 255 **Multi-Residue Pesticide Analysisin Norbixin colour additive oleoresin using GC-MS/MS**; Durvesh Sawant[1]; Rahul Dwivedi[1]; Prashant Hase[1]; Sanket Chiplunkar[1]; Hemant Kesarkar[1]; Jitendra Kelkar[1]; Pratap Rasam[1];

Dheeraj Handique[1]; Satyendra Singh[2]; Mohit Sharma[2]; *[1]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India; [2]Shimadzu Analytical (India) Pvt. Ltd., New Delhi, India*

MP 256 **Simultaneous analysis of siloxanes and synthetic musks in foods using selective biphasic concentration and gas chromatography mass spectrometry**; Woojin Jeong[1]; Sun Koung Joung[1]; Jeewon Lee[1]; Sang Beom Han[1]; *[1]College of Pharmacy, Chung-Ang University, Seoul, South Korea*

MP 257 **PFAS in Food LC-MS/MS Method Comparison - FDA and Nestlé Single Lab Validated Methods**; Manjula Sunkara[1]; Sussan Genualdi[1]; Lowri DeJager[1]; Andrew Savage[2]; Ashten Gibson[2]; Ashley Griffin[2]; Ernest Capraro[2]; *[1]FDA, College Park, MD; [2]Nestlé Quality Assurance Center, Dublin, OH*

MP 258 **Quantification and in vivo Decarboxylation of Cannabinoid Acid Precursors in Commercial Products Using LC-MS/MS**; Abiodun M Adewolu[1]; Cristian D. Gutierrez Reyes[1]; Moyinoluwa Adeniyi[1]; Md Mostofa Al Amin Bhuiyan[1]; Sherifdeen B Onigbinde[1]; Favour Chukwubueze[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock,, TX*

MP 259 **Targeted quantitation of milk and egg allergens in vegan foods**; Sabari Nathan[1]; Lakshmanan Deenadayalan[1]; Sashank Pillai[1]; Holly Lee[2]; Craig Butt[3]; Kendra Adams[4]; *[1]SCIEX - India, Bangalore, India; [2]SCIEX, Concord, ON; [3]SCIEX, Framingham, MA; [4]Sciex, Framingham, MA*

MP 260 **Multi-mycotoxin analysis in cereals and toddler food using a high-end triple quadrupole mass spectrometer**; Julie Brunkhorst[1]; Emilee Easter[1]; Holly Lee[2]; Craig Butt[3]; *[1]Trilogy Analytical Laboratory, Washington, MO; [2]SCIEX, Concord, ON; [3]SCIEX, Framingham, MA*

MP 261 **Quantitation of mycotoxins and tropane alkaloids in food using Triple Quadrupole and advanced technology**; Carlos Bueno[1]; Aidan Harrison[2]; Jianru Stahl-Zeng[3]; Gabriel Ruiz[4]; Lupi Martinez[4]; *[1]SCIEX Spain, Madrid, Spain; [2]SCIEX UK, Macclesfield, United Kingdom; [3]SCIEX, Darmstadt, Germany; [4]Eurofins Ecosur, Lorqui, Spain*

MP 262 **Identifying 4:2 Fluorotelomer Sulfonic Acid (4:2 FTS) Interferences in a Complex Food Matrix with High-Resolution Mass Spectrometry**; Brian Ng[1]; Christine M. Fisher[1]; Susan Genualdi[1]; Wendy Young[1]; Elsie Peprah[1]; Lowri De Jager[1]; *[1]U.S. Food and Drug Administration, College Park, MD*

MP 263 **Determination ofmulticlass residues in meat by green liquid phase microextraction and liquid chromatography-mass spectrometry**; Sandy SO Mookantsa[1, 2]; Rebagamang Tshepho[2]; Elsie D Moema[1]; Simiso Dube[3]; Mathew M Nindi[4]; *[1]University of South Africa, Johannesburg, South Africa; [2]National Agricultural Research and Development Institute, Gaborone, Botswana; [3]University of South Africa, Johannesburg, South Africa; [4]UNISA, Florida Park, Roodepoort, South Africa*

MP 264 **Deep Eutectic Solvent-Based Reverse Dispersive Liquid-Liquid Microextraction and LC-MS/MS determination of antimicrobial drug residues from animal kidneys**; Rebagamang Tshepho[1]; Sandy SO Mookantsa[2, 3]; Mesha Mbisana[4]; Simiso Dube[2]; Mathew M Nindi[5]; *[1]University of South Africa, Johannesburg, South Africa; [2]University of South Africa, Johannesburg, South Africa; [3]National Agricultural Research and Development Institute, Gaborone, Botswana; [4]University of Botswana, Gaborone, Botswana; [5]UNISA, Florida Park, Roodepoort, South Africa*

MP 265 **Black pepper authenticity analysis workflow with LC-QTOF and novel software solution**; Olivier Chevallier[1]; Nick Birse[2]; James Pyke[1]; Christopher Elliott[3]; *[1]Agilent Technologies, Santa Clara, CA; [2]Queen's University Belfast, Belfast, United Kingdom; [3]Thammasat University, Rangsit, Thailand*

MP 266 **Real-time SIFT-MS Monitoring for Safety and Quality in Spray Drying of Milk**; Emma Chachere[1]; Vaughan Langford[2]; Daniel Milligan[2]; *[1]Syft Technologies, Anaheim, CA; [2]Syft Technologies, Inc., Anaheim, CA*

MP 267 **High-Resolution Mass Spectrometric methods to detect and confirm 3ANX and NX producing Fusarium graminearum isolates in Western Canada**; Srinivas Sura[1]; Maria Antonia Henriquez[1]; Sean Walkowiak[2]; David A. Kaminski[3]; Anne Kirk[3]; Mark W. Sumarah[4]; Parthasarathy Santhanam[1]; Nina Kepeshchuk[1]; Jules Carlson[1]; E. RoTimi Ojo[3]; Pam De Rocquigny[3, 5]; Holly Derksen[3, 6]; *[1]Agriculture and Agri-Food Canada, Morden, MB; [2]Canadian Grain Commission, Grain Research Laboratory, Winnipeg, MB; [3]Manitoba Agriculture, Carman, MB; [4]Agriculture and Agri-Food Canada, London, ON; [5]Manitoba Crop Alliance, Carman, MB; [6]UPL AgroSolutions Canada, Guelph, ON*

MP 268 **Analysis of Chlordane by Electrospray Ionization-Liquid Chromatography Mass Spectrometry**; Sarah A Monti[1]; Jennifer Davis[1]; Valeria Zerda-Pinto[1]; Lihini Mendis[1]; Ethan R Hain[1]; Landon Wiest[1]; Christopher T. Gilles[1]; *[1]Shimadzu Scientific Instruments, Columbia, MD*

MP 269 **Characterizing protein sweetener interactions with saliva using crosslinking proteomics**; Sepideh Khaki Firooz[1]; Saiful Chowdhury[1]; *[1]University of Texas at Arlington, Arlington, TX*

MP 270 **Separation of PFAS in Drinking Water (EPA Method OTM-45), Food and Food Packaging by LC-MS/MS**; Stephan Altmaier[1]; Jack A. Wang[2]; Dean Duan[2]; *[1]Merck Life Sciences KGaA, Darmstadt, Germany; [2]Merck Chemicals Co., Ltd., Shanghai, China*

MP 271 **Mass Spectrometry Assisted Exploration of Synthetic Routes for a Recently Identified Arsenical Found in Rice Grain**; Bedraj Pandey[1]; Nicole L Walker[1]; Rachel D Dicken[1]; Kevin Kubachka[1]; *[1]FDA, Cincinnati, OH*

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MP 272 **Chemical attribution signature of organophosphorus pesticide chlorpyrifos syntheses by mass spectrometry-based untargeted metabolomics**; Carla Orlandi[1, 2]; Grégoire Delaporte[3]; Emmanuel Joubert[3]; Christine Albaret[3]; Anne Bossée[4]; Laurent Debrauwer[1, 2]; Emilien Jamin[1, 2]; *[1]Toxalim (Research Center in Food Toxicology), Université Toulouse III, INRAE, ENVT, INP-Purpan, Toulouse, France; [2]MetaboHUB-MetaToul, National Infrastructure of Metabolomics and Fluxomics, Toulouse, France; [3]Analytical Chemistry Department, DGA CBRN Defence, Vert-Le-Petit, France; [4]Chemistry Division, DGA CBRN Defence, Vert-Le-Petit, France*

MP 273 **DEVELOPMENT AND VALIDATION OF A QUANTIFICATION METHOD OF CANNABINOIDS BY UHPLC-MS**; João Victor Macedo de Almeida[1, 2]; Nathália S. Conceição[1, 2]; Alan Reinke Pereira[1, 2]; Marcos Valério V. Lyrio[1]; Rafael S. Ortiz[2, 3]; Nayara A. Dos Santos[1, 2]; Wanderson Romão[1, 2, 4]; *[1]Federal University of Espirito Santo, Vitoria, Brazil; [2]National Institute of Forensic Science and Technology, Porto Alegre, Brazil; [3]Regional Superintendence of the Federal Police Department in Rio Grande do Sul, Brazil, Porto Alegre, Brazil; [4]Federal Institute of Education, Science and Technology of Espírito Santo, Vila velha, Brazil*

MP 274 **LC-MS/MS Software for Identifying Controlled Substances: Utilizing Machine Learning Models, Molecular Networking, and a Variety of Database Search Algorithms**; So Yeon Lee[1]; Han Bin Oh[1]; *[1]Sogang University, Seoul, South Korea*

MP 275 **Using the New Stellar Mass Spectrometer to Confirm and Quantify 31 Drugs of Abuse, Including THC, in Oral Fluid**; Courtney Patterson[1]; Kerry Hassell[1]; Jingshu Guo[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

MP 276 **Hand-held Ion Mobility Spectrometer for in-situ and real-time Drug-added Food Detection**; Chung-Hsuan Chen[1]; Sheng-Ta Tsai[2]; Ju Yao Chang[2]; Jung Lee Lin[2]; Kuan Ju Lin[2]; *[1]Genomic Research Center, Taipei,, Taiwan; [2]Academia Sinica, Taipei, Taiwan*

MP 277 **Characterizing the reproducibility of ambient ionization mass spectral measurements of seized drug samples: An interlaboratory study**; Arun S Moorthy[1]; Dennis Leber[2];

Edward Sisco[2]; [1]*Trent University, Peterborough, ON;* [2]*National Institute of Standards and Technology, Gaithersburg, MD*

MP 278 **Developing a Substrate Spray Mass Spectrometry-Based Method for Processing Fingernail Scraping Evidence for Exogenous Chemical Screening**; Madelynn G. Anderson[1]; Makenna S. Klann[1]; Emily J. Wiggins[1]; Christopher Mulligan[1]; [1]*Illinois State University, Normal, IL*

MP 279 **Rapid, Direct Screening of Opioids from Unwashed Poppy Seeds with 3D-Printed Cone Spray Ionization-Mass Spectrometry (3D-PCSI-MS)**; Emily J. Wiggins[1]; Blaise R. Jones[1]; Kingsley Nwaiwu[1]; Jamie R. Wieland[1]; Patrick W. Fedick[2]; Christopher Mulligan[1]; [1]*Illinois State University, Normal, IL;* [2]*Naval Air Warfare Center, Weapons Division, China Lake, CA*

MP 280 **Forensic hair analysis of illicit drugs using a sequential TOF MS, DDA-MS/MS and DIA-MS/MS method combining quantitative and qualitative workflows**; Benjamin Barrett[1]; Alan Barnes[2]; Emily G. Armitage[2]; Chloe Hutton[2]; Simon Ashton[2]; Ethan Webster[1]; Neil J. Loftus[2]; [1]*AttoLife, Scottow Enterprise Park, Norwich, United Kingdom;* [2]*Shimadzu Corporation, Manchester, United Kingdom*

MP 281 **Screening for unknowns in assessing emerging threats and new developments in the use of illicit drugs**; Emily G Armitage[1]; Chris Bowen[2]; Alan Barnes[1]; Chloe Hutton[1]; Simon Ashton[1]; Neil J Loftus[1]; John Fitzgerald[3]; [1]*Shimadzu Corporation, Manchester, United Kingdom;* [2]*Shimadzu Scientific Instruments, Melbourne, Australia;* [3]*School of Social and Political Sciences, The University of Melbourne, Melbourne, Australia*

MP 282 **Species identification of the DNA-degraded blood drop in the complex matrices by nanoLC-MS/MS**; Katarzyna Staniszewska[1]; Malgorzata Hopcias[1]; Paulina Kret[1]; Piotr Suder[1]; [1]*AGH University of Krakow, Krakow, Poland*

MP 283 **Steroids, stimulants, and transgenes – Mass spectrometry as the common denominator in sports drug testing analytical approaches**; Mario Thevis[1]; Thomas Piper[1]; Oliver Krug[1]; Nana Naumann[1]; [1]*German Sport University, Cologne, Germany*

MP 284 **Untargeted Nitrocellulose Profiling of Smokeless Powders by LC-MS to Determine Geographical Origin**; Samuel G Moore[1]; David A. Gaul[1, 2]; Roman Aranda[3]; Eric J. Pooser[3]; Facundo M. Fernández[1, 2]; [1]*Systems Mass Spectrometry Core, Parker H. Petite Institute for Bioengineering and Biosciences, Georgia Institute of Technology, Atlanta, GA;* [2]*School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA;* [3]*Advanced Concepts Laboratory, Georgia Tech Research Institute, Atlanta, GA*

MP 285 **Collision-induced Dissociation of Protonated Phenethylamine: A Model Study to Aid Peak Annotation in Tandem Mass Spectrometry of Illicit Drugs**; Amina Ihabi[1]; Samuel J. Lenze[1]; Justin G Terhorst[1]; Giel Berden[2]; Jonathan Martens[2]; Jos Oomens[2]; Theodore A Corcovilos[1]; Michael J Van Stipdonk[1]; [1]*Duquesne University, Pittsburgh, PA;* [2]*Radboud University, Nijmegen, Netherlands*

MP 286 **Discovery of Novel Protein Biomarkers for the Identification of Seminal Fluid in Sexual Assault Evidence**; Shelby Morgan[1]; Francis Diamond[2]; Fabio Oldoni[1]; Phillip Danielson[3]; Christian Westring[4]; Kevin Legg[5]; [1]*Arcadia University, Glenside, PA;* [2]*The Center for Forensic Science Research & Education, Willow Grove, PA;* [3]*University of Denver, Denver, CO;* [4]*Niagara County Sheriff's Office, Lockport, NY;* [5]*Protein Metrics, Boston, MA*

MP 287 **Enhancing Forensic Compound Identification: Software-Assisted Approaches in the SWGDRUG Mass Spectral Reference Library**; Weihua Ji[1]; William E. Wallace[1]; [1]*NIST, Gaithersburg, MD*

MP 288 **MALDI-MS and DESI-IM-MS Analysis of Smokeless Powders for Classification by Manufacturer**; David Lewis[1]; Facundo M Fernandez[1]; Xin Ma[2]; [1]*Georgia Institute of Technology, Atlanta, GA;* [2]*University of Virginia, Charlottesville, VA*

MP 289 **Trace Analysis of Alpha-Amanitin in Human Urine: Implications for Poisoning Detection**; Roma Perłowska[1]; Rafał Szewczyk[1]; Katarzyna Krupczyńska-Stopa[1]; Maciej Stopa[2]; Adrian Soboń[1]; Anastasiia Shyian[1]; [1]*LabExperts sp z o.o., Lodz, Poland;* [2]*Bioanalytic Sp. z o.o., Gdańsk, Poland*

MP 290 **HazarDust: Real-Time Detection of Hazardous Dust Particles Using Single-Particle Mass Spectrometry (SPMS) for Security and Environmental Applications**; Sven Ehlert[1]; Robert Irsig[1]; Johannes Passig[1, 2]; Andreas Walte[1]; Ralf Zimmermann[2]; [1]*Photonion GmbH, Schwerin, Germany;* [2]*University of Rostock, Chair of Analytical Chemistry and Dept. of Life, Light and Matter, Rostock, Germany*

MP 291 **Wastewater Surveillance of 68 Novel Psychoactive Substances and Conventional Drug Use in Taipei Metropolitan Area, Taiwan, Before and After COVID-19**; Te-Tien Ting[1]; Pin-Chuan Chen[2]; Ya-Chi Chang[3]; Pin-Ju Chiang[3]; Hsu-Cheng Li[3]; Shih-Hsun Chen[3]; Yi-Hsin Liu[4]; Pai-Shan Chen[3]; [1]*Department of Data Science, School of Big Data Management, Soochow University, Taipei, Taiwan, Taipei, Taiwan;* [2]*Department of Mechanical Engineering, National Taiwan University of Science and Technology, Taipei, Taiwan, Taipei, Taiwan;* [3]*Institute of Toxicology, School of Medicine, National Taiwan University, Zhongzheng District, Taiwan;* [4]*Department of Chemistry, National Taiwan Normal University, Wenshan District, Taiwan*

MP 292 **Testing Explosives and Narcotics Detection Performance on a Novel Ambient Desorption Ionization Compact Single Quadrupole Mass Spectrometer**; Cynthia M. Suarez[1]; Daniel Eikel[1]; Changtong Hao[1]; Jimmie C. Oxley[2]; Michael Chapman[2]; [1]*Advion Interchim Scientific, Ithica, NY;* [2]*University of Rhode Island, Kingston, RI*

MP 293 **Rapid Detection of Explosives, Drugs, Pesticides, and Chemical Warfare Simulants Using Portable Ion Trap Mass Spectrometry with Ambient Ionization**; Venkat Panchagnula[1]; Caleigh O'Connor[1]; Vishal Mahale[2]; Oscar Cabrices[3]; [1]*MassTech Inc., Columbia, MD;* [2]*Barefeet Analytics Private Limited, 100 NCL Innovation Park, Dr. Homi Bhabha Road, Pune, India;* [3]*G-Flo Scientific, Miramar, FL*

MP 294 **Combining DART ionization and trapped ion mobility QTOF mass spectrometry for the analysis of controlled substances**; Ilona Nordhorn[1]; Leon Groeschel[1, 2]; Birgit Schneider[1]; Ben Yong[3]; Carsten Baessmann[1]; [1]*Bruker Daltonics GmbH & Co. KG, Bremen, Germany;* [2]*University of Muenster, Muenster, Germany;* [3]*Bruker Scientific LLC, Billerica, MA*

MP 295 **Comparison of CID, AIF, and IS-CID Activation for the Identification of Nitazene Analogs Using DART Ionization and the NIST DIT**; Emma K. Hardwick[1]; Alleigh N. Couch[1]; J. Tyler Davidson[1]; [1]*Sam Houston State University, Huntsville, TX*

MP 296 **Utilization of Copper Salts to Induce the Formation of Cannabinoid Molecular Ions Enabling Isomer Differentiation**; Alleigh N. Couch[1]; Christopher M. Zall[1]; J. Tyler Davidson[1]; [1]*Sam Houston State University, Huntsville, TX*

MP 297 **Beyond Fingerprint Pattern Evidence: Chemical Imaging of Fingerprints using Laser Mass Spectrometry**; Julia X Morelli[1]; Tessa Monroe[1]; Kenyon Evans-Nguyen[1]; [1]*The University of Tampa, Tampa, FL*

MP 298 **Rapid and reliable DART-MS based screening for benzodiazapenes in urine: calibration, validation, and cross-correlation study**; Terry L Bates[1]; Alex Maggitti[2]; Francois A Espourteille[3]; [1]*Quantera Analytical, Freeville, NY;* [2]*Drug Scan, Horsham, PA;* [3]*Bruker Scientific LLC, Billerica, MA*

MP 299 **In-Field Qualitative and Quantitative Analysis of Illicit Drugs By DART-TOF-MS and DART-QQQ in a Mobile Laboratory Environment**; Edward Sisco[1]; Elizabeth L. Robinson[1]; Thomas P. Forbes[1]; Elise M. Pyfrom[1]; Meghan

G. Appley[1]; Sarah A. Shuda[1]; *[1]National Institute of Standards and Technology, Gaithersburg, MD*

MP 300 **Differentiation of Hair from Individuals with Similarly Colored Light Hair Using Amino Acid Ratios Obtained from GC-MS Analysis**; Emma Brownlie[1]; Timothy Yaroshuk[1, 2]; Robert Powers[1]; Alyssa Marsico[1]; *[1]University of New Haven, West Haven, CT; [2]New Jersey Institute of Technology, Newark, NJ*

MP 301 **Hint in the Print: The application of high-resolution mass spectrometry for the determination of Cannabis-use biomarkers in fingerprint residues**; Niara A Nichols[1]; Rabi A Musah[1]; *[1]Louisiana State University, Baton Rouge, LA*

MP 302 **Source Attribution of Fentanyl via Metals Analysis using ICP-MS/MS**; Edward Bentil[1]; Brian A Eckenrode[1]; Marie Rose Taylor[1]; Mehdi Moini[2]; *[1]George Mason University, Manassas, VA; [2]Picolytics, McLean, VA*

MP 303 **Detection of Volatile Organic Compounds from Lithium-Ion Batteries using GC-MS**; Samuel R DeNight[1]; Brian A. Eckenrode[2]; *[1]University, Manassas, VA; [2]George Mason University, Manassas, VA*

MP 304 **Investigating Odor Signatures of Electronic Storage Devices**; Samuel Friday[1]; Jon Naples[2]; Pauline E Leary[3]; Marisia Fikiet[1]; Alyssa Marsico[1]; Brooke W Kammrath[1]; *[1]University of New Haven, West Haven, CT; [2]Connecticut State Police, Meriden, CT; [3]Noble, Stevensville, MD*

MP 305 **Characteristic GC/MS and DART-MS Spectra for the Detection of of Fatty Acid-based Ignitable Liquid Residues**; Mengliang Zhang[1]; Wen Dong[1]; *[1]Ohio University, Athens, OH*

MP 306 **Developing a method for the analysis of products claiming to treat COVID-19**; Christopher S. Poulos[1]; Travis M. Falconer[2]; Michael D. Thatcher[2]; Adam C. Lanzarotta[2]; Martin M. Kimani[3]; *[1]Oak Ridge Institute for Science and Education, Oak Ridge, TN; [2]US Food and Drug Administration, National Forensic Chemistry Center, Cincinnati, OH; [3]US Food and Drug Administration, Office of Inspections and Investigations, Cincinnati, OH*

MP 307 **Improving compound identification using data-independent acquisition**; David Cox[1]; Hieu Cuong Le[1]; Gordana Ivosev[1]; Nic Bloomfield[1]; *[1]SCIEX, Concord, ON*

MP 308 **Comprehensive Toxicology and TDM by DBS**; Ken Lewis[1]; Robert Wurm[1]; Dana Danger[1]; Salvador Valldeperas[1]; *[1]OpAns, LLC, Durham, NC*

MP 309 **Effect of GC/MS Liner Characteristics on the Analysis of LSD and LSD Analogs**; Sarah A Shuda; *NIST, Gaithersburg, MD*

MP 310 **A Promising Cutting-Edge Multi-Omics Approach for Analyzing Crude Extracts of Ricinus Communis Toxic Seeds Using LC-HRMS/MS for Forensics Investigations.** ; Benoit COLSCH[1]; Kodjo Nouwade[1]; Sylvia Worbs[2]; François Becher[1]; Brigitte Dorner[2]; Eric Ezan[1]; François Fenaille[1]; *[1]Université Paris-Saclay, CEA, INRAE, Département Médicaments et Technologies pour la Santé (MTS), MetaboHUB,, Gif-sur-Yvette, France; [2]Biological Toxins (ZBS 3), Robert Koch Institute, Berlin, Germany*

MP 311 **Determination of 58 abused drugs in a single hair on SCIEX Triple Quad™ 7500+ System**; Chong Zhang[1]; Xiaojie Sun[1]; Bingjie Liu[1]; Zong Yang[1]; Lihai Guo[1]; *[1]SCIEX CHINA Support Center, Shanghai, China, Shanghai, China*

FUNDAMENTALS: ION SPECTROSCOPY
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MP 312 **Structure elucidation in MALDI and MS-imaging using infrared ion spectroscopy**; Jos Oomens[1]; Jelle Schuurman[2]; Lara Van Tetering[2]; Kas J. Houthuijs[3]; Giel Berden[2]; Udo F.H. Engelke[4]; Dirk J. Lefeber[4]; Ron A. Wevers[4]; Michiel Vandenbosch[5]; Ron M. A. Heeren[5]; Jonathan Martens[2]; *[1]Radboud University Nijmegen, Nijmegen, Netherlands; [2]Radboud University, Nijmegen, Netherlands; [3]Vrije Universiteit Amsterdam, Amsterdam, Netherlands; [4]Radboud University Medical Center, Nijmegen, Netherlands; [5]Maastricht University, Maastricht, Netherlands*

MP 313 **The Impact of Metal Ion Binding Motifs on Energy Transfer Efficiency of Gas-Phase tmFRET**; Ceyuan Zheng[1, 2]; Lukas Raphael Benzenberg[2]; Ri Wu[2]; Kim Greis[2]; Renato Zenobi[2]; *[1]University of Zurich, Zurich, Switzerland; [2]ETH Zurich, Zurich, Switzerland*

MP 314 **Cryogenic-Ion Infrared Action Spectroscopy of UNCG RNA Tetraloops**; Maleesha T. Fernando[1]; Madeline Schultz[1]; América Y. Torres-Boy[2]; Katja Ober[2]; Nwanne D. Banor[1]; Gert Von Helden[2]; Daniel A. Thomas[1]; *[1]University of Rhode Island Chemistry Department, Kingston, RI; [2]Fritz Haber Institute of the Max Planck Society, Berlin, Germany*

MP 315 **Gas-Phase Photoelectron Spectroscopy and Reactivity of the Phenylacetylide PhCC-and Copper Bis(phenylacetylide) [Cu(CCPh)2]-Anions**; Howard Z. Ma[1]; Wenjin Cao[2]; Yufei Xie[1]; Xue-Bin Wang[2]; Richard A. J. O'Hair[3]; *[1]The University of Melbourne, Parkville, Australia; [2]Pacific Northwest National Laboratory, Richland, WA; [3]The University of Melbourne, Parkville, Australia*

MP 316 **Best Bang for Your Buck: Meta-analysis of computational methods for predicting IR spectra in small uranium molecular ions**; Theodore Corcovilos[1]; Chloe Bassil[1]; Jonathan K Martens[2]; Giel Berden[2]; Jos Oomens[2]; Samuel J Lenze[1]; Justin G Terhorst[1]; Michael J Van Stipdonk[1]; *[1]Duquesne University, Pittsburgh, PA; [2]Radboud University, Nijmegen, Netherlands*

MP 317 **Sodiated cyclophosphamide fragmentation pattern evaluation by mass spectrometry and helium nanodroplets ion spectroscopy**; Guilherme Obeid[1, 2]; América Torres[2]; Katja Ober[2]; Gert Von Helden[2]; Thiago Correra[1]; *[1]Institute of Chemistry of the University of São Paulo, São Paulo, Brazil; [2]Fritz Haber Institute of the Max Planck Society, Berlin, Germany*

MP 318 **Isomer Characterization Beyond Mass Spectrometry: Vibrational Structures of Ortho-, Meta-, and Para-cyanophenol Anions and Thermochemistry of the Three Cyanophenol Isomers**; Wilson Gichuhi[1]; Lucia Vargas[1]; *[1]Tennessee Tech University, Cookeville, TN*

MP 319 **Exploring the Inter- and Intramolecular Interactions of Phase-Separating Dipeptide Coacervates Using Infrared Action Spectroscopy**; Nwanne D Banor[1]; Katja Ober[2]; América Torres-Boy[2]; Jenna E Lees[1]; Gert Von Helden[2]; Daniel A. Thomas[1]; *[1]University of Rhode Island Chemistry Department, Kingston, RI; [2]Fritz Haber Institute of the Max Planck Society, Berlin, Germany*

FUNDAMENTALS: IONIC CLUSTERS, NANOMATERIALS, AND CATALYSIS
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MP 320 **Potential Magic Numbers of Lithium Oxalate Clusters from Electrospray Ionization**; Secillia Tram[1]; Mike McCallum[1]; *[1]University of the Pacific, Stockton, CA*

MP 321 **Matrix-Free Laser Desorption/Ionization Mass Spectrometry of Bismuth Salts: Fragmentation Patterns Provide Structural Insights**; Chanbopha Tho[1]; Daniil G Ivanov[2]; Igor A. Kaltashov[2]; *[1]University of Massachusettes, Amherst, MA; [2]University of Massachusetts Amherst, Amherst, MA*

MP 322 **Investigation of Structural Motifs in Glycol/Quaternary Ammonium Halide Deep Eutectic Solvents by Ion Infrared Action Spectroscopy**; Miyuru M. Wellalage[1]; Maleesha T. Fernando[1]; América Y. Torres-Boy[2]; Katja Ober[2]; Gert Von Helden[2]; Daniel A. Thomas[1]; *[1]University of Rhode Island Chemistry Department, Kingston, RI; [2]Fritz Haber Institute of the Max Planck Society, Berlin, Germany*

MP 323 **Ambient catalyst-free conversion of methane to methanol by water radical cations**; Xiaoping Zhang[1]; Huanwen Chen[2]; *[1]East China University of Technology, Jiangxi Key Laboratory for Mass Spectrometry and Instrumentation, Nanchang, China; [2]Jiangxi University of Chinese Medicine, Nanchang, China*

FUNDAMENTALS: IONIZATION
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MP 324 **Optimization of spray and solvent conditions for functional oligonucleotide analysis by cVSSI-MS**;

Chandrima Banerjee[1]; Thomas Hughart[1]; Vikum K. Dewasurendra[2]; Matthew B. Johnson[2]; Peng Li[1]; Stephen J. Valentine[1]; *[1]Department of Chemistry, West Virginia University, Morgantown, West Virginia; [2]Department of Physics, West Virginia University, Morgantown, West Virginia*

MP 325 **Silver Coated Microcapillaries in a Contained ESI Source Provide Enhanced Analyte Ionization and Expand the Repertoire of Microdroplet Condensation Reactions**; Adam J Reed[1]; Abraham K. Badu-Tawiah[2]; *[1]The Ohio State University, Columbus, OH; [2]Ohio State University, Columbus, OH*

MP 326 **Dynamic Plasma-in-Droplet Ionization for Liquid Chromatography-Mass Spectrometry**; Purva S. Damale[1]; Dmytro S. Kulyk[1]; Alexander P. Zumock[1]; Abraham K. Badu-Tawiah[1]; *[1]Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH*

MP 327 **Protein Signal Enhancements with Polar Organic Ester Vapor Addition in Desorption and Electrospray Ionization**; Christopher Taylor[1]; Andre R Venter[1]; *[1]Western Michigan University, Kalamazoo, MI*

MP 328 **Ionization Efficiency of Intact Proteins in LC-ESI, nanoESI, and femtoESI**; Ian T Ferraro[1]; Tolulope Idiat Ogunsanya[1]; Kanwal Jeet[1]; Nathan Kenyon[1]; Anyin Li[1]; *[1]University of New Hampshire, Durham, NH*

MP 329 **Evaluating a next generation ion source for proteomics**; Dong-Gi Mun[1]; Benjamin J. Madden[1]; Steven Draper[1]; Kiran Kumar Mangalaparthi[2]; Joshua A Silveira[3]; Daniel Jackson[3]; Katherine Walker[4]; Eloy R. Wouters[3]; Cornelia Boeser[4]; Akhilesh Pandey[1]; *[1]Mayo Clinic, Rochester, MN; [2]Mayo Clinic, Rochester; [3]ThermoFisher Scientific, San Jose, CA; [4]Thermo Fisher Scientific, San Jose, California*

MP 330 **Submerged Electrospray: Charge Transfer in Liquid Environments**; Cristian A. Blanco-Combariza[1]; Jeffrey E Dick[2]; *[1]Purdue University, West Lafayette, IN; [2]Purdue Univeristy, West Lafayette, IN*

MP 331 **Analysis of Individual Non-Summed TOF Mass Spectra: Comparing Aspirated ESI Droplet Signatures with APCI**; Chris Vico Heintz[1]; Walter Wissdorf[1]; Hendrik Kersten[1]; Thorsten Benter[1]; *[1]University of Wuppertal, Wuppertal, Germany*

MP 332 **Superoxide radical anion oxidative ionization in negative LDTD-MS/MS analysis of Serotonin**; Sylvain Letarte[1]; Jonathan Rochon[2]; Mégane Moreau[2]; Sarah Demers[2]; Serge Auger[2]; Pierre Picard[2]; Jean Lacoursière[2]; *[1]Ingenio, Calgary, Alberta; [2]Phytronix Technologies, Quebec, QC*

MP 333 **Charge Monitoring of Electrosprayed Methanol and Micrometer-sized Polystyrene droplets at ambient temperature**; Shao-Yu Liang[1]; Shiu-Yao Yeh[1]; Wei-Chun Chiu[1]; Avinash A Patil[1]; Wen-Ping Peng[1]; *[1]National Dong Hwa University, Shoufeng, Taiwan*

MP 334 **Characterization of the Dynamic Behavior of Charged Aspirated Droplets and Their Fragments within the SelexIon DMS Cell**; Patricia Itzenhäuser[1]; Walter Wissdorf[1]; Thorsten Benter[1]; Hendrik Kersten[1]; *[1]University of Wuppertal, Wuppertal, Germany*

MP 335 **Development of a vendor agnostic, optical fiber based IR-MALDESI interface for high throughput sample analysis**; Jonathan Wingfield[1]; Adria Escobet Montalban Escobet Montalban[1]; *[1]TTP Plc, Royston, United Kingdom*

MP 336 **Evaluation of hydrophobic emitters on sensitivity and reproducibility of electrospray ionization-mass spectrometry-based proteomics**; Ha T. H. Cung[1]; Adam J. Cusick[1]; Joseph P. Thekkekkara[1]; Ralf Schittenhelm[2]; Scott Blundell[2]; *[1]Trajan Scientific and Medical, Ringwood, Australia; [2]Monash University, Clayton, Australia*

GC/MS: INSTRUMENTATION AND APPLICATIONS
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MP 337 **Pushing the Limits of Sample Identification by GC-MS with Cold EI**; Aviv Amirav[1]; Benny Neumark[2]; Oneg Elkabets[2]; Alex Yakovchuk[2]; *[1]Tel-Aviv University, Tel-Aviv, Israel; [2]Tel Aviv University, Tel Aviv, Israel*

MP 338 **From Uncertainty to Clarity: See with Cold EI What You Are Missing with Standard EI**; Alex Yakovchuk[1]; Aviv Amirav[1]; *[1]Tel Aviv University, Tel Aviv, Israel*

MP 339 **Advancing Phthalates and Mixed Alkyl Phthalates Analysis in Plastics Using GC-MS with Cold EI**; Oneg Elkabets[1]; Benny Neumark[1]; Aviv Amirav[1, 2]; *[1]Tel Aviv University, Tel Aviv, Israel; [2]Aviv Analytical, Hod Hasharon, Israel*

MP 340 **Development of non-targeted analytical method for comprehensive 2-dimensional gas chromatography using high-resolution mass spectrometry and machine learning**; Masaaki Ubukata[1]; Azusa Kubota[1]; Takuhiro Hizume[1]; Haruki Ishioka[1]; Ayumi Kubo[1]; *[1]JEOL Ltd., Tokyo, Japan*

MP 341 **Screening of volatile organic compounds (VOC's) in 'e-liquids' using atmospheric pressure gas chromatography coupled to a high resolution mass spec**; Chris Henry[1]; Joanne Ballantyne[2]; *[1]Waters Corportaion, Cheshire, United Kingdom; [2]Waters Corporation, Wilmslow, United Kingdom*

MP 342 **Toward Automated Solutions for Higher Confidence Identification with Combined EI and CI HR-TOFMS Data**; Craig Fowler[1]; Albert Lebedev[2]; Viatcheslav Artaev[1]; *[1]LECO, St. Joseph, MI; [2]Shenzhen MSU-BIT University, Shenzhen, China*

MP 343 **An automated approach for the analysis of VOCs in drinking and surface water by using a VOC Sample Prep Station**; Andy Fornadel[1]; Adam Ladak[2]; Jason Cole[3]; Rick Phillips[3]; Jerry Holycross[3]; Matthew Menesini[3]; Amit Gujar[3]; Giulia Riccardino[4]; Daniela Cavagnino[4]; Manuela Bergna[4]; Xin Zheng[3]; *[1]Thermo Scientific, Bannockburn, IL; [2]Thermo Scientific, Macclesfield, United Kingdom; [3]Thermo Fisher Scientific, San Jose, CA; [4]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

MP 344 **Streamlined untargeted workflow for priority and unknown pollutant identification in industrial stack particulate by GC-Orbitrap high resolution mass spectrometry**; Dominic Roberts[1]; Xin Zheng[2]; Nick Warner[3]; Kjell Hope[4]; Jason Cole[5]; *[1]Thermo Fisher Scientific, Runcorn, United Kingdom; [2]Thermo Fisher Scientfic, San Jose, CA; [3]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [4]Pacific Rim Laboratories, Vancouver, BC; [5]Thermo Fisher Scientific, 355 River Oaks Pkwy, San Jose, CA95134*

MP 345 **Non-targeted analysis of whisky using SPME Arrow and Orbitrap Exploris GC 240 mass spectrometer**; Dominic Roberts[1]; Jason Cole[2]; Xin Zheng[2]; Nick Warner[3]; Andy Fornadel[4]; *[1]Thermo Fisher Scientific, Runcorn, United Kingdom; [2]Thermo Fisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [4]Thermo Fisher Scientific, Rockford, IL*

MP 346 **Gas Chromatography-Mass Spectrometry Evaluation of Chemical Compounds in Perfumes Across the Market**; Gianna Anguiano[1]; Danna Aguirre[1]; Araceli Nunez[2]; Sophia Hernandez[1]; Stephanie Garcia[1]; Karen L. Lohnes[1]; *[1]Huntington Park Institute of Applied Medicine at Linda Marquez HS, Huntington Park, CA; [2]California State University, Long Beach, Long Beach, CA*

MP 347 **GC-APCI-MS/MS Analysis of Polychlorinated Dibenzo-p-dioxins and Furans to Revised US EPA1613 Guidelines**; Gareth Rhys Jones[1]; David Douce[1]; Douglas Stevens[2]; Ignatius J Kass[2]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Waters Corporation, Milford, MA*

MP 348 **Performance comparison of different GC-HRMS analytical methods for quantitation of fragrance allergens in perfume concentrates**; Aurélien Cuchet[1]; Christian-Sebastiano TOPPI[1]; Thierry Bernard[2]; Tatiana Cucu[3]; Franck David[3]; Christophe Mauduit[1]; *[1]L'Oréal, CHEVILLY LARUE, France; [2]L'Oréal Research and Innovation, Aulnay-sous-Bois, France; [3]Research Institute for Chromatography, Kortrijk, Belgium*

MP 349 **From Extraction to Detection: The Synergy of Acetonitrile-Ethyl Acetate Mixtures in Advanced**

Multiresidue Analysis by GC-MS/MS; José Antonio Martínez[1]; José Luis Oller-Serrano[1]; Victor Manuel Cutillas[1]; Amadeo R. Fernández-Alba[1]; María Dolores Hernando[2]; *[1]European Union Reference Laboratory for Pesticide Residues in Fruits & Vegetables, Almería, Spain; [2]CSIC Spanish Research Council, Almería, Spain*

MP 350 **A Highly Sensitive Approach for Analysis of PFAS in Water Using Vacuum Assisted Sorbent Extraction and GCMS**; Daniel Cardin; *Entech Instruments, Simi Valley, CA*

MP 351 **Ensuring drinking water quality through a single method of VOCs analysis and taste- and odor-causing substances**; Ana C Martimiano[1]; Isabela De Oliveira E Silva[1]; Rodrigo Ossamu Saga Kitamura[1]; *[1]Shimadzu do Brasil, Barueri, Brazil*

MP 352 **Highly sensitive and efficient analysis of aroma components using trapped Headspace GC-MS**; Ana C Martimiano[1]; Isabela De Oliveira E Silva[1]; Rodrigo Ossamu Saga Kitamura[1]; *[1]Shimadzu do Brasil, Barueri, Brazil*

MP 353 **Analysis of allergens in fragrance samples using a comprehensive GCxGC in combination with a high-resolution mass spectrometry**; Sofia Nieto[1]; Matthew Curtis[1]; Nick Harden[1]; *[1]Agilent Technologies, Inc., Santa Clara, CA*

MP 354 **Unveiling VOC Complexity: High-Resolution Quantitation with GC-EI-Orbitrap**; Justin Y Elliott[1]; Priya Viathee[2]; Bashar Amer[2]; Susan S Bird[2]; Hussain Abdulla[1]; *[1]Department of Physical and Environmental Sciences, Texas A&M University Corpus Christi, Corpus Christi, TX; [2]Thermo Fisher Scientific, San Jose, CA*

MP 355 **Workflows for Non-Target Investigation of Battery Electrolyte Solutions by Gas Chromatography Coupled to Nominal Mass and High-Resolution Time-of-Flight Mass Spectrometry**; Christina N Kelly[1]; Joe Binkley[1]; Martin R Trujillo[2]; Bicy Kottathodi[2]; Wan Si Tang[2]; Judith A Jeevarajan[2]; *[1]Leco Corporation, St. Joseph, MI; [2]UL Research Institutes - Electrochemical Safety Research Institute, HOUSTON, TX*

MP 356 **Chemical profiling of cannabinoid hemp products using multidimensional gas chromatography-time-of-flight mass spectrometry (GC×GC-TOFMS)**; Sarah Prebihalo; *U.S. Food and Drug Administration, College Park, MD*

MP 357 **Hydrogen as the Future of GC-MS – Revolutionizing Carrier Gas Solutions**; Reuven Mery; *M. Snir Ltd, K. Ata, Israel*

MP 358 **Optimizing Hydrogen Carrier Gas on GC/MS Using the HydroInert EI Source and Q Columns**; Samuel Haddad[1]; Paul Tripp[1]; Alex Graettinger[2]; *[1]Agilent Technologies, Wilmington, DE; [2]Agilent Technologies, Inc., Wilmington, Delaware*

MP 359 **Analysis of Phthalates Using GC/MS With Hydrogen Carrier Gas: The Importance of Reducing Interferences and Contamination**; Bruce Quimby[1]; Anastasia Andrianova[1]; Eric Fausett[1]; *[1]Agilent Technologies, Inc., Wilmington, Delaware*

MP 360 **Improved Determination of Polychlorinated Biphenyl Compounds by US EPA Method 1628**; Jennifer Sanderson; *Agilent Technologies, Inc., Wilmington, DE*

MP 361 **Full Evaporative Vacuum Extraction (FEVE) – Greater Sensitivity, Wider Analyte Range, and Cleaner GC-MS Injection than Large Volume Liquid Injection**; VICTORIA VOGEL[1]; Daniel B. Cardin[2]; Weier Hao[2]; *[1]Entech Instruments, Simi Valley, CA; [2]Entech Instruments, Simi Valley, California*

MP 362 **Optimized GC/MS/MS Analysis of Semi-volatile Organic Compounds (sVOCs) concurrent with Organochlorine Pesticides using hydrogen carrier gas**; Johnny Mitchell[1]; Bill Mock[1]; Eric Fausett[2]; Anastasia Andrianova[2]; Bruce Quimby[2]; *[1]Pace Analytical, Roseville, MN; [2]Agilent Technologies, Inc., Wilmington, Delaware*

MP 363 **Beyond the Ion Source: Optimizing GC/MS Sensitivity with Capillary Chromatography**; Vanessa Abercrombie[1]; Ashlee Gerardi[2]; Gustavo Serrano-Izaguirre[2]; Rick Lake[2]; Amanda McQuay[2]; *[1]Agilent Technologies, Folsom, CA; [2]Agilent Technologies, Inc., Wilmington, Delaware*

MP 364 **Chip-Scale Mass Spectrometry for Point-of-Care Breath Diagnostics**; Spiros Manolakos[1]; Dustin McRae[1]; Ashish Chaudhary, Ph.D. [1]; *[1]Detect-ION, Tampa, FL*

MP 365 **Optimizing the Efficiency and Productivity of GC/MS workflows to Improve Laboratory Sustainability** ; Ashlee M Gerardi[1]; Vanessa Abercrombie[2]; Gustavo Serrano-Izaguirre[2]; Rick Lake[2]; *[1]Agilent, WILMINGTON, DE; [2]Agilent Technologies, Inc., Wilmington, Delaware*

MP 366 **Developing a Combined System with Diffusive Sorbent Pen Thermal Desorption and Canister Preconcentrator for Analysis of VOCs in Ambient Air**; Weier Hao[1]; Daniel B. Cardin[1]; Victoria Vogel[1]; Daniel J. Cardin[1]; *[1]Entech Instruments, Simi Valley, CA*

MP 367 **Unusual Rearrangements in the Electron Ionization Mass Spectra of Silylated Per- and Polyfluoroalkyl Compounds**; Yufang Zheng[1]; Edward Erisman[1]; Weihua Ji[1]; Quanlong Pu[1]; Stephen E. Stein[1]; William E Wallace[1]; *[1]NIST, Gaithersburg, MD*

MP 368 **The versatility of Sliding Window in Ion Mobility-Mass Spectrometry for targeted and non-targeted analysis of chemicals of emerging concern**; Gauthier Eppe[1]; Hugo B Muller[1]; Johann Far[1]; Georges Scholl[1]; Edwin De Pauw[1]; *[1]Liege University, Liège, Belgium*

MP 369 **Automated analysis of combined CI and EI mass spectral data for enhanced compound identification**; Steffen Bräkling[1]; Eliska Ceznerova[1]; Sonja Klee[1]; *[1]TOFWERK, Thun, Switzerland*

GLYCOPROTEINS I
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MP 370 **PNGaseF-generated N-glycans adduct onto peptides in the gas phase**; Joann Chongsaritsinsuk[1]; Valentina Rangel-Angarita[1]; Keira E. Mahoney[1]; Lea Kim[1]; Ryan J. Chen[1]; Akua A. Appah-Sampong[2]; Isabella P. Tran[1]; Alexandra D. Steigmeyer[1]; Marie A. Hollenhorst[2]; Stacy A. Malaker[1]; *[1]Yale University, New Haven, CT; [2]Brigham and Women's Hospital, Harvard Medical School, Department of Medicine, Boston, MA*

MP 371 **Extensive Domain-specific N-glycan Analysis in mAbs and Fusion Proteins via a Sequential Deglycosylation Scheme and HILIC-FLR-MS**; Charles Nwosu[1]; Samali Lwanga[1]; Johnathon Li[1]; Lei Wang[1]; Brian Flaherty[1]; Chris Barton[1]; *[1]Takeda Pharmaceuticals International Co, Lexington, Massachusetts*

MP 372 **Uncovering the tear fluid O-glycoproteome in dry eye disease**; Vincent Chang[1]; Keira E. Mahoney[1]; Stacy A. Malaker[1]; Niclas G. Karlsson[2]; *[1]Yale University, New Haven, CT; [2]Oslo Metropolitan University, Oslo, Norway*

MP 373 **Selective Exo-Enzymatic Labeling for Glycoform-Specific Biomarker Discovery in a Pancreatic Cancer Model**; Sydney Bedillion[1]; Michael Tiemeyer[1]; Lance Wells[1]; *[1]University of Georgia, Athens, GA*

MP 374 **Understanding the role of lysosomal membrane protein (LAMP) family glycosylation in the tumor microenvironment**; Valentina Rangel Angarita[1]; Joann Chongsaritsinsuk[1]; Ryan J. Chen[1]; Lea M. Kim[1]; Taryn M. Lucas[1]; Nara Chung[1]; Keira E. Mahoney[1]; Stacy A. Malaker[1]; *[1]Yale University, New Haven, CT*

MP 375 **Quantification of sialylated O-glycopeptides of serum IgA1 by LC-MS**; Mary A. Cunningham[1]; Stacy Hall[1]; Stephen E. Cunningham[2]; Hogan Morton[1]; Dana V. Rizk[1]; Jan Novak[1]; Matthew B. Renfrow[1]; *[1]University of Alabama at Birmingham, Birmingham, AL; [2]Independent researcher, Birmingham, AL*

MP 376 **Charge detection mass spectrometry and proton transfer charge reduction reveal complex glycosylation of HIV-1 envelope protein, gp120**; Kyle Juetten[1]; Jennifer Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX*

MP 377 **Development of a Comprehensive Proteomics Workflow for In Vivo Characterization of mRNA-Expressed IgA2**; Ding Liu; *Moderna, Inc., Cambridge, MA*

MP 378 **Two's a crowd: quantifying co-isolation in glycoproteomics experiments using Proton Transfer Charge Reduction (PTCR)**; Kayla Markuson[1]; Ruby Zhang[1]; Nicholas M. Riley[1]; *[1]University of Washington, Seattle, WA*

MP 379 **Expanding Autonomous Dissociation-type Selection to include GlcNAc-containing O-glycopeptides**; Jacob H. Russell[1]; Emmajay Sutherland[1]; Ruby Zhang[1]; Nicholas M. Riley[1]; *[1]University of Washington, Seattle, WA*

MP 380 **Leveraging offline fractionation methods for in-depth glycoproteomics**; Ruby Zhang[1]; Kayla A. Markuson[1]; Nicholas M. Riley[1]; *[1]University of Washington, Seattle, WA*

MP 381 **Comparing methods to access the intact cell surface N-glycoproteome**; Emmajay Sutherland[1]; Nicholas M. Riley[1]; *[1]University of Washington, Seattle, WA*

MP 382 **Characterization of the interactions between high mannose glycans and a novel prokaryotic lectin using mass spectrometry based approaches**; Lindsay J Morrison[1]; Johnny Zhu[1]; Kevin Wyndham[1]; *[1]Waters Corp., Milford, MA*

MP 383 **Characterizing integrin glycosylation using real-time decision making**; Anna G. Duboff[1]; Kathryn Kothlow[1]; Tim S. Veth[1]; Jacob H. Russell[1]; Emmajay Sutherland[1]; Chris D. McGann[1]; Fengchao Yu[2]; Daniel A. Polasky[2]; Alexey I. Nesvizhskii[2]; Devin K. Schweppe[1]; Nicholas M. Riley[1]; *[1]University of Washington, Seattle, WA; [2]University of Michigan, Ann Arbor, MI*

MP 384 **Profiling of O-fucose proteome of POFUT1 and POFUT2 using 6-alkynyl fucose**; Huilin Hao[1]; Zilei Liu[2]; Peng Wu[3]; Robert S. Haltiwanger[1]; *[1]Complex Carbohydrate Research Center, University of Georgia, Athens, GA; [2]Department of Molecular Medicine, Scripps Research, La Jolla, CA; [3]Department of Molecular and Cellular Biology, Scripps Research, La Jolla, CA*

MP 385 **Comprehensive glycosylation mapping in human erythropoietin by RPLC- ECD and CID mass spectrometry**; Takashi Baba[1]; Ryo Yokoyama[2]; Ushio Takeda[2]; Stanislav Beloborodov[1]; Pavel Ryumin[1]; Yves Le Blanc[1]; *[1]SCIEX, Concord, ON; [2]SCIEX, Shinagawa, Japan*

MP 386 **Mass spectrometry analysis reveals fucosylated, complex, and mannose-6-phosphorylated N-glycans at distinct asparagine binding sites of the cancer metastasis-linked protein EpCAM**; Nicole M Jenkinson[1]; Joshua W Smith[2]; Lauren R DeVine[2]; Robert N Cole[2, 3]; Kristine Glunde[1, 3, 4]; *[1]Division of Cancer Imaging Research, The Russell H. Morgan Department of Radiology and Radiological Science, The Johns Hopkins University School of Medicine, Baltimore, Maryland; [2]The Mass Spectrometry and Proteomics Facility, The Johns Hopkins University School of Medicine, Baltimore, Maryland; [3]Department of Biological Chemistry, The Johns Hopkins University School of Medicine, Baltimore, Maryland; [4]Sidney Kimmel Comprehensive Cancer Cancer, Johns Hopkins University School of Medicine, Baltimore, Maryland*

MP 387 **Comparative Evaluation of GlycanFinder and Byonic for Glycopeptide Identification and Quantitation in High-Throughput Glycoproteomics Using LC-MS/MS**; Shafia Shafiq Nishe[1]; Vishal Sandilya[1]; Sherifdeen Onigbinde[1]; Sarah Sahioun[1]; Yehia Mechref[1]; *[1]Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, Texas*

MP 388 **Oligomeric State Characterization of Human Cytomegalovirus Surface Protein by Native Mass Spectrometry and Single Particle Methods**; Zhixin Xu[1, 2]; Michael Mor[3, 4]; Jeremy p. Kamil[5]; Christopher Benedict[3]; Erica Ollmann Saphire[3, 4]; Vicki H. Wysocki[1, 2]; *[1]Ohio State University, Columbus, OH; [2]Native Mass Spectrometry Guided Structural Biology Center, The Ohio State University, Columbus, OH; [3]Center for Vaccine Innovation, La Jolla Institute for Immunology, La Jolla, CA; [4]Department of Medicine, University of California San Diego, La Jolla, CA; [5]University of Pittsburgh, Pittsburgh, PA*

MP 389 **High sensitivity identification of N-linked glycopeptides in human plasma using alternative fragmentation**; Remco Van Soest[1]; Kristina Jurcic[2]; Patrick Pribil[3]; *[1]SCIEX, Redwood City, CA; [2]Bioinformatics Solution Inc., Waterloo, CA; [3]SCIEX, Concord, ON*

MP 390 **Glycoproteomics reveal glycoform-specific regulation of glycoproteins in hiPSC-CM cardiomyocytes upon ER Stress**; Alexander W Black[1]; Boomathi Pandi[1]; Dominic Ng[1]; Maggie P Y Lam[1]; *[1]University of Colorado Anschutz, Aurora, CO*

MP 391 **Site-Specific Glycosylation Profiling of Etanercept and Biosimilars Using TMT Labeling and ZIC-HILIC HPLC Chromatography**; Hyojin Kim[1]; Heeyoun Hwang[2]; Geul Bang[2]; Myung Jin Oh[3]; Hyun Joo An[3]; Jong Shin Yoo[3]; Jin Young Kim[2, 4]; *[1]Department of Bio and Brain Engineering, Korea Advanced Institute of Science and Technology, Daejeon, South Korea; [2]Digital Omics Research Center, Korea Basic Science Institute, Ochang, South Korea; [3]Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, South Korea; [4]Critical Diseases Diagnostics Convergence Research Center, Korea Research Institute of Bioscience and Biotechnology, Daejeon, South Korea*

MP 392 **Optimized HILIC-Based Enrichment and Characterization of O-Linked Glycopeptides from Human Serum Using Nano-LC–ESI–MS/MS**; Jyoti Kannoujia[1]; Andrew D Couse[1]; Jonathan C Trinidad[1]; *[1]Indiana University, Bloomington, IN*

MP 393 **Characterization of Site-Specific N- and O-Glycopeptides from Recombinant Spike and ACE2 Glycoproteins Using LC-MS/MS Analysis**; Ju Hwan Song[1, 2]; Sangeun Jang[1]; Jin-Woong Choi[1]; Seoyoung Hwang[1]; Kyoung Heon Kim[2]; Hye-Yeon Kim[1]; Sun Cheol Park[1]; Wonbin Lee[1]; Ju Yeon Lee[1, 3, 4]; *[1]Korea Basic Science Institute (KBSI), Ochang, Cheongju, South Korea; [2]Korea University, Seoul, South Korea; [3]University of Science and Technology, Daejeon, South Korea; [4]Korea Research Institute of Bioscience and Biotechnology, Daejeon, South Korea*

MP 394 **Electron Activated Dissociation (EAD) of O-fucosylated Peptides from Human Samples Identifies New Substrates of the Protein O-fucosyltransferases FUT10 and FUT11**; Benjamin M. Eberand[1]; Michelle Cielesh[1]; Huilin Hao[2]; Yvonne Kong[1]; Jemma Fenwick[1]; Freda H. Passam[1]; Robert S. Haltiwanger[2]; Mark Larance[1]; *[1]The University of Sydney, Camperdown, Australia; [2]University of Georgia, Athens, GA*

HIGH MASS ACCURACY / HIGH PERFORMANCE MS: APPLICATIONS, AUTOMATION, AND INSTRUMENTATION

395-411

MP 395 **AQbD-Based LC-Q Orbitrap MS Method for NDMA Determination and Genotoxic Nitrosamine Mitigation in Metformin Products**; Dande Aishwarya[1]; Rajkumar Malayandi[1]; Subramanian Natesan[2]; Abhishek Sahu[1]; Murali Kumarasamy[1]; Ramalingam Peraman[1]; *[1]National Institute of Pharmaceutical Education and Research (NIPER) Hajipur, Hajipur, India; [2]National Institute of Pharmaceutical Education and Research (NIPER) Kolkata, Kolkata, India*

MP 396 **Assessing the impact of Parts-per-billion Mass Accuracy Upon Forensic Toxicology Data-Independent Analysis Screening**; NAYAN S MISTRY[1]; Michael McCullagh[1]; Hans Vissers[2]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Waters Corporation, Wilmslow, United Kingdom*

MP 397 **From Automated Covalent Hit Finding to Characterizing Target Protein Covalent Modifiers**; Yecenia Peraza[1]; Patrick Bingham[1]; Patrick Shelton[1]; Seth Darensburg[1]; Karen Maegley[1]; Matthew Petroski[1]; Taran Dodd[1]; *[1]Pfizer, San Diego, CA*

MP 398 **Breaking Velocity Focusing Limitations in MALDI Linear TOF MS: Experimental Verification of High Resolution**; Yi-Hong Cai[1]; Yi-Sheng Wang[2]; *[1]Genomics Research Center, Academia Sinica, Taipie, Taiwan; [2]Genomics Research Center, Academia Sinica, Taipei, Taiwan*

MP 399 **Development of an Automated Food Glycomics Workflow Using UHPLC/QqQ-dMRM-MS and Open Source Robotics**; Christopher Suarez[1]; Aaron D. Stacy[2]; Shawn Ehlers Cheang[2]; Cheng-Yu Charlie Weng[1]; Jiani Jiang[1]; Carlito B. Lebrilla[1]; *[1]University of California, Davis, Davis, CA; [2]University of California Davis, Davis, CA*

MP 400 **On-demand Online Reduction of Intact Antibodies for Automated Workflows on SampleStream coupled to a timsTOF**; Dodge Baluya[1]; Philip Compton[2]; Jared Drader[2]; Sheri Manalili[2]; Guillaume Tremintin[1]; *[1]Bruker, San Jose, CA; [2]Integrated Protein Technologies, Evanston, IL*

MP 401 **Finding the Best Fit: Comparison of Automated Sample Preparation Workflows for Bottom-Up Proteomics**; Serena Wu[1]; Strassheim Strassheim[1]; Amit Dey[1]; Yue Andy Qi[2]; Nathan Basisty[1]; *[1]NIA, Baltimore, MD; [2]NIH, BETHESDA, MD*

MP 402 **On-the-fly Retention Time Adjustment on a modified Orbitrap Hybrid Mass Spectrometer enabling Targeted and Discovery Workflows with high efficiency**; Markus Kellmann[1]; Hanno Resemann[2]; Julia Kraegenbring[2]; Yovany Cordero Hernandez[2]; Jordi Bertran Vincente[2]; Jesse D. Canterbury[3]; William Barshop[4]; Philip Remes[4]; Heiner Koch[2]; *[1]Thermo Fisher Scientific, Bremen, Germany; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [3]ThermoFisher Scientific, San Jose, CA; [4]Thermo Fisher Scientific, San Jose, CA*

MP 403 **Towards Dual Fecal Metabolomics and Lipidomics: Design of Experiments-Driven Optimization of Biphasic Extraction and Two-dimensional UHPLC-HRMS**; Kimberly De Windt[1]; Vera Plekhova[1]; Tiffany De Troyer[1]; Beata Pomian[1]; Ellen De Paepe[1]; Lynn Vanhaecke[1, 2]; *[1]Ghent University, Ghent, Belgium; [2]Queens University Belfast, Belfast, United Kingdom*

MP 404 **Metabolite and lipid analysis (MLA) profiling using mass spectrometry with data visualization and a chemometrics workflow**; Hoon Park[1]; Gobind Sah[1]; Stephen Dearth[2]; Sam Mwilu[1]; Ronny Dosanjh[1]; *[1]Thermo Fisher Scientific, Hunt Valley, MD; [2]biocrates life sciences ag, Innsbruck, Austria*

MP 405 **Abandoning the Quadrupole for MS Fragmentation Analysis: Towards 1,000 Hz Speeds with 100% Ion Utilization Using HRIM Precursor Isolation**; Leonard Rorrer[1]; Lauren Royer[1]; Liulin Deng[1]; Bennett Kalafut[1]; Isabel Uribe[1]; Benjamin Orsburn[2]; Oliver M. Bernhardt[3]; Tejas Gandhi[3]; Lukas Reiter[3]; Daniel DeBord[1]; *[1]MOBILion Systems, Inc., Chadds Ford, PA; [2]University of Pittsburgh, Pittsburgh, PA; [3]Biognosys, Schlieren, Switzerland*

MP 406 **Enhanced Reproducibility and Robustness of Ultrasensitive Spray-capillary CE-MS**; Ahmed Mohamed Amin Abdelhamed[1, 2]; Zhitao Zhao[3]; Samin Anjum[1]; Kellye A. Cupp-Sutton[1]; Si Wu[1]; *[1]The University of Alabama, Tuscaloosa, AL; [2]Ain Shams University, Cairo, Egypt; [3]Oklahoma University, Norman, OK*

MP 407 **Out-of-the-box 5 GSPS data acquisition system with 16-bit performance for mass spectrometers**; Jan-Erik Eklund[1]; Mans Persson[1]; Joe Sharp[1]; *[1]Teledyne Signal Processing Devices Sweden AB, Linkoping, Sweden*

MP 408 **Non-targeted LC-Orbitrap Collision Cross Section Measurements to Enhance Lipid Annotation**; Ziqin Ni[1]; Konstantin Aizikov[2]; Alexander Makarov[2]; Kyle L. Fort[2]; Facundo M Fernández[1]; *[1]Georgia Institute of Technology School of Chemistry and Biochemistry, Atlanta, GA; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

MP 409 **Simultaneous Quantitation and Discovery (SQUAD): an intelligent combination of targeted and untargeted workflows using a modified Orbitrap Astral mass spectrometer**; Bashar Amer[1]; Eugen Damoc[2]; Martin Zeller[2]; Anna V. Pashkova[2]; Tabiwang N. Arrey[2]; Rahul Deshpande[3]; Daniel Hermanson[3]; Thomas Moehring[2]; Susan S Bird[3]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [3]ThermoFisher Scientific, San Jose, CA*

MP 410 **Using large spectral models for simultaneous annotation and quantitation of complex metabolomic samples**; Ana S. H. Costa[1]; Gabriel Asher[1]; Rahul Deshpande[2]; Devesh Shah[1]; Bashar Amer[2]; Susan S Bird[2]; Timothy Kassis[1]; Mimoun Cadosch Delmar[1]; Jennifer M Campbell[1]; *[1]Matterworks, Somerville, MA; [2]ThermoFisher Scientific, San Jose, CA*

MP 411 **Quantitative proteomic analysis of WT and nudC mutant E. coli strains by in-cell digestion and single-shot LC-MS/MS**; Yogeshwari Singh[1]; Jeremy Bird[1]; Yanbao Yu[1]; *[1]University of Delaware, Newark, DE*

IMAGING MS: COMPUTATIONAL METHODS, SOFTWARE, AND ANALYSIS
412-424

MP 412 **Image fusion to improve the spatial resolution of LA-ICP-MS imaging of nanomaterial biodistributions**; Teerapong Jantarat[1]; Jeerapat Doungchawee[1]; Richard W Vachet[1]; *[1]University of Massachusetts Amherst, Amherst, MA*

MP 413 **Unsupervised Segmentation for Mass Spectrometry Imaging of in vivo Isotope Labeled Duckweed**; Raven Johnson[1]; Vy Tat[1]; Young Jin Lee[1]; *[1]Iowa State University, Ames, IA*

MP 414 **Optimized Delocalization Analysis Software for Mass Spectrometry Imaging Data**; Alejandro Catacora[1]; Wan Kyu Paul Choi[1]; Cole C. Johnson[1]; Nathan Riemann[1]; Ethan Yang[1]; Jason Fan[1]; Kristine Glunde[1]; Cay Tressler[1]; *[1]Johns Hopkins Applied Imaging Mass Spectrometry Core, Johns Hopkins University School of Medicine, Baltimore city, MD*

MP 415 **Integrated annotation pipeline using in-silico prediction for on-target chemical derivatization MALDI Imaging**; Arne Behrens[1]; Nikolas Kessler[2]; Sofie Weinkouff[3]; Bram Heijs[4]; Tobias Boskamp[3]; Sarah Diez[5]; Achim Buck[5]; Michael Becker[5]; Kevin Zematis[6]; Dusan Velickovic[6]; Christopher R Anderton[6]; Andrew DelaCourt[7]; Azad Eshghi[7]; Nannan Tao[7]; Michael Easterling[7]; *[1]Bruker Daltonics, Bremen, Germany; [2]Bruker Daltonics GmbH & Co. KG, Billerica, MA; [3]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [4]Bruker Nederland B.V., Leiderdorp, Netherlands; [5]Boehringer Ingelheim, Biberach, Germany; [6]Pacific Northwest National Laboratory, Richland, WA; [7]Bruker Scientific LLC, Billerica, MA*

MP 416 **Unbiased Feature Down-Selection to Improve Classification by Machine Learning on MS Imaging Data**; Braysen J Miller[1]; Aleesa E Chua[1]; Emily R. Sekera[2]; Amanda B. Hummon[2]; Heather Desaire[1]; *[1]University of Kansas, Lawrence, KS; [2]THE OHIO STATE UNIVERSITY, Columbus, OH*

MP 417 **Statistical Principles Define an Open-Source Analysis Workflow for Mass Spectrometry Imaging Experiments with Complex Designs: A Case Study of Osteoarthritis**; Ethan B Rogers[1]; Sai Srikanth Lakkimsetty[1]; Kylie Ariel Bemis[1]; Charles A Schurman[2]; Birgit Schilling[2]; Peggi M Angel[3]; Olga Vitek[1]; *[1]Northeastern University, Boston, MA; [2]Buck Institute for Research on Aging, Novato, CA; [3]Department of Cell & Molecular Pharmacology & Experimental Therapeutics at the Medical University of South Carolina, Charleston, SC*

MP 418 **Enhanced tissue compartmentalization by applying segmentation algorithms on reduced spatial omics data**; Bram Heijs[1]; Ryan Marsico[2]; Sören-Oliver Deininger[3]; Arne Behrens[3]; Janina Oetjen[3]; Azad Eshghi[4]; Tobias Boskamp[3]; *[1]Bruker Nederland B.V., Leiderdorp, Netherlands; [2]Bruker Scientific LLC, San Jose, California; [3]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [4]Bruker Scientific LLC, Billerica, MA*

MP 419 **TIMSImaging: a Python package for trapped-ion mobility mass spectrometry imaging data visualization and preprocessing**; Yinyue Zhu[1]; Kylie Bemis[1]; Sai Lakkimsetty[1]; Andreas Weber[2]; Mujia Li[2]; Larissa Meyer[2]; Melanie Föll[2]; Olga Vitek[1]; *[1]Northeastern University, Boston, MA; [2]Institute of Surgical Pathology, Medical Center, University of Freiburg, Faculty of Medicine, Freiburg, Germany*

MP 420 **Combining AP-SMALDI with data independent analysis to enable localization and improved identification of compounds in MALDI MS imaging**; Carmen Paschke[1]; Kerstin Strupat[1]; Carolin M Morawietz[2,3]; Karl-Christian Schaefer[3]; Christoph Henrich[1]; Bernhard Spengler[2,3]; *[1]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [2]Justus Liebig University, Institute of Inorganic and Analytical Chemistry, Giessen, Germany; [3]Transmit GmbH, Giessen, Germany*

MP 421 **Evaluation of Novel Clustering Algorithms for Identifying Spatial Patterns in Imaging Mass Spectrometry**; Mahshid Manouchehri[1]; Yingchan Guo[1]; Lexin Chen[1]; Ramón Alain Miranda-Quintana[1]; Boone M. Prentice[1]; *[1]University of Florida, Gainesville, FL*

MP 422 **Teardrop: Unsupervised Co-registration of H&E microscopic Images and Mass Spectrometry Images (MSI) with Neural Networks** ; Sai Srikanth Lakkimsetty[1]; Andreas Weber[2]; Kylie Ariel Bemis[1]; Melanie Föll[2,3]; Olga Vitek[1]; *[1]Northeastern University, Boston, MA; [2]Institute of Surgical Pathology, Medical Center, University of Freiburg, Faculty of Medicine, Freiburg, Germany; [3]German Cancer Consortium (DKTK) and German Cancer Research Center (DKFZ), partner site, Tübingen, Germany*

MP 423 **FlexPro: Development of automated data analysis framework to resolve the complexity of spatial metabolomics, lipidomics and proteomics based on MALDI-IMS-MSI**; Reza Aalizadeh[1]; Varvara Nikolopoulou[1]; Georgia Charkoftaki[1]; Athina Lisgara[1]; Jordan Hartig[2]; Scott Pennino[2]; Vladimir V. Papov, Jr. [2]; Vasilis Vasiliou[1]; *[1]Department of Environmental Health Sciences, Yale School of Public Health, Yale University, New Haven, CT; [2]Boehringer Ingelheim Pharmaceuticals, Inc., Ridgefield, CT*

MP 424 **Raw spectra processing with accurate peak alignment in mass spectrometry imaging data using open Python code**; Andrey Kuzin[1]; Maria Derkach[1]; Igor Popov[1]; Stanislav I. Pekov[1,2]; *[1]Moscow Institute of Physics and Technology, Dolgoprudniy, Russian Federation; [2]Skoltech, Skolkovo, Russia*

IMAGING MS: DISEASE MARKERS
425-440

MP 425 **Defining tri- and tetra-antennary sialylated N-glycan isomer distributions using N-glycan MALDI MSI in a large cohort of prostate tumor tissues**; Kameisha Rashford[1]; Caroline Kittrel[1]; Bettina F Drake[2]; Ariana Ahmed[2]; Alesksandra Klim[2]; Eric Kim[2]; Peggi M Angel[1]; Joseph E Ippolito[2]; Richard R Drake[1]; *[1]Medical University of South Carolina, Pharmacology & Immunology, Charleston, South Carolina; [2]Washington University School of Medicine, St. Louis, MO*

MP 426 **Nano-DESI MS Imaging Reveals Metal-Deficient hSOD1G37R Localisation to Hindbrain Motor Nuclei in Transgenic ALS Mouse Models**; Cameron Baines[1]; Oliver J Hale[1]; Peter J Crouch[2]; Helen J Cooper[1]; *[1]University of Birmingham, Birmingham, United Kingdom; [2]University of Melbourne, Melbourne, Australia*

MP 427 **IR-MALDESI Mass Spectrometry Imaging of Mouse Brain Tissue with Globoid Cell Leukodystrophy (Krabbe Disease): Interrogation of the Cytotoxic Sphingolipid Psychosine**; Sierra N. Hunter[1]; Brittany N. Thomas[2,3]; Mary F. Wang[1]; Anthony J. Filiano[2,3]; David C. Muddiman[1]; *[1]The Biological Imaging Laboratory for Disease and Exposure Research (BILDER) Center, Department of Chemistry, North Carolina State university, Raleigh, NC; [2]Marcus Center for Cellular Cures, Department of Neurosurgery, Duke University, Durham, NC; [3]Department of Pathology, Duke University, Durham, NC*

MP 428 **Investigating the relationship between off target pharmacology and the DMPK of methapyrilene using lipidomics and MS imaging**; Robert S Plumb[1]; Andrew Leightner[2]; Steven Lai[2]; Ian Wilson[3]; *[1]Waters, Milford, MA; [2]Waters Corp., Milford, MA; [3]Imperial College London, London, United Kingdom*

MP 429 **Comparative Analysis of Lipids in a Metabolic Dysfunction-Associated Steatohepatitis (MASH) Mouse Model using Imaging MS and LCMS**; Doug Carlton[1]; Jeff Dahl[1]; Toshiya Matsubara[1]; Min Kyounghee[2]; Eiichi Matsuo[3]; Philipp Scherer[2]; Ruth Gordillo[2]; *[1]Shimadzu Scientific Instruments, Columbia, Maryland; [2]University of Texas Southwestern Medical Center, Dallas, TX; [3]Shimadzu Corporation, Kyoto, Japan*

MP 430 **MALDI Imaging of Patient iPSC-derived Hindbrain Organoids to Evaluate the Effects of Escitalopram on Neurotransmitter and Lipid Metabolism**; Dalton Brown[1]; Cristina Zivko[2,3]; Rachel Boyd[2,3]; Ram Sagar[2,3]; Waqar Ahmed[2,3]; Caitlin M. Tressler[4,5]; Kristine Glunde[4,5,6]; Vasiliki Mahairaki[2,3]; *[1]Johns Hopkins AIMS Core, Baltimore, MD; [2]Department of Genetic Medicine, Johns Hopkins School of Medicine, Baltimore, MD; [3]The Richman Family Precision Medicine Center of Excellence in Alzheimer's Disease, Johns Hopkins School of Medicine, Baltimore, MD; [4]Johns Hopkins Applied Imaging Mass Spectrometry Core, Russell H. Morgan Department of Radiology and Radiological Science, Johns Hopkins School of Medicine, Baltimore, Maryland; [5]The Sidney Kimmel Comprehensive Cancer Center, The Johns Hopkins University School of Medicine, Baltimore, MD; [6]Department of Biological Chemistry, The Johns Hopkins University School of Medicine, Baltimore, Maryland*

MP 431 **Differential lysolipid production in functional spaces in the lungs during bacterial infection**; Tialfi Bergamin De Castro[1]; Kelsey Gregg[2]; Alison Scott[1]; *[1]Department of Microbial Pathogenesis, University of Maryland School of Dentistry, Baltimore, Maryland; [2]Division of Bacterial, Parasitic and Allergenic Products, Center for Biologics Evaluation and Research, FDA, Silver Spring, Maryland*

MP 432 **Multimodal Study of Murine Cardiovascular Remodeling in Myocardial Infarction and Aging: 4D Ultrasound and Mass Spectrometry Imaging**; Anna Colleen Crouch; *University of Tennessee, Knoxville, TN*

MP 433 **Investigating the metabolic landscape of atypical hemolytic-uremic syndrome: Insights into DGKE deficiency using MALDI-MSI**; Laurentiu Dabija[1]; Demian Ifa[1]; Mathieu Lemaire[2]; *[1]York University, Toronto, ON; [2]University of Toronto, Toronto*

MP 434 **High resolution multimodal molecular maps of the vasculature in human cortex reveal molecular markers of cerebral amyloid angiopathy**; Cody R Marshall[1,2,3]; Claire F Scott[3,4]; Lissa Ventura-Antunes[5,6]; Wilber Romero-Fernandez[6]; Alena Shostak[5,6]; Felipe A Moser[7]; Lukasz G Migas[7]; Madeline E Colley[3,8]; Martin Dufresne[3,8]; Raf Van De Plas[3,7]; Matthew S Schrag[5,6]; Jeffrey M Spraggins[2,3,4,8,9]; *[1]Vanderbilt University, Nashville, TN; [2]Chemical Physical Biology Program, Vanderbilt University, Nashville, TN; [3]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [4]Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; [5]Vanderbilt Medical Center, Nashville, TN; [6]Department of Neurology, Vanderbilt University, Nashville, TN; [7]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [8]Department of Biochemistry, Vanderbilt University, Nashville, TN; [9]Department of Chemistry, Vanderbilt University, Nashville, TN*

MP 435 **Mapping the Influence of Pseudomonas aeruginosa (Pa) Infection on Host Lipid Profiles Using a Multi-Factorial CF-like Mouse Model**; Shanaliz Natta[1]; Janette M. Harro[1]; Tialfi Bergamin De Castro[1]; Natalia Islam[1]; Manita Shakya[1]; Robert K. Ernst[1,2]; Alison Scott[1,2]; *[1]Department of Microbial Pathogenesis, University of Maryland School of Dentistry, Baltimore, Maryland; [2]Department of Microbiology and Immunology, University of Maryland School of Medicine, Baltimore, Maryland*

MP 436 **Imaging mass spectrometry-based multiplexedMALDI-IHCfor assessment of ER, PR and HER2 protein expression in breastcancer**; Kiran Kumar Mangalaparthi[1]; Daigo Gunji[1]; Olajide E Olaleye[1]; Amy J French[1]; Gunveen

Sachdeva[1]; Shilpa Venkataraman[1]; Neha Joshi[1]; Tianqi Gao[1]; Sumankalai Ramachandran[2]; Kenneth J. Rothschild[3]; Mark J Lim[3]; Gargey Yagnik[3]; Akhilesh Pandey[1, 4]; *[1]Department of Laboratory Medicine and Pathology, Mayo Clinic, Rochester, MN; [2]Bruker Scientific LLC, Billerica, MA; [3]AmberGen Inc., Billerica, MA; [4]Center for Individualized Medicine, Mayo Clinic, Rochester, MN*

MP 437 **Exploring the Aβ Plaque microenvironment in Alzheimer's disease model mice by multimodal Lipid-Protein-Histology Imaging on a benchtop mass spectrometer**; Elisabeth Müller[1, 2]; Thomas Enzlein[1]; Dagmar Niemeyer[3]; Livia Von Ammon[1]; Katherine Stumpo[4]; Knut Biber[5]; Corinna Klein[5]; Michael Easterling[4]; Carsten Hopf[1, 2, 6]; *[1]Center for Mass Spectrometry and Optical Spectroscopy (CeMOS), Mannheim University of Applied Sciences, Mannheim, Germany; [2]Medical Faculty, Heidelberg University, Heidelberg, Germany; [3]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [4]Bruker Scientific, Billerica, MA; [5]AbbVie Deutschland GmbH & Co., KG, Knollstrasse 50, 67061, Ludwigshafen, Germany; [6]Mannheim Center for Translational Neurosciences (MCTN), Medical Faculty Mannheim, Heidelberg University, Mannheim, Germany*

MP 438 **The Lipid Awakens: A T Cell Activation Story**; Sutirtha Chattopadhyay; *Technical University of Munich, Munich, Germany*

MP 439 **Spatial multi-omics study delineates significant link between amyloid pathology and sphingolipids in Alzheimer's Disease brain**; Yumiko Toyama[1]; Takashi Nirasawa[2]; Kohei Yuyama[3]; Yuko Saito[4]; Shigeo Murayama[4]; Colin L. Masters[5]; Masaya Ikegawa[1]; *[1]Doshisha University, Kyotanabe City, Japan; [2]Bruker Japan, Yokohama, Japan; [3]Hokkaido University, Sapporo, Japan; [4]Tokyo Metropolitan Geriatric Hospital and Institute of Gerontology, Tokyo, Japan; [5]Florey Institute and University of Melbourne, Melbourne, Australia*

MP 440 **MALDI imaging mass spectrometry reveals lipid alterations in physiological and Sertoli cell-only syndrome human testicular tissue sections**; Alexandra Sulc[1]; Stefania Bankuti[1]; Mate Reti[1]; Laszlo Mark[2, 3]; *[1]University of Pecs, Institute of Biochemistry and Medical Chemistry, Pécs, Hungary; [2]Institute of Biochemistry and Medical Chemistry, University of Pecs, Pecs, Hungary; [3]National Human Reproduction Laboratory, Pécs, Hungary*

INFORMATICS: GENERAL, SRM, AND DIA
441-446

MP 441 **timsplot: A Python Shiny App for Visualizing tims-TOF Proteomics Results**; Zachary J Kirsch[1]; Manubhai Kadayil Prabhakaran[1]; Diego Assis[1]; Ruben Shrestha[2]; Matthew Willetts[1]; *[1]Bruker, Billerica, MA; [2]Bruker, San Jose, CA*

MP 442 **Phosphomatics 2025: Expanded Capabilities for Kinase Prediction, Missing Data Handling, and Data Visualization**; Michael G Leeming[1]; Ching-Seng Ang[1]; Swati Varshney[1]; Keshava Datta[1]; Nicholas A Williamson[1]; *[1]The University of Melbourne, Parkville, Australia*

MP 443 **Hybrid-DIA and SureQuant on a Modified Orbitrap Astral MS**; Max Hoek[1]; Johannes Petzoldt[1]; Arne Kreutzmann[1]; Till Zickmantel[1]; Ankit Dwivedi[1]; Christopher Rathje[1]; Sophia Steigerwald[1]; Vinodkumar Mhetre[1]; Eugen Damoc[1]; Christian Hock[1]; *[1]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

MP 444 **MRMAssayDB: An Expansive and Integrated Resource for Targeted Proteomics Assays**; Yassene Mohammed[1, 2]; Pallab Bhowmick[3]; Christoph H. Borchers[2, 3, 4, 5]; *[1]LUMC, Leiden, Netherlands; [2]Gerald Bronfman Department of Oncology, Montreal, QC; [3]Segal Cancer Proteomics Centre, Jewish General Hospital, Montreal, QC; [4]Division of Experimental Medicine, McGill University, Montreal, QC; [5]Department of Pathology, McGill University, Montreal, QC*

MP 445 **MS1-based alignment improves chromatographic accuracy and precision of monitoring windows with the GoDig multiplexed targeted proteomics platform**; Caleb M Lindgren[1]; David R Vanderwall[1]; Steven P Gygi[1]; Steven R Shuken[1]; *[1]Harvard Medical School, Boston, MA*

MP 446 **A Scalable Approach to Assess Statistical Confidence of Peptides in Targeted Proteomics Assays**; Ariana E Shannon[1]; Alex W Joyce[2]; Lilian Heil[3]; Cristina Jacob[4]; Philip M Remes[3]; Lukas Käll[5]; Brian C. Searle[1]; *[1]The Ohio State University, Columbus, OH; [2]Ohio State University, Colubus, OH; [3]ThermoFisher Scientific, San Jose, CA; [4]Thermo Fisher Scientific, San Jose, California; [5]KTH Royal Institute of Technology, Stockholm, Sweden*

INFORMATICS: MULTIOMICS INTEGRATION
447-468

MP 447 **Comprehensive Multiomics Data Integration: Bridging Proteomics and Genomics**; Khatereh Motamedchaboki[1]; Dave Abramowitz[1]; Eric M Wilson[1]; Mark R Ressler[1]; Samad Jahandideh[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

MP 448 **Probabilistic Modeling and Functional Clustering in Multi-Omics Data Integration**; Chi Yen Tseng[1]; Emilio S. Rivera[1]; Tara Harvey[1]; Joshua Breidenbach[1]; Brett Blackwell[1]; Salvator Palmisano[1]; Madison Grace Thornhill[1]; Emilia Solomon[1]; Claire Sanders[1]; Kes Luchini[1]; Ethan M. McBride[1]; Jessica A. Salguero[1]; Francie E. Rodriguez[1]; Philip Mach[1]; Trevor Glaros[1]; *[1]Los Alamos National Laboratory, Los Alamos, NM*

MP 449 **Multi-omics analysis of lung tissue through integrated study of MALDI-mass spectrometry imaging and co-detection by indexing-based multiplexed fluorescence microscopy**; Naina A Beishembieva[1]; Brittney L Gorman[1]; Geremy C Clair[1]; Christopher R Anderton[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

MP 450 **Evaluation towards the genetic compensation from globin gene mutations to hemoglobin subunit abundance responses**; Xiaotong Zhang[1, 2]; Yixi Cai[1, 2]; Guixue Hou[1, 2]; Siqi Liu[1, 2]; *[1]University of Chinese Academy of Sciences, Beijing, China; [2]BGI-Shenzhen, Shenzhen, China*

MP 451 **Automated Cell Type Annotation by AI for Multiomic Workflows Using Laser Microdissection**; Dave Mitchell[1]; Joshua P Schaaf[1]; Sakiyah Taqee[1]; Kathleen M. Darcy[1]; Christopher M. Tarney[1]; George L Maxwell[2]; Thomas P Conrads[2]; Nicholas W. Bateman[1]; *[1]Gynecologic Cancer Center of Excellence, Annandale, Virginia; [2]Women's Health Integrated Research Center, Annandale, Virginia*

MP 452 **Multi-omics of intestinal lymphatic fluid and plasma using bead-based sample preparation, DIA proteomics, and lipidomics enabled by real-time library search**; Benton J. Anderson[1]; Corinne E. Moss[1]; Daniel D. Lee[2]; Kento Kurashima[3]; Ajay K. Jain[3]; Katherine A. Overmyer[1, 4]; Gwendalyn J. Randolph[2]; Joshua J. Coon[1, 4, 5]; *[1]Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI; [2]Department of Pathology and Immunology, Washington University School of Medicine, St. Louis, MO; [3]Department of Pediatrics, St. Louis University, St. Louis, MO; [4]Morgridge Institute for Research, Madison, WI; [5]Department of Chemistry, University of Wisconsin-Madison, Madison, WI*

MP 453 **Multi-Omics Characterization of SCA34-Associated Molecular Alterations in Rat Skin: Integrating LC-MS/MS Proteomics and DESI-MSI Lipidomics**; Dan Chen[1]; Eniola A Adewunmi[2]; Asa J Brown[3]; Richard S Brush[3]; Zhu Zou[1]; Martin-Paul Agbaga[2, 3]; Zhibo Yang[1]; *[1]Department of Chemistry and Biochemistry, University of Oklahoma, Norman, Oklahoma; [2]University of Oklahoma Health Science Center, Departments of Cell Biology, Oklahoma City, Oklahoma; [3]University of Oklahoma Health Sciences Center, Ophthalmology, Oklahoma City, Oklahoma*

MP 454 **A Metabolomics/Proteomics-Inspired Workflow to Probe Prebiotic Chemical Systems**; Alex Deans-Rowe[1, 2]; Kavita Matange[2, 3]; Anton S Petrov[2, 4]; Pau Capera-Aragonès[1, 2]; Facundo M. Fernández[1, 2]; Loren Dean Williams[1, 2]; *[1]School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA; [2]NASA iCOOL (Center for Integration of the Origins of Life), Atlanta, GA; [3]Cold Spring*

Harbor Laboratory, Laurel Hollow, NY; [4]School of Biological Sciences, Georgia Institute of Technology, Atlanta, GA

MP 455 **Biological Age prediction via LC-MS/MS steroid profiling using a DNN model based on metabolic pathways**; Zi Wang[1]; Qiuyi Wang[1]; Kenji Mizuguchi[1]; Toshifumi Takao[1, 2]; *[1]Osaka University, Suita, Japan; [2]Rigaku Co., Akishima, Japan*

MP 456 **Hnet: Hierarchical Network Visualization for xMWAS**; Sami Teeny[1]; Zachery R Jarrel[1]; Barbara Cohn[2]; Jessica Alvarez[1]; Cecile Lahiri[1]; Young-Mi Go[1]; Dean P Jones[1]; *[1]Emory University, Atlanta, GA; [2]Child Health and Development Studies, Berkeley, CA*

MP 457 **Spatially Resolved Multiomic Correlative Analysis Software for MALDI-MSI of Lipids and Targeted Transcripts and Proteins on the Same Tissue Section**; Leonardo Garcia Dettori[1]; Jonathan Bell[1]; Gargey B. Yagnik[1]; Zhi Wan[1]; Philip Carvalho[1]; Mark J. Lim[1]; Kenneth J. Rothschild[1, 2]; *[1]AmberGen, Billerica, MA; [2]Department of Physics and Photonics Center, Boston University, Boston, MA*

MP 458 **Combining Multi-Omics Factorization Methods for Robust Biomarker Identification**; Ivo Kwee; *BigOmics Analytics, Lugano, Switzerland*

MP 459 **Integrated Phosphoproteomic and Metabolomic Analysis in Wild-Type and KRAS-Mutant Colorectal Cancer Cells Connects Signaling Pathways to Metabolic Hubs**; Adam D Richardson[1]; Ethan Stancliffe[1]; Ashima Mehta[1]; Sharla Friend[1]; Monil Gandhi[1]; Douglas V. Guzior[1]; Cassandra G Kempf[2]; Kevin Cho[2]; Tom Cohen[1]; Gary J Patti[2]; *[1]Panome Bio, St Louis, MO; [2]Washington University, St. Louis, MO*

MP 460 **Plasma multi-omics analysis to define Long-COVID molecular signatures**; William F Beimers[1]; Joseph Balnis[2]; Salma Ibrahim Abouelhassan[1]; Benton J. Anderson[1]; Katherine A. Overmyer[1, 3]; Joshua J. Coon[1, 3]; Ariel Jaitovich[2]; *[1]University of Wisconsin-Madison, Madison, WI; [2]Albany Medical College, Albany, NY; [3]Morgridge Institute for Research, Madison, WI*

MP 461 **Proteomic Data Commons: Empowering Cancer Research Through Comprehensive Proteomic Data**; Alexander Pilozzi[1]; Yin Lu[1]; Karen A Ketchum[1]; Nathan Edwards[2]; Michael Holck[1]; Deepak Singhal[1]; Paul A Rudnick[3]; Michael MacCoss[4]; Aaron Maurais[4]; Sudha Venkatachari[5]; Ratna R Thangudu[1]; *[1]ICF, Rockville, MD; [2]Georgetown University, Washington, DC; [3]Spectragen Informatics, Bainbridge Island, WA; [4]University of Washington, Seattle, WA; [5]Frederick National Laboratory, Rockville, MD*

MP 462 **Cracking the egg: uncovering the molecular mechanism of rapidly evolving species-specific fertilization in abalone using a multiomics approach**; Stella M Lai[1, 2]; Regina M Edgington[1]; Trevor G Stepanyan[1]; Damien B Wilburn[1, 2]; *[1]Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH; [2]Ohio State Biochemistry Program, The Ohio State University, Columbus, OH*

MP 463 **Multi-omics analysis reveals membrane remodeling and extracellular matrix alterations as key drivers' of cisplatin resistance in Triple-Negative Breast Cancer**; Shashwati Parihari[1]; Saheli Sarkar[1]; Vidhi Vashishtha[1]; Sanjeeva Srivastava[1]; *[1]Indian Institute of Technology Bombay, Mumbai, India*

MP 464 **Metadata driven discovery: a global effort towards more interoperable and interpretable multiomics data**; Sarah C Brinkley[1]; Jenny Johana Gallo-Franco[2]; Marie-Angélique Laporte[3]; Chi-Ming Chien[4]; Jessica E. Prenni[5]; Maya Rajasekharan[2]; Elizabeth Arnaud[3]; Selena Ahmed[6]; John De La Parra[7]; *[1]Bioversity International, Rome, Italy; [2]International Center for Tropical Agriculture (CIAT), Palmira, Colombia; [3]Bioversity International, Montpellier, France; [4]Periodic Table of Food Initiative, San Francisco, CA; [5]Colorado State University, Department of Horticulture and Landscape Architecture, Fort Collins, CO; [6]American Heart Association, Dallas, TX; [7]The Rockefeller Foundation, New York City, NY*

MP 465 **Systems-level multi-omics analysis identifies biomarkers and metabolic perturbations in arginine and sphingolipid pathways associated with oral squamous cell carcinoma progression**; Avinash Singh[1]; Pratibha Sharma[1]; Richa Vaish[2]; Sudhir Nair[3]; Sanjeeva Srivastava[1]; *[1]Indian Institute of Technology Bombay, Mumbai, India; [2]Tata Memorial Hospital, Mumbai, India; [3]Advanced Centre for Treatment Research and Education in Cancer, Tata Memorial Centre, Mumbai, India*

MP 466 **The Impact of Pseudomonas aeruginosa Specialized Metabolites on Chronic Lung Allograft Dysfunction Pathogenesis**; Christian Martin[1, 2]; Cely T. Gonzalez[2]; Ani Winkler[2]; Tara E. Jager[3]; Girgis Reda[3]; Xiaopeng Li[4]; Robert A. Quinn[2]; *[1]Mass Spectrometry and Metabolomics Core, Michigan State University, East Lansing, Michigan; [2]Department of Biochemistry and Molecular Biology, Michigan State University, East Lansing, Michigan; [3]Corewell Health, Grand Rapids, Michigan; [4]Department of Pediatrics and Human Development, Michigan State University, East Lansing, Michigan*

MP 467 **RaMP-DB 3.0: Annotations and data interpretation analyses for metabolomic and multi-omic data**; Khyati Y. Mehta[1]; Keith J. Kelleher[1]; Tim Sheils[1]; Andrew Patt[1]; Adam Tisch[1]; Jaden Sayer[1]; John Braisted[1]; Ewy A. Mathé[1]; *[1]National Center For Advancing Translational Sciences, Rockville, MD*

MP 468 **A Workflow Integrating Generative AI and Parallel Fold-Change Analysis for Enhanced Interpretation of Large-Scale Omics Data**; Manhoi Hur; *The University of California, Riverside, Riverside, CA*

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MP 469 **A Novel high pressure, High Space Charge Capacity Ion Separation Device Based on Opposing Travelling Wave and DC potentials**; Martin Green[1]; Keith Richardson[1]; David Langridge[1]; Thomas Moore[1]; *[1]Waters Corporation, Wilmslow, United Kingdom*

MP 470 **Single File Injections (SFIs): Untargeted Metabolomics Analysis of 1000 Samples per Day with 10 Minutes Chromatography Separation**; Miao Yu[1]; Shujian Zheng[1]; Shuzhao Li[1]; Vivek Philip[2]; *[1]The jackson laboratory, Farmington, CT; [2]The Jackson Laboratory, Bar Harbor, ME*

MP 471 **Advances in hardware design and function of the new timsOmni MS platform**; Dimitris Papanastasiou[1]; Athanasios Smyrnakis[1]; Mariangela Kosmopoulou[1]; Anastasios Grigoriadis[1]; Ioannis Orfanopoulos[1]; Nikolaos Manolis[1]; Ilias Panagiotopoulos[1]; Rafail Gioves[1]; Alexandros Lekkas[1]; Florian Busch[2]; Jean-François Greisch[2]; Stuart Pengelley[3]; Christoph Gebhardt[3]; Amalia Apalategui[3]; Jonas Koehling[3]; Michael Krause[3]; Jens Decker[3]; Niels Goedecke[3]; Eduardo Carrascosa[3]; Oliver Raether[3]; *[1]Fasmatech Science & Technology, Chalandri, Greece; [2]Bruker Switzerland AG, Fällanden, Switzerland; [3]Bruker Daltonics, Bremen, Germany*

MP 472 **Digital QTOF Narrows Precursor Selectivity to Clean Chimeric MS/MS Spectra**; Elizabeth Groetsema[1]; Sumeet Chakravorty[1]; Fatima Olayemi Obe[1]; Gordon A. Anderson[2]; Shane Tichy[3]; Adam P. Huntley[1]; Peter T.A. Reilly[1]; Brian H. Clowers[1]; *[1]Washington State University, Pullman, WA; [2]GAA Custom Electronics, LLC, Kennewick, WA; [3]Agilent Technologies, Santa Clara, CA*

MP 473 **Improving mass spectrometer robustness using a slotted bandpass ion guide**; Benjamin Jones[1]; Kate Whyatt[1]; *[1]Waters Corporation, Wilmslow, United Kingdom*

MP 474 **Ultrahigh Resolution Ion Mobility Separation Achieved using "Iterative SLIM" for Targeted Mobility Analysis**; Miriam Fico[1]; Liulin Deng[1]; Daniel DeBord[1]; *[1]Mobilion Systems Inc., Chadds Ford, PA*

MP 475 **Four Quadrant Mass Spectrometry: A Versatile Approach for Complex Mixture Analysis**; Dmytro S Kulyk[1]; Abraham K. Badu-Tawiah[1]; *[1]OSU, Columbus, OH*

MP 476 **SQUAD analysis of plasma using modified Orbitrap Hybrid MS for enhanced dynamic range, reduced unintentional MS1 fragmentation, and improved sensitivity**; Bashar Amer[1]; Michal Kaczmarek[2]; Claire Dauly[2]; Christian Klass[2]; Susan Gelman[3]; Rahul R. Deshpande[3]; Thomas Moehring[2]; Susan S Bird[3]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [3]ThermoFisher Scientific, San Jose, CA*

MP 477 **A band-pass filter quadrupole ion guide on a Time-of-Flight instrument**; Yang Kang[1]; Bill Loyd[1]; David Cox[1]; Calvin Chan[1]; Bradley Schneider[1]; *[1]SCIEX, Concord, ontario*

MP 478 **Exploring Helical Electric Fields in Transmitting Ions at Ambient Pressure**; Adam L. Hollerbach[1]; Aneesh Prabhakaran[1]; Jung Lee[1]; Sandilya V.B. Garimella[1]; Randolph V. Norheim[1]; Gordon A. Anderson[2]; Adam G. Ryan[1]; John M. Lindquist[1]; Yehia M Ibrahim[3]; *[1]Pacific Northwest National Laboratory, Richland, Washington; [2]GAA Custom Electronics, LLC, Kennewick, WA; [3]Pacific Northwest National Laboratory, Richland, WA*

MP 479 **Enhanced Mass Spectrometry Detection of Organic Explosives Using Adducting Agents in Ambient Desorption Ionization**; Changtong Hao[1]; Daniel Eikel[1]; Jimmie C Oxley[2]; Michael Chapman[2]; Cynthia M. Suarez[1]; *[1]Advion Inc., Ithaca, NY; [2]University of Rhode Island, Kingston, RI*

MP 480 **Development of novel ICP-MS-CRIS instrumentation hyphenating collinear resonance ionisation spectroscopy (CRIS) with ICP-MS for ultra-trace analysis of radionuclides**; Giles Edwards[1, 2]; Matthew Duggan[1]; Holly Perrett[1]; Samuel Smithies[2]; Chris Yates[2]; Kieran Flanagan[1, 2]; *[1]The University of Manchester, Manchester, United Kingdom; [2]Artemis Analytical Ltd, Manchester, United Kingdom*

MP 481 **You Too Can LTQ: Revitalizing Linear Ion Traps Using Digital Waveform Technology**; Christopher Anderson[1]; Adam P. Huntley[2]; Gordon A. Anderson[1]; Brian H. Clowers[2]; *[1]GAA Custom Electronics, LLC, Kennewick, WA; [2]Washington State University Department of Chemistry, Pullman, WA*

MP 482 **AI-enabled Machine Vision of Graphical Mass Spec Data: Rapidly Enabling AI Mass Specs in the Lab and the Field**; David P Fries[1]; Andre Serafim[1]; *[1]Guided Particle Systems, Pensacola, FL*

INSTRUMENTATION: NEW DEVELOPMENTS IN IONIZATION AND SAMPLING
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MP 483 **Handheld Probe with Position Sensor Feedback for Real-time, Minimally-invasive Analysis of Objects In Situ**; G. Asher Newsome; *Smithsonian Museum Conservation Institute, Suitland, MD*

MP 484 **Hydrophobic coated nanoelectrospray emitters increase sensitivity in proteomics applications**; Ireshyn S Govender; *Council for scientific and industrial research, Pretoria, South Africa*

MP 485 **Impact of environmental factors on EUV-induced plasma ions during sampling with an ion transfer and high-resolution TOF-MS analysis**; Niklas Pengemann[1]; Sanna Benter[1]; Laura Lehmann[1]; Lena Mokros[1]; Franziska Schuler[1]; Linus Nagel[2]; Adelind Elshani[2]; Sascha Brose[2]; Annika Bonhoff[2]; Carlo Holly[2]; Peter Gust[1]; Hendrik Kersten[1]; Thorsten Benter[1]; *[1]University of Wuppertal, Wuppertal, Germany; [2]RWTH Aachen, Aachen, Germany*

MP 486 **Mass spectrometer interface visualisation techniques in atmospheric pressure and vacuum sections**; Roch Andrzejewski[1]; Andrew Entwistle[1]; Philip Albericci[1]; Jeff Chadbourne[1]; Benjamin Brown[1]; *[1]Shimadzu Research Laboratory (Europe) Ltd, Manchester, United Kingdom*

MP 487 **Design of a Dual Ion Source coupled to HRMS to enhance the chemical characterization of comprehensive 2D-LC approaches**; Marvin Häßler[1]; Katharina Wetzel[1]; Juan F Ayala-Cabrera[2]; Oliver J Schmitz[1]; *[1]University of Duisburg-Essen Applied Analytical Chemistry (AAC), Essen, Germany; [2]Department of Analytical Chemistry, University of the Basque Country, Leioa, Spain*

MP 488 **Novel Photoionization Sources for Improved Sensitivity in Economical Mass Spectrometers for Atmospheric Trace Gas Monitoring**; Kevin Wokosin[1]; Steven J. Kregel[2]; Eric Chow[2]; Timothy H. Bertram[1]; *[1]University of Wisconsin-Madison, Madison, WI; [2]Bradley University, Peoria, IL*

MP 489 **Multi-Pressure Chemical Ionization Mass Spectrometry: Comprehensive Analysis of Complex Gas Mixtures**; Henning Finkenzeller[1, 2]; Aleksei Shcherbinin[2]; H.-J. Jost[2]; Netta Vinkvist[1]; Jyri Mikkilä[2]; Jussi Kontro[2]; Juha Kangasluoma[1]; Matti Rissanen[3, 4]; *[1]Institute for Atmospheric and Earth System Research/ Department of Physics, Faculty of Science, University of Helsinki, Helsinki, Finland; [2]Karsa Ltd., Helsinki, Finland; [3]Aerosol Physics Laboratory, Physics Unit, Faculty of Engineering and Natural Sciences, Tampere University, Tampere, Finland; [4]Department of Chemistry, Faculty of Science, University of Helsinki, Helsinki, Finland*

MP 490 **State-of-the-art Rapid Stepped Collision Energy in a modified Orbitrap Astral MS**; Matthew James Garland[1]; Bernd Hagedorn[2]; Hamish Stewart[1]; Eduard Denisov[1]; Tabiwang Arrey[1]; Johannes Petzoldt[1]; Eugen Damoc[1]; Christian Hock[1]; *[1]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

MP 491 **Probing Ions from Deeply Embedded Plasmas Energy Distribution Analysis and Comparison of Ion Transfer Units**; Sanna Benter[1]; Niklas Pengemann[1]; Hendrik Kersten[1]; Thorsten Benter[1]; *[1]University of Wuppertal, Wuppertal, Germany*

MP 492 **Developing an ultra-sensitive metabolomics platform for low-abundance sample analysis using advanced annotation tools for molecular identification**; Nicholas S Ly[1]; Andrew T Quaile[1]; J. Rafael Montenegro-Burke[1]; *[1]University of Toronto, Toronto, ON*

MP 493 **Signal-to-Noise Ratio Enhancement Using a High-Speed Ion Shutter for IR-MALDESI-MS**; David C Muddiman[1]; Seth M Eisenberg[1]; Fan Pu[2]; James W Sawicki[3]; David Chang-Yen[3]; David Hernandez[3]; Jonathan D Trumbull[3]; Russell R Kibbe[1]; Alena N Joignant[1]; Jon D Williams[3]; Nathaniel L Elsen[3]; Andrew Radosevich[3]; *[1]North Carolina State University, Raleigh, NC; [2]AbbVie Inc, North Chicago, IL; [3]AbbVie, Inc., North Chicago, IL*

MP 494 **Robust ultra-sensitive positive mode chemical ionization mass spectrometry enabled by Uronium: ion production via X-ray-assisted sublimation of solids**; Aleksei Shcherbinin[1]; Henning Finkenzeller[2, 3]; Fariba Partovi[3, 4]; Netta Vinkvist[5]; Joona Mikkilä[3]; Jussi Kontro[3]; Jyri Mikkilä[3]; H.-J. Jost[3]; Juha Kangasluoma[2]; Siddharth Iyer[4]; Matti Riisanen[4, 5]; *[1]Karsa Ltd., Helsinki, Finland; [2]Institute for Atmospheric and Earth System Research/ Department of Physics, Faculty of Science, University of Helsinki, Helsinki, Finland; [3]Karsa Ltd, Helsinki, Finland; [4]Aerosol Physics Laboratory, Physics Unit, Faculty of Engineering and Natural Sciences, Tampere University, Tampere, Finland; [5]Department of Chemistry, Faculty of Science, University of Helsinki, Helsinki, Finland*

MP 495 **Laser Desorption on Water Microdroplets for Gas Phase Characterization**; Ayoub Badri[1]; Charles Desfrancois[1]; Frederic Lecomte[1]; Bruno Manil[1]; Nicolas Nieuwjaer[1]; *[1]Laser Physics Laboratory, CNRS UMR7538, University Sorbonne Paris Nord, VILLETANEUSE, France*

MP 496 **Coated Blade Spray-Miniature MS for On-site Analysis**; Wei Zhou[1]; Yiming Wang[2]; Wenjian Sun[2]; Janusz Pawliszyn[1]; *[1]University of Waterloo, Waterloo, ON; [2]Shimadzu Research Laboratory (Shanghai) Co., Ltd., Shanghai, China*

MP 497 **Quick bacterial differentiation from smears using filter paper, vacuum matrix-assisted ionization (vMAI)**; Jessalyn Aquilino[1, 2]; Charles N McEwen[1, 2]; Milan Pophristic[1, 2]; Adetoun Adeniji-Adele[1]; John Tomsho[1]; I-Chung Lu[3]; Sarah Trimpin[2, 4]; Barbara Larsen[5]; *[1]Saint*

Joseph's University, PHILADELPHIA, PA; [2]MSTM, Newark, DE; [3]National Cheng Kung University, Tainan, Taiwan; [4]Wayne State University, Detroit, MI; [5]Larsen Scientific Consulting, West Chester, Pennsylvania

MP 498 **Coupling Accelerated Microdroplet Reactions on LC-MS Systems: Toward Absolute Quantification and Deep Lipidomics**; Abraham Kwame Badu-Tawiah[1]; Niraj Panday[1]; *[1]The Ohio State University, Columbus, OH*

MP 499 **Development of a ThermoGravimetric Analysis-Time of Flight Mass Spectrometer for the Analysis of Thermal and Chemical Characteristics of Battery Materials**; ByungGwun Jin[1]; Euiyoung Ji[1]; So-yeon Kim[2]; Yeu Young Youn[2]; Hyunsik Kim[1]; Yangsun Kim[1]; *[1]ASTA, Suwon, South Korea; [2]LG Energy Solution, Yuseong-Gu, South Korea*

MP 500 **Sensitive, Accurate, Affordable, and Rapid Detection of Lanthanide and Actinide Complexes using the Plate Source on a Multi-Port Ionization System**; Ravin A Rayes[1]; Sarah Trimpin[1]; *[1]Wayne State University, Detroit, MI*

MP 501 **Novel Nano-Electrospray Ion Source for Charge Detection Mass Spectrometry**; Jakub Ujma[1]; Dale A Cooper-Shepherd[1]; Anisha Haris[1]; Rachel Koerber[2]; Nicholas Smith[1]; Hong Ly[1]; Charles Murphy[2]; Chris Wheeldon[1]; Joseph Michienzi[2]; Kevin Giles[1]; Ian Trivett[1]; Nick Tomczyk[1]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Waters Corporation, Milford, MA*

MP 502 **Miniaturization and integration of SICRIT into the inlet capillary of a LC-MS instrument – towards kinetic control of ionization**; Jan-Christoph Wolf[1]; Ciara Conway[1, 2]; Atsuhiko Toyama[3]; Markus Weber[1, 2]; *[1]Plasmion GmbH, Augsburg, Germany; [2]Technical University of Munich, München, Germany; [3]Shimadzu Scientific Instruments, Columbia, MD*

MP 503 **Intact (t-BuLi)4+• radical ions and [(n-BuLi)6Li]+ even electron ions by LIFDI MS**; H. Bernhard Linden[1]; Mathias H. Linden[1]; Pim Puylaert[2]; Jens Beckmann[2]; *[1]Linden CMS GmbH, Weyhe, Germany; [2]University Bremen, Bremen, Germany*

MP 504 **Orbitrap Exploris without downtime between LIFDI and ESI spectra acquisitions**; Mathias H. Linden[1]; Kerstin Strupat[2]; H. Bernhard Linden[3]; *[1]Linden CMS GmbH, Weyhe, Germany; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [3]Linden CMS GmbH, Weyhe, Germany*

MP 505 **Photoionization Mass Spectrometry as an Advanced Tool for Process Control and Technological Advancements**; Sven Ehlert[1]; Jan Heide[1, 2]; Kevin Schnepel[2]; Fabian Carl[2]; Hendryk Czech[2]; Ralf Zimmermann[2]; *[1]Photonion GmbH, Schwerin, Germany; [2]University of Rostock, Chair of Analytical Chemistry and Dept. of Life, Light and Matter, Rostock, Germany*

MP 506 **Simultaneous Sulfur and Fluorine Detection by Nitrogen Microwave ICP-Chemical Ionization MS in Negative Mode for Standard-free Quantitation of Compounds**; Mustakim Zaman[1]; Jordan L Tanen[1]; Kaveh Jorabchi[2]; *[1]Georgetown University, Washington, DC; [2]Georgetown Univ., Washington, DC*

MP 507 **Flow Rate Influences Ionization Efficiency and Not Droplet Size for Vibrating Sharp-Edge Spray Ionization (VSSI)**; Thomas Hughart[1]; Chandrima Banerjee[1]; Christina Denison[1]; Vikum K. Dewasurendra[2]; Amanda DeVor[1]; Matthew B. Johnson[2]; Peng Li[1]; Stephen J Valentine[1]; *[1]Department of Chemistry, West Virginia University, Morgantown, West Virginia; [2]Department of Physics, West Virginia University, Morgantown, West Virginia*

MP 508 **Tailoring Ionization Response and Mitigating Ion Suppression by Thermal Analysis Hyphenation and Advanced Laser Ionization Mass Spectrometry**; Fabian Etscheidt[1, 2]; Christopher Paul Rüger[2, 3]; Anika Neumann[2]; Carolin Schwarz[2]; Silvia Vesga Martínez[2]; Paul Kösling[2]; Sven Ehlert[1]; Andreas Walte[1]; Thorsten Streibel[2, 4]; Ralf Zimmermann[2, 4]; *[1]Photonion GmbH, Schwerin, Germany; [2]University of Rostock, Chair of Analytical Chemistry and Dept. of Life, Light and Matter, Rostock, Germany; [3]International Joint Laboratory, iC2MC: Complex Matrices Molecular Characterization, Harfleur, France; [4]Helmholtz Munich, Munich, Germany*

MP 509 **Nanobubbles in bulk solution and in electrosprayed microdroplets accelerate chemical reactions during ESI-MS**; Bincy Binny[1]; George Joseph[1]; Andre R Venter[1]; *[1]Western Michigan University, Kalamazoo, MI*

MP 510 **Surface Acoustic Wave-Based Sampling of Extracellular Vesicles for Lipidomic Screening**; Theresa Evans-Nguyen[1]; Ashton Taylor[1]; Yuqi Huang[1]; Brianna Jones[1]; Qian Ma[1]; Larry Campbell[2]; Niketa Patel[1]; Venkat Bhethanabotla[1]; *[1]University of South Florida, Tampa, FL; [2]Bedrock Scientific, Milton, ontario*

MP 511 **Improved Analysis of His-Tagged Proteins by DESI-MS with Ni-NTA Magnetic Beads**; Christopher J Taylor[1]; Sumana Parvin[1]; Andre R Venter[1]; *[1]Western Michigan University, Kalamazoo, MI*

MP 512 **Further Development and Optimization of a Successfully Implemented Accumulation Ion Source**; Laura Lehmann[1]; Niklas Pengemann[1]; Hendrik Kersten[1]; Thorsten Benter[1]; *[1]University of Wuppertal, Wuppertal, Germany*

ION MOBILITY: FUNDAMENTALS
513-522

MP 513 **Assessing the Effects of Ionization Parameters on Formation of Protomers for Fentanyl Analogues and Novel Psychoactive Substances**; Copeland Johnson[1]; Heidi Sabatini[1]; Ralph Aderorho[1]; Christopher Chouinard[1]; *[1]Clemson University, Clemson, SC*

MP 514 **A Derivation of Ion Drift Velocity for Ion Mobility Spectrometry using Statistical Mechanics**; Glenn E. Spangler; *Technispan LLC, Lutherville, MD*

MP 515 **Ion transport via a travelling wave in a cylindrical guide**; Anson Lee[1]; Duncan Lockerby[1]; Steve Bajic[2]; Gordon Jones[2]; James Kermode[1]; *[1]University of Warwick, Coventry, United Kingdom; [2]Waters Corporation, Wilmslow, United Kingdom*

MP 516 **Investigation of molecular dynamics methods for predicting high and low field ion mobilities of small molecular ions**; Michelle Rajkovic[1]; Walter Wissdorf[1]; Thorsten Benter[1]; *[1]University of Wuppertal, Wuppertal, Germany*

MP 517 **Rapid Compaction of Activated Protein Ions in the Gas Phase**; Talitha K Richards[1]; Nicholas B. Borotto[1]; *[1]University of Nevada Reno, Reno, NV*

MP 518 **Comparison of Tristate Ion Shutter used in a HiKE-IMS between experimental data and simulations with IDSimF**; Adem Bulut[1]; Walter Wissdorf[1]; Thorsten Benter[1]; *[1]University of Wuppertal, Wuppertal, Germany*

MP 519 **Characterizing the Effects of PFAS Binding on Protein Structure and Stability**; EBUNOLUWA O KUKOYI[1]; Kenneth W Lee[1]; *[1]Brigham Young University, Provo*

MP 520 **Accurate Modeling of Ion Mobility and Ion Loss Processes Using a Hard Sphere Collision Model in SIMION**; Sidney E. Buttrill, Jr.; *Consultant, Palo Alto, CA*

MP 521 **Identification of isotopic mobility shifts at arbitrary fields and the tendency of ions to minimize rotational kinetic energy**; Carlos Larriba Andaluz; *Purdue University, Indianapolis, IN*

MP 522 **Addressing Limitations in Cyclic Ion Mobility Spectrometry Separations of Isomers using Non-Covalent Complexation**; Kenneth W Lee; *Brigham Young University, Provo, UT*

ION MOBILITY: STRUCTURE
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MP 523 **Rapid Differentiation of Amino Acid Enantiomers via Crown Ether Complexation Using Ion Mobility-Mass Spectrometry**; Michael J Kelley[1]; GAOYUAN LU[2]; Zhijun Zhu[1]; Shuling Xu[2]; Vu Ngoc Huong Tran[2]; Lingjun Li[1, 2]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [2]School of Pharmacy, University of Wisconsin-Madison, Madison, WI*

MP 524 **Structural Insights into Enantiomer Differentiation using Computational Modeling and Ion Mobility – Mass Spectrometry**; Emma R. Remish[1]; Benjamin K. Blakley[1];

Eric Dybeck[2]; Valeria Guidolin[3]; Jody C. May[1]; John A. McLean[1]; [1]*Department of Chemistry, Vanderbilt University, Nashville, TN; [2]MedDesign, Pfizer, Cambridge, MA; [3]PharmSci Smal Molecule, Analytical Research and Development, Pfizer, Groton, CT*

MP 525 **Superior Differential Ion Mobility Spectrometry of Pendular Macromolecules Using Flexible Low-Frequency Rectangular Waveforms**; Egor Gusachenko[1]; Hayden A Thurman[1]; Gordon A. Anderson[2]; Alexandre A Shvartsburg[1]; [1]*Wichita State University, Wichita, KS; [2]GAA Custom Electronics, LLC, Kennewick, WA*

MP 526 **Investigating the Structural Stability of Ribonucleic Acid Hairpins Encapsulated in Lipid Nanoparticles by Native Ion Mobility-Mass Spectrometry**; Caela P Fedraw[1]; Courteney R Dufrene[1]; Brandon T. Ruotolo[1]; [1]*University of Michigan, Ann Arbor, MI*

MP 527 **Collision-Induced Unfolding of High-m/z Native-like Protein Ions within a Trapped Ion Mobility Device**; Olakunle Akinola[1]; Nicholas B. Borotto[2]; [1]*University of Nevada, Reno, Reno, NV; [2]University of Nevada, Reno, Nevada*

MP 528 **Two-Step Thermal Unthreading Mechanism of Lasso Peptide Syanodin I**; Kevin Jeanne Dit Fouque[1]; Miguel Santos-Fernandez[1]; Ukesh Karki[1]; Severine Zirah[2]; Prem P Chapagain[1]; Julian D Hegemann[3]; Francisco Fernandez-Lima[1]; [1]*Florida International University, Miami, FL; [2]National Museum of Natural History, Paris, France; [3]Technical University of Braunschweig, Braunschweig, Germany*

MP 529 **Streamlining Small Molecule Identification with Ion Mobility-Mass Spectrometry, Computational Chemistry and Bayesian Statistics**; Valeria Guidolin[1]; Eric Dybeck[2]; Md Kamrul Hasan Khan[3]; Ke Wang[3]; [1]*Pfizer, Groton, CT; [2]Pfizer Inc., Cambridge, MA; [3]Pfizer Inc., Groton, CT*

MP 530 **Characterizing gas-phase protein structures using ion-mobility mass-spectrometry and adaptive biased molecular dynamics, through solvent accessible-surface guided compaction**; Viraj D Gandhi[1, 2]; Carlos Larriba-Andaluz[1]; [1]*Purdue Univeristy, West Lafayette, IN; [2]AUBURN UNIVERSITY, Auburn, AL*

MP 531 **Unraveling the Mobility-Aligned Collision-Induced Dissociation (CID) Pathways of Fentanyl Analogues**; Bradley B Garrison[1]; Drew Whitman[1]; Ralph Aderorho[1]; Christopher Chouinard[1]; [1]*Clemson University, Clemson, SC*

MP 532 **Applying trapped ion mobility spectrometry to engineer switchable domains mimicking regulatory RNAs involved in cancers and infectious diseases**; Michael Addo[1]; Thomas Kenderdine[2]; Yassaghi Ghazaleh[2]; Daniele Rollo[2]; Margrate Anyawu[2]; Daniele Fabris[2]; [1]*University of Connecticut, Storrs, CT; [2]University of Connecticut, Storrs*

MP 533 **Metal Induced Rearrangements in Polyproline Using Ion Mobility Mass Spectrometry**; Anthony J Pestritto[1]; David E. Clemmer[2]; [1]*Indiana University, Bloomington, IN; [2]Indiana University Bloomington, Bloomington, IN*

MP 534 **Leveraging electron capture dissociation to elucidate the gas-phase unfolding pathway of large proteins**; Michael R. Armbruster[1]; Joseph C. Meeuwsen[2]; Yury V. Vasil'ev[2]; Brandon T. Ruotolo[1]; [1]*Department of Chemistry, University of Michigan, Ann Arbor, MI; [2]Agilent Technologies, Inc., Corvallis, OR*

MP 535 **Structural Characterization of Unsaturated Fatty Acids and Lipids via Chemical Epoxidation of C=C Positional and Geometrical Isomers using PS-IM-MS/MS**; Iffat Jerin[1]; Kimberly Youandi Kartowikromo[1]; Alexis Rae Toney[1]; Kristen Marshall[1]; Ahmed M Hamid[1]; [1]*AUBURN UNIVERSITY, Auburn, AL*

MP 536 **Cyclic Ion Mobility and High Resolution-Mass Spectrometry to Study Dependence of Degradation Pathway on PFAS Structure**; Meagan Gadzuk-Shea[1]; Zekun Liu[1]; Andrew Healy[1]; Zijie Beryl[1]; [1]*Claros Technologies, Minneapolis, MN*

MP 537 **Identifying the stability determinants of siRNA biotherapeutics by trapped ion mobility spectrometry mass spectrometry**; Sarah Mutchek[1]; William McIntyre[1]; Michael Addo[1]; Vladimir V. Papov[2]; Scott Pennino[2]; Daniele Fabris[1]; [1]*University of Connecticut, Storrs, CT; [2]Boehringer Ingelheim Pharmaceuticals, Inc., Ridgefield, CT*

MP 538 **Thermal Stability Analysis of RNase A Conformations Using vT-ESI-IMS-MS**; Minh Tram Ha[1]; Sarah O'Keefe[1]; David E. Clemmer[1]; [1]*Indiana University Bloomington, Bloomington, IN*

MP 539 **Structural Analysis of Divalent Cation Bound α-Synuclein by Cross-linking Ion Mobility-Mass Spectrometry**; Ankita B Gurav[1]; Ian K. Webb[1]; [1]*Indianapolis University- Indianapolis, Indianapolis, IN*

LC/MS: GENERAL
540-570

MP 540 **Validation of LC-MS/MS Method for Quantification of Iodixanol in AAV Gene Therapy Product**; Pamela Kell[1]; Xuntian Jiang[1]; [1]*Washington University School of Medicine, St. Louis, MO*

MP 541 **Simultaneous Chiral Determination of Ten Tobacco Alkaloids in E-liquids Using Liquid Chromatography-Tandem Mass Spectrometry Method**; Shulei Han[1]; Lili Cui[1]; Yaning Fu[1]; Hongjuan Wang[1]; Yushan Tian[1]; Xiao Li[1]; Huan Chen[1]; Hongwei Hou[1]; [1]*China National Tobacco Quality Supervision & Test Centre, Zhengzhou, China*

MP 542 **Analysing the HYE Species Mix: A Comprehensive Reference Standard for Mass Spectrometry Quality Control and Method Development**; Marco Harms[1, 2]; Stephan Michalik[2]; Jana Richter[3]; Tabiwang Arrey[3]; Eugen Damoc[3]; Kristin Surmann[1, 2]; [1]*ProTec Diagnostics GmbH, Greifswald, Germany; [2]University Medicine Greifswald, Greifswald, Germany; [3]Thermo Fisher Scientific, Dreieich, Germany, Bremen, Germany*

MP 543 **Identifying Tautomeric Metabolite Substrates of Macrophage Migration Inhibitory Factor (MIF) Tautomerase Activity**; Michael W Christopher[1]; Liulin Deng[2]; Daniel Debord[2]; Boone M Prentice[1]; Timothy J Garrett[1]; [1]*University of Florida, Gainesville, FL; [2]MOBILion Systems, Inc., Chadds Ford, PA*

MP 544 **Untargeted Metabolomics Reveals the Effects of Cricket Powder on the Intestinal Microbiome in High-LDL Individuals**; Pitchayaporn Sukkha[1]; NACHON RAETHONG[1]; DUNYAPORN TRACHOOTHAM[1]; AREE PRACHANSUWAN[1]; SARUNYA KITDUMRONGTHUM[1]; WARANGKANA SRICHAMNONG[1]; JARUWAN CHIMASANGKANAN[1]; WIMONPHAN CHATHIRAN[1]; [1]*Institute of Nutrition, Mahidol University, Phutthamonthon, Thailand*

MP 545 **Accurate LC-MS/MS quantification of hyaluronic acid in biological matrices using a double isotopic standard addition method**; Giovanna Baron[1]; Simone Manzi[1]; Giacomo Mosconi[1]; Alessandra Anna Altomare[1]; Marina Carini[1]; Giancarlo Aldini[1]; [1]*University of Milan, Milano, Italy*

MP 546 **Analysis of PFAS in Water Using Solid-Phase Extraction and LC-MS/MS with a High-Purity Activated Carbon Delay Column**; YUKINORI KONNO[1]; Yuko Yui[2]; Takumi Kunieda[2]; Reika Takahara[2]; Kazuyuki Ishii[2]; Manabu Takayanagi[2]; Shigenori Ota[2]; Kousuke Kabe[2]; Hiroshi Hayashida[2]; [1]*GL Sciences Inc, Fukushima, Japan; [2]GL Sciences Inc., Iruma-shi, Japan*

MP 547 **Mass Spectral Analysis of Secondary Metabolites in Pepper Cultivars Grown Under Saline Conditions**; Devanand Luthria; *USDA, Beltsville, MD*

MP 548 **Highly Sensitive Quantification of N-Nitroso Timolol Impurity in Timolol API Using Liquid Triple qudrupole chromatography mass spectrometry**; Preeti Bharatiya; *Agilent technologies, Bangalore, India*

MP 549 **Using Agilent Hybrid Multisampler with Triple Quadrupole Mass Spectrometer to Solve Solvent Effect in PFCAs and its Precursor FTOHs Analysis**; Zhihui Lin[1]; Jianzhong Li[2]; Chunye Sun[3]; Winnie Hung[4]; [1]*Agilent Technologies (China), Guangzhou, China; [2]Agilent Technologies (China), Beijing, China; [3]Agilent Technologies (China), Shanghai, China; [4]Agilent Technologies (China), Hong Kong, China*

MP 550 **Correlating HCD and CID Energies for Reliable MS/MS Spectral Matching Across Different LCMS Systems**; Feng Qiu[1]; Li Chen[1]; Michel Van Strien[2]; Tarang Nema[3]; Danielle Dinallo[1]; Yanpeng Hou[1]; *[1]Advanced Analytical, International Flavors and Fragrances, Union Beach, NJ; [2]Advanced Analytical, International Flavors and Fragrances, Tilburg, Netherlands; [3]Consumer Product Analytics, International Flavors and Fragrances, Singapore, Singapore*

MP 551 **Evaluating System Robustness of a High-Sensitivity Triple Quadrupole LC/MS for PFAS Analysis in Food Matrix Over an Extended Period**; PETER WEIDNER[1]; Behrooz Zekavat[1]; Anabel Fandino[1]; *[1]Agilent Technologies, Inc., Santa Clara, CA*

MP 552 **Quantification of HbA1C via Tryptic Digestion using Tandem Mass Spectrometry and Ion Mobility**; Esabella R Powers[1]; Michael W Christopher[1]; Boone M. Prentice[1]; Richard A. Yost[1]; Timothy J Garrett[1, 2]; *[1]University of Florida, Department of Chemistry, Gainesville, FL; [2]University of Florida, College of Medicine, Department of Pathology, Immunology, and Laboratory Medicine, Gainesville, FL*

MP 553 **Analysis of Synthetic Peptide Mixture to Improve Understanding of Breakthrough Peptides in Liquid Chromatography**; Meghan Burke[1]; Anh Tran[1]; Guanghui Wang[1]; William E Wallace[1]; Steve E Stein[1]; *[1]National Institute of Standards and Technology, Gaithersburg, MD*

MP 554 **Optimizing Trapping Column Parameters and Loading Conditions for Nanoflow LC-MS**; Siqi Huang[1]; Thy Truong[2]; Chao Wang[1]; Xiaofeng Xie[2]; Ryan Kelly[1, 2]; *[1]Brigham Young University, Provo, UT; [2]MicrOmics Technologies LLC, Spanish Fork, UT*

MP 555 **A Comparative Analysis of siRNA Applications Across Various LC-MS Platforms**; Sergio Madera[1]; Ryan Hill[2]; *[1]Eli Lilly and Company, INDIANAPOLIS, IN; [2]Eli Lilly and Company, Indianapolis, IN*

MP 556 **Adapting a low-cost pipetting robot for autosampling in custom nanoLC workflows**; Nathaniel B Axtell[1]; Kei G. I. Webber[1]; Andrew Sandberg[1]; Ryan Kelly[1]; *[1]BYU, Provo, UT*

MP 557 **Modular nanoLC system with single-cell sensitivity and a measurement throughput of 200 samples per day**; Xiaofeng Xie[1]; Thy Truong[1]; Ryan Kelly[1]; *[1]MicrOmics Technologies LLC, Spanish Fork, UT*

MP 558 **A low level, carryover free and wide Range, LC-MS/MS method for quantitation of Semaglutide from human plasma**; Nitin Satish Shukla[1]; Samruddha Chavan[1]; Nitish Ramchandra Suryawanshi[1]; Devika Tupe[1]; Siddhesh Ghadi[1]; Ramesh Manigiri[1]; Shalu Nair[1]; Jitendra Kelkar[1]; Pratap Rasam[1]; Satyajit Ghavane[1]; *[1]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India*

MP 559 **Enhanced separation performance with reduced carry-over for proteomics analyses using novel nanoLC and the timsTOF HT**; Ines Metatla[1]; Chiara Guerrera[1]; Cerina Chhuon[1]; Petra Martinović[2]; Mario Mirabelli[3]; Pierre-Olivier Schmit[4]; Goran Mitulović[5]; *[1]Necker Proteomics, Université Paris Cité - Structure Fédérative de Recherche Necker, INSERM US24/CNRS UAR3633, Paris, France; [2]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [3]Bruker Switzerland AG, Fällanden, Switzerland; [4]Bruker France SAS, Wissembourg, France; [5]Bruker Austria GmbH, Vienna, Austria*

MP 560 **Minimizing the impact of sample carryover affinity purification mass spectrometry (AP-MS) experiments**; W. Hayes McDonald[1]; Kaeli N Bryant[1]; Timothy L Cover[2]; Goran Mitulovic[3]; Mario F Mirabelli[4]; *[1]Vanderbilt University, Nashville, TN; [2]Vanderbilt Medical Center, Nashville, TN; [3]Bruker Austria GmbH, Vienna, Austria; [4]Bruker Switzerland AG, Fällanden, Switzerland*

MP 561 **StayClean Ion Source LC-MS/MS for Analysis of PFAS in Surface Water/Wastewater Using Automated SPE Based on EPA Method 1633**; Jingcun Wu[1]; Sheng-Suan (Victor) Cai[2]; Autumn Payne[2]; Jesse Leonard[2]; Jacob Jalalib[2]; *[1]PerkinElmer Inc., Woodbridge, ON; [2]PerkinElmer US, LLC, Shelton, CT*

MP 562 **Quantitation of Methyl Pentose from Pneumococcal Polysaccharide vaccine using LC-MS/MS**; Nitish Ramchandra Suryawanshi[1]; Chetan Dhatunde[2]; Swapnil Sawant[2]; Samruddha Chavan[1]; Nitin Satish Shukla[1]; Devika Tupe[1]; Siddhesh Ghadi[1]; Ramesh Manigiri[1]; Shalu Nair[1]; Satyajit Ghavane[1]; Jitendra Kelkar[1]; Pratap Rasam[1]; *[1]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India; [2]Spinco Biotech Pvt. Ltd.,, Chennai, India*

MP 563 **A Next Generation Ion Source for Robust, Low-Flow LC/MS Workflows Enables Sensitive and Precise Peptide Quantitation and Global Proteomics Analysis**; John Crellin[1]; Katherine Walker[1]; Yuan Lin[1]; Kevin Yang[1]; Colin Paul[2]; Dominique Figueroa[1]; Pradip Shahi Thakuri[1]; Joshua Silveira[1]; Eloy Wouters[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientfic, San Jose, CA*

MP 564 **Evaluation of post-column dead volume for nanoLC when using integrated and separate electrospray emitters**; Ryan Kelly[1]; Chao Wang[1]; Siqi Huang[1]; Thy Truong[2]; Xiaofeng Xie[2]; *[1]Brigham Young University, Provo, UT; [2]MicrOmics Technologies LLC, Spanish Fork, UT*

MP 565 **Evaluation of system robustness for a high performance small form factor LC/MS Single Quadrupole System**; Patrick M Batoon[1]; Xiaoli Dong[1]; Lee Bertram[2]; Russell Burge[2]; Olivier Chevallier[2]; *[1]Agilent Technologies Inc., Santa Clara, CA; [2]Agilent Technologies, Santa Clara, CA*

MP 566 **Evaluating a tandem LC workflow for eliminating mass spectrometer idle time**; Runsheng Zheng[1]; Martin Rendl[1]; Alec C Valenta[2]; Yuan Lin[3]; Christopher Pynn[1]; Maksim Daniliuk[4]; Ece Aydin[1]; Robert Van Ling[5]; Wim Decrop[6]; Martin Samonig[7]; Anne Morgenstern[1]; *[1]Thermo Fisher Scientific, Germering, Germany; [2]Thermo Fisher Scientific, Somerset, NJ; [3]Thermo Fisher Scientific, Sunnyvale, CA; [4]Thermo Fisher Scientific, Vilnius, Lithuania; [5]Thermo Fisher Scientific, Breda, Netherlands; [6]Thermo Fisher Scientific, Courtaboeuf, France; [7]Thermo Fisher Scientific, Vienna, Austria*

MP 567 **A comparative assessment of DIA and DDA mass spectrometry approaches for tear fluid proteomics**; Saleh Ahmed[1]; Jeremy Altman[1]; Garrett Jones[1]; Drew Mayernik[1]; Eliza Williams[1]; Tae Jin Lee[1]; Wenbo Zhi[1]; Shruti Sharma[1, 2]; Ashok Sharma[1, 2]; *[1]Center for Biotechnology and Genomic Medicine, Medical College of Georgia, Augusta University, Augusta, GA; [2]Department of Ophthalmology, Medical College of Georgia, Augusta University, Augusta, GA*

MP 568 **A Gas-shield Corona Discharge Atmospheric Pressure Chemical Ionization Interface for Liquid Chromatography Mass Spectrometry**; Shin-Ting Wang[1]; Jenn-Feng Sheen[1]; *[1]National Formosa University, Yunlin County, Taiwan*

MP 569 **Optimized plasma proteomics pipeline from sample to figure enhancing large-scale studies for biomarker discovery**; Marcello F Stein[1]; Martin Schirmer[2]; Leander Runtsch[1]; Katrin Hartinger[1]; Kuan-Ting Pan[1]; Petra Martinovic[2]; Florian Busch[3]; Nils Kulak[1]; *[1]PreOmics GmbH, Martinsried, Germany; [2]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [3]Bruker Switzerland AG, Fällanden, Switzerland*

MP 570 **Extended Lifespan of Innovative Column Assemblies in Low-Flow Ion Sources**; Katherine Walker[1]; Robertas Žilinskas[2]; Vytautas Tamosiunas[2]; Jeff Op De Beeck[3]; Joshua A Silveira[1]; Runsheng Zheng[4]; Cornelia Boeser[1]; Romain Huguet[1]; Eloy R. Wouters[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Vilnius, Lithuania; [3]Thermo Fisher Scientific, Ghent, Belgium; [4]Thermo Fisher Scientific, Germering, Germany*

LIPIDS: TARGETED AND QUANTITATIVE ANALYSIS
571-584

MP 571 **Optimizing Sphingolipid Quantitation: Evaluating Base Hydrolysis and Chromatographic Strategies in LC-MS/MS Analysis**; Josie Daldegan Rezende[1]; Yuanyan Ji[1]; Anh Tran[1]; Jace W. Jones[1]; *[1]University of Maryland, School* *of Pharmacy, Department of Pharmaceutical Sciences, Baltimore, MD*

MP 572 **Targeted MS3 Approach for Quantifying Triacylglycerols with Resolved Fatty Acid Composition in Breast Milk using Stellar Mass Spectrometer**; Hector Gallart Ayala[1]; Magdalena Vagnerova[1]; Julijana Ivanisevic[1]; Brittany Lee[2]; Rahul Deshpande[2]; Susan Bird[3]; Philip Remes[2]; Cristina Jacob[2]; *[1]University of Lausanne, Lausanne, Switzerland; [2]Thermo Fisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific, Boston, MA*

MP 573 **Targeting Lipid Peroxidation in Barth Syndrome: LC-MS/MS Analysis of a Novel Therapeutic Approach Using Bis-Allylically-Deuterated Arachidonic Acid**; Ecem Saritas[1]; Svetlana N. Samovich[1]; Haider H. Dar[2]; Louis J. Sparvero[2]; Mert Akdogan[2]; Yulia Y. Tyurina[2]; Michail S. Shchepinov[2]; Valerian E. Kagan[2]; Hülya Bayir[1]; *[1]Columbia University, New York City, NY; [2]University of Pittsburgh, Pittsburgh, PA*

MP 574 **Development of a highly multiplexed and quantitative lipidomics panel as a laboratory diagnostic approach**; Jinyong Kim[1]; Ramesh Bokka[1]; Jisha Chandran[1]; Paul Norris[2]; Paul RS Baker[3]; Matthew J Schultz[1]; Dietrich Matern[1]; Jeff W Meeusen[1]; Akhilesh Pandey[1]; Seul Kee Byeon[1]; *[1]Mayo Clinic, Rochester, MN; [2]Sciex, Framingham, MA; [3]SCIEX, Concord, ON*

MP 575 **LC/MS detection and MS imaging of pro-ferroptotic death signals in ileum of irradiated mice. Effect of NO-donor**; Yulia Y. Tyurina[1]; Hua Tian[1]; Louis J. Sparvero[1]; Vladimir Tyurin[1]; Haider H. Dar[1]; Mert Akdogan[1]; Ecem Saritas[2]; Alexander Kapralov[1]; Michael Epperly[1]; Galina Shurin[1]; Yuri L. Bunimovich[1]; Joel Greenberger[1]; Hülya Bayir[2]; Valerian E. Kagan[1, 2]; *[1]University of Pittsburgh, Pittsburgh, PA; [2]Columbia University, New York City, NY*

MP 576 **Elucidating the reaction mechanism behind the sulfo-phospho-vanillin assay (SPVA) for quantitation total lipids as a pre-quantitation method in untargeted lipidomics**; Kari B Basso[1]; Katie Heiden[1]; Laura Bailey[1]; *[1]University of Florida, Gainesville, FL*

MP 577 **Comprehensive Profiling of Lipid Mediators Using a Charge-Switch Chemical Derivatization Strategy**; Ritchie Ly[1]; Caleb Porter[1]; Harrison Kim[1]; Adrienne Boire[1]; Justin R. Cross[1]; *[1]Memorial Sloan Kettering Cancer Center, New York, NY*

MP 578 **Analysis of lipid content and purity in LNPs with HPLC-ELSD and HPLC-MS/MS**; Till Myrach[1]; Mareike Prüfer[1]; Carsten Losch[1]; *[1]KNAUER Wissenschaftliche Geräte GmbH, Berlin, Germany*

MP 579 **Detecting edible oil adulteration using a highly sensitive triple quadrupole mass spectrometer**; Kiran Maan[1]; Dipankar Malakar[1]; Ankush Gupta[2]; Uttam Tripathi[2]; Pranav Choksi[2]; *[1]SCIEX - India, Bangalore, India; [2]Gufic Biosciences Limited, Indore, India*

MP 580 **Evaluation of the Quantification Capabilities of Untargeted Lipidomics Approaches**; Paul D Kennedy[1]; Dilrukshika S.W. Palagama[1]; Matthew J Kwiatkowski[1]; Samantha K Goodwin[1]; Miguel A Gijon[1]; *[1]Cayman Chemical Company, Ann Arbor, MI*

MP 581 **Characterization of human plasma as a reference material for lipid analysis using LC-MS**; Matthew J. Kwiatkowski[1]; Samuel L. DeLoy[1]; Dilrukshika S.W. Palagama[1]; Miguel A. Gijón[1]; Paul D. Kennedy[1]; *[1]Cayman Chemical Company, Ann Arbor, MI*

MP 582 **Development of LC-coaxial electrospray mass spectrometry method for absolute quantification of polar lipids using a single internal standard**; Niraj Kumar Panday[1]; Abraham K. Badu-Tawiah[2]; *[1]THE OHIO STATE UNIVERSITY, Columbus, OH; [2]The Ohio State University, Columbus, OH*

MP 583 **Ether Phosphatidylethanolamines Are Favored Targets For 15LOX-Derived Oxidation During Ferroptosis: LC-ESI-MS/MS Analysis Of Oxygenated Phospholipids**; Vladimir A. Tyurin[1]; Yulia Y. Tyurina[1]; Karolina Mikulska-Ruminska[2]; Alexander Kapralov[1]; Louis J. Sparvero[1]; Brian A. Kleiboeker[1]; Kazuhiro Yamada[3]; Jinming Zhao[1]; Taha Kelestemur[4]; Theodore R. Holman[5]; Yuri L. Bunimovich[1]; Yulia Nefedova[6]; Ayumi Hashimoto[7]; Dmitry I. Gabrilovich[7]; Sally E. Wenzel[1]; Ivet Bahar[8]; Valerian E. Kagan[1, 4]; Hülya Bayir[4]; *[1]University of Pittsburgh, Pittsburgh, PA; [2]Nicolaus Copernicus University in Torun, Torun, Poland; [3]Osaka Metropolitan University, Osaka, Japan; [4]Columbia University, New York City, NY; [5]University of California Santa Cruz, Santa Cruz, CA; [6]The Wistar Institute, Philadelphia, PA; [7]AstraZeneca, Gaithersburg, Maryland; [8]Stony Brook University, Stony Brook, NY 11794, USA, Stony Brook, NY*

MP 584 **Improving Selectivity and Sensitivity of Lipid Mediator Analyses by Coupling Nano-flow Chromatography with the Stellar Mass Spectrometer**; Ciara J Myer[1]; Thiago Mattos[1]; Rahul R Deshpande[1]; Susan S Bird[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

MALDI: APPLICATIONS
585-603

MP 585 **Analysis of soluble and particulate fraction of wastewaters by shotgun green proteomics MALDI-TOF MS and Aquasearch novel software application**; Damia Barcelo[1]; Montserrat Carrascal[2]; Joaquin Abian[2]; Ester Sanchez-Jimenez[2]; Carlos Perez-Lopez[3]; Antoni Ginebrada[3]; *[1]UNIVERSITY OF ALMERIA, Almeria, Spain; [2]Institute of Biomedical Research of Barcelona, CSIC, Barcelona, Spain; [3]Institute of Environmental Assessment and Water Studies,CSIC, Barcelona, Spain*

MP 586 **AD-associated Myelin Lipid Sulfatide Deficiency Leads to Spatial Lipidome and Metabolome Reorganization Revealed by MALDI/-ESI Imaging**; Ziying Xu[1]; Sylwia Stopka[2]; Srada Karmacharya[2]; Juan Henao[2]; Michael A. Kiebish[2]; Xianlin Han[1, 3]; *[1]Sam and Ann Barshop Institute for Longevity and Aging Studies, UT Health San Antonio, San Antonio, TX; [2]BPGbio, Inc., Framingham, MA; [3]Department of Medicine, UT Health San Antonio, San Antonio, TX*

MP 587 **Enabling the Detection of Per- and Polyfluoroalkylphosphonic acids with MALDI-TIMS-TOF Mass Spectrometry**; Kira Baker[1]; Tian (Autumn) Qiu[1, 2]; *[1]Michigan State University, Department of Chemistry, East Lansing, Michigan; [2]Center for PFAS Research, Michigan State University, EAST LANSING, Michigan*

MP 588 **Rapid Screening for PFAS in water samples using a benchtop linear MALDI-TOF Mass Spectrometer**; Caroline Jones[1]; Tom Abban[1]; Milaan Thirukumaran[2]; Francine E Yanchik-Slade[2]; Matthew E. Openshaw[1]; *[1]Kratos Analytical Ltd., Manchester, United Kingdom; [2]Shimadzu Scientific Instruments, Columbia, MD*

MP 589 **Quantification of PFAS in the ppb-ppm Range Using AP/MALDI and High-Resolution Mass Spectrometry**; Eugene Moskovets[1]; Caleigh O'Connor[2]; Nivedita Bhattacharya[2]; Konstantin Novoselov[2]; *[1]MassTech Inc, Columbia, MD; [2]MassTech, Columbia, MD*

MP 590 **Nanoparticle-Assisted LDI MS and Machine Learning Enable Non-Invasive Diagnosis of Moyamoya Disease**; Yudian Xu[1, 2]; Kun Qian[2]; Wei Xu[1]; *[1]RenJi Hospital, School of Medicine, Shanghai Jiao Tong University, Shanghai, China; [2]Shanghai Jiao Tong University, Shanghai, China*

MP 591 **Mechanistic insights decode laser desorption/ionization effect of self-assembled TiO2/Au nanoarray**; Yanyan Li; *shanghai jiaotong university, shanghai, China*

MP 592 **Rapid Diabetes Diagnosis in Biological Fluids Using Chemiluminescence and Mass Spectrometry**; Li-Ting Wang[1]; He-Hsuan Hsiao[1]; *[1]Department of Chemistry, National Chung Hsing University, Taichung City, Taiwan*

MP 593 **IDBac: An Open-Access Web Platform for Bacterial Identification via MALDI-TOF Mass Spectrometry**; Michael Strobel[1]; Nyssa K Krull[2]; Robert A Shepherd[3]; Laura M Sanchez[3]; Brian T Murphy[2]; Mingxun Wang[4]; *[1]University of California, Riverside, Riverside, CA; [2]University of Illinois at Chicago, Chicago, IL; [3]University of California, Santa Cruz, Santa Cruz, CA; [4]University of California, Riverside, CA*

MP 594 **On-plate Digestion and Analysis of Immunoglobulins using MALDI-TOF-MS**; Francine E Yanchik-Slade[1]; Milaan Thirukumaran[1]; Nazim Boutaghou[1]; *[1]Shimadzu Scientific Instruments, Columbia, MD*

MP 595 **Co-crystallization effects in FluoMALDI imaging: Comparison of sublimation and spraying methods**; Taehun Hahm[1]; Wanyue Wang[2]; Maxime A. Siegler[3]; Dalton Brown[2]; Caitlin M. Tressler[2]; Scot C. Kuo[4, 5]; Kristine Glunde[5, 6, 7]; *[1]Johns Hopkins Applied Imaging Mass Spectrometry Core, Russell H. Morgan Department of Radiology and Radiological Science, Johns Hopkins School of Medicine, Baltimore, Maryland; [2]Johns Hopkins Applied Imaging Mass Spectrometry Core, Johns Hopkins University School of Medicine, Baltimore city, MD; [3]Department of Chemistry, Johns Hopkins University, Baltimore city, MD; [4]Microscope Facility, Johns Hopkins University School of Medicine, Baltimore city, MD; [5]Sidney Kimmel Comprehensive Cancer Cancer, Johns Hopkins University School of Medicine, Baltimore city, MD; [6]Applied Imaging Mass Spectrometry Core, Johns Hopkins University School of Medicine, Baltimore city, MD; [7]Russell H. Morgan Department of Radiology and Radiological Science, Johns Hopkins University School of Medicine, Baltimore city, MD*

MP 596 **Enhancing Detection and MALDI-MS Imaging of Carbonyl Compounds and Oxidized Lipids Using On-Tissue Chemical Derivatization**; Monika Mahmud[1]; Jeerapat Doungchawee[1]; Fiona McEvoy[1]; Richard W. Vachet[1]; *[1]Department of Chemistry, University of Massachusetts Amherst, Amherst, MA*

MP 597 **Speciation of Algae geneses using Matrix-Assisted Laser Desorption Ionization to Build a Mass Spectra Database**; Cheyenne Copling[1]; Kevin R. Tucker[1]; João Nail[1]; *[1]Southern Illinois University Edwardsville, Edwardsville, IL*

MP 598 **Magnetic Nanoparticle Modified DNAzyme Applied to Paraffin Membrane Channel Microfluidic Device to Detect Lead Ions in Aqueous Solution**; Chang-Yu Chen[1]; He-Hsaun Hsiao[1]; *[1]Department of Chemistry, National Chung Hsing University, Taichung City, Taiwan*

MP 599 **MALDI-TOF/TOF mass spectrometry of astrobiology-relevant peptides with noncanonical residues**; Julianna E. DeMauro[1]; Amanda K. Peterson[1]; Undergraduate Students From CHEM 423 (Bioanalytical Chemistry) [1]; Eric T. Parker[2]; Michael W. Giuliano[1]; Jay G. Forsythe[1]; *[1]College of Charleston, Charleston, SC; [2]NASA Goddard Space Flight Center, Greenbelt, MD*

MP 600 **Automatic differentiation of Clostridioides difficileribotypes from clinical isolates using MALDI-TOF MS and web-based machine learning classification models**; Mario Blázquez-Sánchez[1]; José Miguel Moreno[2]; Alejandro Guerrero-López[2]; Mark Gutiérrez-Pareja[1]; Vanessa Gómez-Verdejo[2]; Patricia Muñoz[1]; Mercedes Marín[1]; Luís Alcalá[1]; David Rodriguez-Temporal[1]; Belén Rodríguez-Sánchez[1]; *[1]Health Research Institute Hospital Gregorio Marañón, Madrid, Spain; [2]Universidad Carlos III, Madrid, Spain*

MP 601 **MALDI-MS based million-screening platform using W/O droplet**; Ryogo Takai[1, 2]; Masamune Morita[2]; Satoko Matsukura[2]; Satoshi Matsuoka[1, 2]; Masaki Kanai[1]; Koretsugu Ogata[1]; Naohiro Noda[2]; Daisuke Miura[3]; *[1]Shimadzu, Kyoto, Japan; [2]National Institute of Advanced Industrial Science and Technology, Japan, Ibaraki, Japan; [3]Nat'l Inst. of Advanced Industrial Science & Technology, Ibaraki, Japan*

MP 602 **Nanoparticle-enhanced metabolic histopathology for rapid, label-free lymphoma diagnosis and subtype classification**; Juxiang Zhang; *Shanghai JIao Tong University, Shanghai, China*

MP 603 **Optimized MALDI-TOF Method for Enhanced Detection and Accurate Mass Characterization of Synthetic Oligonucleotides**; Mirandia Szramowski[1]; Mohsin Ali[1]; Steven Fletcher[1]; Jace W. Jones[1]; *[1]University of Maryland, School of Pharmacy, Department of Pharmaceutical Sciences, Baltimore, MD*

MALDI: INNOVATION IN INSTRUMENTATION AND SAMPLE PREPARATION
604-612

MP 604 **Solvent-free preparation for MALDI-MS analysis of virgin and recycled polyethylene terephthalate (PET)**; Nina Timmer[1]; Matthew E. Openshaw[2]; Andreas Baumeister[1]; Nils Garnebode[1]; *[1]Shimadzu Europa GmbH, Duisburg, Germany; [2]Kratos Analytical Ltd, Manchester, United Kingdom*

MP 605 **LAP-MALDI – an alternative ionization technique on commercial instrumentation**; Rainer Cramer[1]; Lily R Adair[1]; Kerstin Strupat[2]; *[1]University of Reading, Reading, United Kingdom; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

MP 606 **From Sample to Species: Automated MALDI-TOF MS Workflows for Streamlined Bacterial Identification**; Jeremy Provoost[1]; Hagen M. Gegner[2]; Stefan Gaugler[1]; Timm Hettich[1]; Guenter Boehm[2]; Valentin Pflueger[3]; Jonathan Beck[2]; *[1]Institute of Chemistry and Bioanalytics, University of Applied Sciences and Arts Northwestern Switzerland, Muttenz, Switzerland; [2]CTC Analytics AG, Zwingen, Switzerland; [3]Mabritec AG, Riehen, Switzerland*

MP 607 **Optimized method for N-glycan imaging of fixed frozen tissues for mapping multicellular functional tissue units in human kidney tissue**; Audra Judd[1, 2]; Madeline E. Colley[2, 3]; Jamie L. Allen[2, 4]; Lukasz G Migas[5]; Angela R. S. Kruse[2, 3]; Melissa A. Farrow[2, 3]; Raf Van De Plas[2, 4, 5]; Jeffrey M Spraggins[2, 3, 4, 6, 7, 8]; *[1]Vanderbilt University, Nashville, TN; [2]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [3]Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; [4]Department of Biochemistry, Vanderbilt University, Nashville, TN; [5]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [6]Chemical and Physical Biology Program, Vanderbilt University, Nashville, TN, United States 2. Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [7]Department of Chemistry, Vanderbilt University, Nashville, TN; [8]Department of Pathology, Microbiology, and Immunology, Vanderbilt University Medical Center, Nashville, TN*

MP 608 **Mass Spectrometry Imaging of Neurotransmitters Enabled by a Reactive Radical Generation MALDI Matrix**; Thao U Duong[1]; Hua Zhang[2]; Zicong Wang[2]; Cameron John Kaminsky[1]; Lingjun Li[1, 2]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [2]School of Pharmacy, University of Wisconsin-Madison, Madison, WI*

MP 609 **Development of a high sensitivity atmospheric MALDI-2 source for imaging mass spectrometer**; Zhi Geng[1]; Qiao Jin[1]; Jiankui Liu[1]; Zhenhe Chen[2]; Xiaoqiang Zhang[1]; Wenjian Sun[1]; *[1]Shimadzu Research Laboratory (Shanghai) Co., Ltd., Shanghai, China; [2]Shimadzu China Innovation Center, Shimadzu Corporation, Beijing, China*

MP 610 **Visualizing the Neuropeptide Distribution in the Common Eastern Bumble Bee using trapped ion mobility MALDI Imaging**; Daniel C. Castro[1, 2]; Callum J. Kingwell[3, 4]; Ian M. Traniello[3, 4]; Sarah D. Kocher[3, 4]; *[1]Bruker Scientific LLC, Billerica, MA; [2]Bruker Daltonics GmbH & Co.KG, Bremen, Germany; [3]Department of Ecology and Evolutionary Biology, Princeton University, Princeton, NJ, USA., Princeton, New Jersey; [4]Lewis-Sigler Institute for Integrative Genomics, Princeton University, Princeton, NJ*

MP 611 **Charge inversion ion/ion reactions for improved resolution of MALDI-generated proteins in Fourier transform ion cyclotron resonance mass spectrometry**; Nicholas R Ellin[1]; Matthias-Erich N Born[2]; Ariana E Stratton[2]; Woo-Young Kang[2]; Boone M Prentice[2]; Scott A. McLuckey[1]; *[1]Department of Chemistry, Purdue University, West Lafayette, IN; [2]Department of Chemistry, University of Florida, Gainesville, FL*

MP 612 **Extending the mass range of MALDI-generated proteins via charge inversion ion/ion reactions on an FT-ICR mass spectrometer**; Matthias-Erich N Born[1]; Nicholas R. Ellin[2]; Ariana E. Stratton[1]; Woo-Young Kang[1]; Scott A.

McLuckey[2]; Boone M. Prentice[1]; *[1]University of Florida, Gainesville, Florida; [2]Purdue Univeristy, West Lafayette, IN*

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MP 613 **Targeted Liquid Chromatography-Mass Spectrometry based profiling of cysteine, cystine and other critical metabolites in cell culture supernatant: application in biopharma**; Francesca Ferlenghi[1]; Maria Sani[1]; Nicole Bradshaw[1]; James Graham[1]; *[1]Lonza Biologics plc, Slough, United Kingdom*

MP 614 **High throughput analysis of NPH-derivatized central carbon metabolites using prm-Pasef**; Matthias Anagho-Mattanovich[1]; Ondrej Hodek[2]; Nikolas Kessler[3]; Sofie Weinkouff[4]; Aiko Barsch[4]; Cristian De Gobba[4]; Matthew R. Lewis[4]; Thomas Moritz[1]; *[1]Novo Nordisk Foundation Center for Metabolic Research, University of Copenhagen, Copenhagen, Denmark; [2]Swedish Metabolomics Centre, Swedish University of Agricultural Sciences, Umeå, Sweden; [3]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [4]Bruker Daltonics GmbH & Co. KG, Bremen, Germany*

MP 615 **LC-MS quantification of short chain fatty acids revealed that inulin increased short chain fatty acid production in mice**; Zhentian Lei[1]; Lucille M. Yanckello[2]; Ya-Hsuan Chang[2]; McKenna Sun[2]; George Chlipala[3]; Stefan J. Green[4]; Aaron C. Ericsson[5]; Xin Xing[2]; Tyler C. Hammond[2]; Adam D. Bachstetter[2]; Lloyd W. Sumner[1]; Ai-Ling Lin[6]; *[1]Metabolomics Center, University of Missouri, Columbia, MO; [2]Sanders Brown Center on Aging, University of Kentucky, Lexington, KY; [3]Research Informatics Core, University of Illinois, Chicago, IL; [4]Genomics and Microbiome Core Facility, Rush University, Chicago, IL; [5]Department of Veterinary Pathobiology, University of Missouri, Columbia, MO; [6]Department of Radiology, University of Missouri, Columbia, MO*

MP 616 **HILIC-HRMS/MS method for the analysis of purines in foods using acid hydrolysis extraction**; Manasi Kamat[1]; Katherine Heydorn[2]; Pamela Pehrsson[2]; Xianli Wu[2]; Timothy J Garrett[1]; *[1]University of Florida, Gainesville, Florida; [2]USDA, Beltsville, MD*

MP 617 **Measurement of Redox Metabolites Using Liquid Chromatography–Mass Spectrometry: Application in Cancer Research**; Chandra Shekar Reddy Ambati[1]; Abu Hena Mostafa Kamal[1,2]; Vasanta Putluri[1]; Karthik Reddy Kami Reddy[3]; Nagireddy Putluri[4,5]; *[1]Advanced Technology Core, Dan L Duncan Comprehensive Cancer Center, Baylor College of Medicine, Houston, Texas, United States., Houston, TX; [2]Department of Molecular and Cell Biology, Baylor College of Medicine, Houston, Texas, United States., Houston, TX; [3]Department of Molecular and Cell Biology., Houston, TX; [4]Advanced Technology Core, Dan L Duncan Comprehensive Cancer Center, Houston, TX; [5]Department of Molecular and Cell Biology, Baylor College of Medicine, Houston, Texas, United States, Houston, TX*

MP 618 **Single-Cell Metabolomic Characterization via CE-NanoESI-MS with Nanoflow Sheath Liquid Interface**; Shuangshuang Chen[1]; Chen Huang[1]; Yash Nelavelli[1]; Stanislav S. Rubakhin[1]; Michael Knierman[2]; Jonathan Sweedler[1]; *[1]University of Illinois Urbana-Champaign, Urbana, IL; [2]Agilent Technologies, Inc., Santa Clara, CA*

MP 619 **3-NPH derivatization improves coverage of polar metabolome in LC-MS**; Ondrej Hodek[1,2]; Thomas Moritz[3]; Annika I. Johansson[4,5]; *[1]Swedish Metabolomics Centre, Swedish University of Agricultural Sciences, Umeå, Sweden; [2]Department of Forest Genetics and Plant Physiology, Swedish University of Agricultural Sciences, Umeå, Sweden; [3]Novo Nordisk Foundation Center for Metabolic Research, University of Copenhagen, Copenhagen, Denmark; [4]Swedish Metabolomics Centre, Swedish University of Agricultural Sciences, Umeå, Sweden; [5]Department of Plant Physiology, Umeå, Sweden*

MP 620 **Targeted LC-MS/MS metabolomics reveals age-associated metabolic dysregulations and cardiovascular risk biomarkers in advanced maternal age pregnancies**; Muhammad Imran[1,2,3]; Rupasri Mandal[2,3]; Sandra Davidge[1,4,5]; David Wishart[3,6,7,8]; *[1]Women and Children's Health Research Institute, Faculty of Medicine & Dentistry, University of Alberta, Edmonton, Alberta; [2]The Metabolomics Innovation Centre (TMIC), University of Alberta, Edmonton, Alberta; [3]Department of Computer Science and Biological Sciences, University of Alberta, Edmonton, Alberta; [4]Department of Obstetrics and Gynecology, Faculty of Medicine & Dentistry, University of Alberta, Edmonton, Alberta; [5]Department of Physiology, Faculty of Medicine & Dentistry, University of Alberta, Edmonton, Alberta; [6]The Metabolomics Innovation Centre (TMIC), University of Alberta, Edmonton; [7]Department of Laboratory Medicine & Pathology, Faculty of Medicine & Dentistry, University of Alberta, Edmonton, Alberta; [8]Faculty of Pharmacy and Pharmaceutical Sciences, University of Alberta, Edmonton, Alberta*

MP 621 **Combining targeted MS2 and MS3 approaches for the quantitation of bile acids in biological specimens using the Stellar Mass Spectrometer**; Cristina C. Jacob[1]; Britanny Lee[1]; Charles E. Maxey[1]; Bashar Amer[1]; Susan Bird[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

MP 622 **Broad profiling, quantitative metabolomics using the MxP® Quant 500 XL kit on TSQ Altis series mass spectrometers**; Stephen Dearth[1]; Markus Langsdorf[1]; Tuan-Hai Pham[1]; Gregor Ömer[1]; Edmund Moy[2]; Susan Bird[2]; *[1]biocrates life sciences ag, Innsbruck, Austria; [2]Thermo Fisher Scientific, San Jose, CA*

MP 623 **Quantitative, large panel metabolomics with the MxP® Quant 500 XL kit optimized and validated for the 6495D triple quadrupole LC/MS**; Stephen Dearth[1]; Markus Langsdorf[1]; Tuan-Hai Pham[1]; Fadi Abdi[1]; Ian Edwards[2]; Peter Weidner[2]; Kevin Cho[3]; Ethan Stancliffe[3]; Monil Gandhi[3]; Ashima Mehta[3]; Adam Richardson[3]; *[1]biocrates life sciences ag, Innsbruck, Austria; [2]Agilent Technologies, Santa Clara, CA; [3]Panome Bio, Saint Louis, MO*

MP 624 **Investigating Metabolism During Mammalian Cell Bioproduction using High Throughput Targeted Microchip Capillary Electrophoresis Tandem Mass Spectrometry**; Maikel Gaitkoski[1,2]; Noemí Dorival-García[1]; Aaron Richardson[1]; J. Will Thompson[3]; Erin Redman[3]; Graziella Piras[4]; Jonathan Bones[1,2]; *[1]Nat'l Inst. for Bioprocessing Research & Training, Dublin, Ireland; [2]University College Dublin, Belfield, Ireland; [3]908 Devices, Inc., Morrisville, NC; [4]908 Devices Inc., Boston, MA*

MP 625 **Improving compound identification and quantitation using ZT Scan DIA on a novel QTOF instrument**; Wen Jin[1]; Anjali Chelur[1]; Gordana Ivosev[1]; Cuong Le[1]; David M Cox[1]; *[1]SCIEX, Concord, ON*

MP 626 **A Scalable Machine Learning-Based Platform for Absolute Quantitation of Metabolitesto Elucidate CHO Cell Metabolism**; Elsa Gorre[1]; Kathryn Dorst[1]; Bo Zhai[1]; Andrew Mahan[2]; Javier Gomez Castro[2]; Jack Howland[3]; Baljit K. Ubhi[3]; *[1]Johnson and Johnson Innovative Medicine, Spring House, PA; [2]JOHNSON AND JOHNSON, Spring House, PA; [3]Matterworks, Somerville, MA*

MP 627 **UHPLC-Orbitrap-MS Method for Simultaneous Quantitation and Discovery of metabolites in Waste Biomass and Paludicultured Crops**; Pius K Kairigo[1]; Roosa-Maria Liimatainen[1]; Aniina Kiesilä[1]; Elina Kalenius[1]; *[1]University of Jyväskylä, Jyväskylä, Finland*

MP 628 **Ultra-High-Throughput analysis for the upregulation of Triacetic acid lactone (TAL) in R.toruloides via Random Mutagenesis.**; Blake E Mirman[1]; Hyunjoon Oh[2]; Quanhui Ye[2]; Jonathan Sweedler[2]; Yong-Su Jin[1]; *[1]University of Illinois at Urbana Champaign, Urbana, IL; [2]University of Illinois at Urbana-Champaign, Urbana, IL*

MP 629 **Unveiling quantitative secondary metabolome in plants and natural products through low-resolution global targeted and untargeted approaches**; Alberto AA Asteggiano[1]; Federica Dal Bello[1]; Alex Affricano[1]; Alice Di Bernardo[1]; Claudio Medana[1]; *[1]Dipartimento di Biotecnologie Molecolari e Scienze per la Salute, Turin, Italy*

MP 630 **Ultrafast high throughput screening of energy metabolism using Sciex Echo-DMS MS system**; Stephan Siebel[1]; Robert Hale[1]; Richard G Kibbey[1]; John Janiszewski[2]; Chang Liu[3]; Thomas R. Covey[3]; Jon Shrimp[4]; Matthew Hall[4]; *[1]Yale University, New Haven, CT; [2]J2.Bioanalytical, Westerly, RI; [3]SCIEX, Concord, ontario; [4]National Center for Advancing Translational Sciences (NCATS), Rockville, MD*

MP 631 **Expanding the analyte coverage of Pyxis, an AI tool for rapid, broad coverage, absolute quantification of metabolites in biological samples**; Ana S. H. Costa[1]; Devesh Shah[1]; Gabriel Asher[1]; Luke S Ferro[1]; Craig Knisley[1]; Aubrey Brueckner[1]; Jennifer M Campbell[1]; *[1]Matterworks, Somerville, MA*

MP 632 **Quantification of over 1,200 metabolites across four different LC-MS platforms using a cloud-based workflow management software with AI-driven peak picking**; Tuan-Hai Pham[1]; Cornelia Röhring[1]; Ulf Sommer[1]; Stephen Dearth[1]; Guido Dallmann[1]; Markus Langsdorf[1]; *[1]biocrates life sciences ag, Innsbruck, Austria*

MP 633 **Quantification of 1,200+ metabolites in human plasma, urine and feces using optimized calibration standards, quality controls, and acquisition methods**; Gordian Adam[1]; Tuan-Hai Pham[1]; Cornelia Röhring[1]; Ulf Sommer[1]; Guido Dallmann[1]; Markus Langsdorf[1]; Alice Limonciel[1]; *[1]biocrates life sciences ag, Innsbruck, Austria*

MP 634 **Fast-Tracking Cancer Metabolism Research: Integrating Discovery and Targeted Metabolomics for Comprehensive Biological Insights**; Crystal L. Pace[1, 2]; Wen-Hsuan Chang[2]; Clint A. Stalnecker[2, 3]; Channing J. Der[2, 3]; Erin Redman[4]; J. Will Thompson[4]; Laura E. Herring[1, 2]; Whitney L. Stutts[1, 2]; *[1]UNC Metabolomics & Proteomics Core, Chapel Hill, NC; [2]Department of Pharmacology, University of North Carolina at Chapel Hill, Chapel Hill, NC; [3]Lineberger Comprehensive Cancer Center, University of North Carolina at Chapel Hill, Chapel Hill, NC; [4]908 Devices, Morrisville, NC*

MP 635 **Characterization of amine conjugated bile acids in healthy donors and patients with liver disease**; Amber R Rose[1]; Michael W Mullowney[1]; Ashley M Sidebottom[1]; Anitha Sundararajan[1]; Ramanujam Ramaswamy[1]; Eric G Pamer[1, 2, 3]; Samuel H Light[1, 3]; Matthew A Odenwald[1, 4]; *[1]Duchossois Family Institute, The University of Chicago, Chicago, IL; [2]Department of Medicine, Section of Infectious Disease and Global Health, The University of Chicago, Chicago, IL; [3]Department of Microbiology, The University of Chicago, Chicago, IL; [4]Department of Medicine, Section of Gastroenterology, Hepatology, and Nutrition, The University of Chicago, Chicago, IL*

MP 636 **An improved internal standards-based metabolomics workflow for accurate, absolute quantitation of metabolites in urine**; Debasish Ghosh[1]; Michael Neugent[2]; Alexander Raskind[3]; Nicole J. De Nisco[2, 4]; Felice A. De Jong[3]; Chris Beecher[3]; Vladimir Shulaev[1]; *[1]UNIVERSITY OF NORTH TEXAS, Denton, TX; [2]The University of Texas at Dallas, Richardson, Texas; [3]IROA Technologies LLC, Nellysford, VA; [4]The University of Texas Southwestern Medical Center, Dallas, Texas*

MP 637 **Mapping Every Cell Metabolome during early Vertebrate Embryonic (frog) Development using Mass Spectrometry**; Yayra T Tuani[1]; Navid Ayon[2]; Peter Nemes[2]; *[1]University of Maryland, College Park, MD; [2]University of Maryland, College park, Hyattsville, MD*

MP 638 **Quantification of underivatized acylcarnitines and carnitine intermediates using RP chromatography and ion funnel triple quadrupole in fecal samples**; Bianca Ferreira da Silva[1]; Ruben Jose Jesus Faustino Ramos[2]; Justin Cross[3]; Karen Yannell[4]; Daniel Cuthbertson[5]; *[1]Agilent Technologies, Lexington, MA; [2]Memorial Sloan Kettering Cancer Center, New York, NY; [3]. Marron Cancer Metabolism Center Memorial Sloan Kettering Cancer Center, New York, NY, Kettering, NY; [4]Agilent Technologies, Santa Clara, CA; [5]Agilent Technologies, Inc., Santa Clara, CA*

MP 639 **Targeted metabolomics and lipidomics approaches for evaluation of biomarker candidate for HCC in patients with liver cirrhosis**; Md Mamunur Rashid[1]; Rency S Varghese[1]; Habtom W Ressom[1]; *[1]Georgetown University, Lombardi Cancer Center, Washington, DC*

MP 640 **Evaluation of the importance of high-resolution in targeted metabolomics**; Rachel Buckley[1]; Gabriella Handford[1]; Anita Brinker[1]; Ill Yang[1]; Lauren Aleksunes[1]; Brian T Buckley[1]; *[1]Rutgers University, Piscataway, NJ*

MP 641 **Tackling Noise and Redundancy in LC-MS metabolomics data**; Pramod P Wangikar[1]; Aviral Singh[2]; *[1]Indian Institute of Technology Bombay, Mumbai, India; [2]Clarity Bio Systems India Pvt. Ltd, Mumbai, India*

MP 642 **Development of a Comprehensive Reverse-Phase Liquid Chromatography-Mass Spectrometry Method for Measuring Short- to Long-Chain Acyl-Coenzyme A Compounds**; Daniel Kantner[1]; Nathaniel W. Snyder[1]; *[1]Temple University, Philadelphia, PA*

MP 643 **Quantitative Bioreactor Metabolomics Using a New Metabolomics Platform Reveals Key Differences Between Isolated CHO Clones**; Jeremy J. Wolff[1]; Sean G. Mack[1]; Daniel B. Gowetski[1]; Q. Paula Lei[1]; Jason G. Gall[1]; *[1]NIH, Gaithersburg, MD*

MP 644 **Quantitative metabolomics and lipidomics screening of serum samples for detecting prenatal cyanotic congenital heart disease**; Nadia Ashrafi[1]; Romana Ashrafi Mimi[1]; Stephen Dearth[2]; Ciara Talbot[3]; Perry Friedman[4]; Onur Turkoglu[5]; Stewart Graham[1, 5, 6]; Ray Bahado-Singh[5]; *[1]Corewell Health Research Institute, Royal Oak, MICHIGAN; [2]biocrates life sciences ag, Innsbruck, Austria; [3]Kaiser Permanente, Altanta, Georgia; [4]Memorial Division of Maternal Fetal Medicine, Pembroke Pines, Florida; [5]Corewell Health East William Beaumont University Hospital, Royal Oak, Michigan; [6]Oakland University-William Beaumont School of Medicine, Rochester, Michigan*

MP 645 **Solid Phase Extraction and Multiplex LC-MS/MS Assay for Quantification of STK-001 and Potential Metabolites in Human Urine**; Qianyun Zhang; *Stoke Therapeutics, Bedford, MA*

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MP 646 **Capillary electrophoresis hyphenated with inductively coupled plasma mass spectrometry for the study of GHK-Cu tripeptide-loaded liposomes**; Joanna Zajda[1]; Karolina Ogórek[1]; Kinga Nowak[1]; Magdalena Matczuk[1]; *[1]Warsaw University of Technology, Warsaw, Poland*

MP 647 **Separation and structural analysis of therapeutic cyclic peptides using UVPD-MS with capillary electrophoresis and liquid chromatography**; Malcolm A. Barnard[1]; Jennifer S. Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX*

MP 648 **Development of Hydrodynamic Surface Sampling for Capillary Electrophoresis Mass Spectrometry for Spatial Metabolomics**; Natalia Remper[1]; Ingela Lanekoff[1]; *[1]Uppsala University, Uppsala, Sweden*

MP 649 **Is CE-ICP-MS or HPLC-ICP-MS more effective in examining the formation of metallic and organic anticancer drug delivery nanosystems?**; Magdalena Matczuk[1]; Joanna Zajda[1]; Damian Dąbrowski[1]; Marta Stępień[1]; *[1]Warsaw University of Technology, Warsaw, Poland*

MP 650 **Determination of sgRNA and mRNA Sequence Identity by Low-Micro Flow Ion-Pair Reversed-Phase Chromatography and High-Resolution Tandem Mass Spectrometry**; Sergio Guazzotti[1]; Roxana Eggleston-Rangel[2]; Jason Anspach[2]; *[1]Phenomenex, Alcobendas, Madrid, Spain; [2]Phenomenex, Torrance, California*

MP 651 **Exploring determinant factors in the application of capillary electrophoresis-mass spectrometry (CE-MS) to the analysis of divide-and-conquer mixtures from larger RNAs**; Daniele Rollo[1]; Daniele Fabris[1]; *[1]University of Connecticut, Storrs, CT*

MP 652 **Enabling High-throughput, Automated nanoESI Workflows for Intact and Native analysis with Inline Tangential Flow Filtration via DynaChip**; Austin Culberson[1]; Casey Vantucci[1]; Carter Asef[1]; Patrick Spencer[1]; Mason Chilmonczyk[1]; *[1]Andson Biotech, Atlanta, GA*

MP 653 **Novel LCMS-Compatible icIEF Fractionation for Characterization of Innovator and Biosimilar mAbs**; Srinivasa Rao[1]; Samantha Ippoliti[2]; Ying Qing Yu[2]; Nick Pittman[3]; Chris Heger[1]; *[1]Bio-techne, San Jose, CA; [2]Waters Corp, Milford , MA; [3]Waters Corp, Wilmslow, United Kingdom*

MP 654 **Integrated PLOT-SPE-CE-MS to Enable Online Fractionation and Multi-Omic Profiling of ng-Level Biological Samples**; Yunfan Gao[1]; Michal Gregus[1]; Yifan Liu[1]; Owen S. Skinner[1]; Alexander R. Ivanov[1]; *[1]Northeastern University, Boston, MA*

MP 655 **DynaChip Online Buffer Exchange and Desalting Coupled to Charge Detection Mass Spectrometry for the Analysis of Large Biologics**; Lohra M Young[1]; Carter K Asef[2]; Benjamin E Draper[1]; Casey E Vantucci[2]; Jim Filippini[2]; Martin F Jarrold[3]; Mason A Chilmonczyk[2]; *[1]Megadalton Solutions, Bloomington, IN; [2]Andson Biotech, Atlanta, GA; [3]Indiana University, Bloomington, IN*

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MP 656 **Investigation on the Retention and Separation of Glucosinolates with a Mixed-Mode Reversed-Phase/Weak Anion-Exchange Column by UPLC-IMS-HRMS**; Yanfang Li[1, 2]; Pei Chen[1]; Mengliang Zhang[2]; Jianghao Sun[1]; *[1]USDA, Beltsvile, MD; [2]Department of Chemistry, Ohio University, Athens, OH*

MP 657 **Determination of NNN and NAT enantiomers in tobacco and tobacco products**; Huihua Ji[1]; Ying Wu[1]; *[1]University of Kentucky, Lexington, KY*

MP 658 **Characterization of sea urchin footprints using MALDI-MSI to uncover new underwater adhesives**; Luciana V Rivera Molina[1]; Zachary Baker[2]; Alyssa Stark[2]; Chrys Wesdemiotis[1]; *[1]University of Akron, Akron, OH; [2]Villanova University, Villanova, Pennsylvania*

MP 659 **Investigating LoaP's Effect on the Proteome and Secondary Metabolite Production by Mass Spectrometry**; Conor C Jenkins[1]; Madison Jermain[1]; Benjamin Nasisi[1]; Wade Winkler[1]; *[1]University of Maryland, College Park, MD*

MP 660 **Characterization of the Glycosyltransferase Responsible for the Observed Glucosamine Chemistry in Sphingomonas paucimobilisin Glycosphingolipids**; Tahir Ali[1]; Paul D. Boudreau[2]; *[1]University of Mississippi, Oxford, MS; [2]University of Mississippi, University, MS*

MP 661 **A comprehensive workflow for non-targeted profiling and comparison of complex essential oils by GC-APCI-IMS mass spectrometry**; Thilani M Anthony[1]; Samuel Putnam[2]; *[1]Bruker Scientific LLC, Bilerica, MA; [2]Bruker Scientific LLC, Billerica, MA*

MP 662 **Enhanced methods for identifying compounds by gc/ms in plants using the NIST 2023 EI Library: Example of Calendula officinalis**; Nirina Rabe Andriamaharavo[1]; Edward P Erisman[1]; Lewis Y Geer[1]; Douglas J Slotta[1]; William E Wallace[1]; Steve Stein[1]; *[1]National Institute of Standards and Technology, Gaithersburg, MD*

MP 663 **Noncovalent Modulation of Chemoselectivity in the Gas Phase studied by IM-QTOF mass spectrometry**; Elina Kalenius; *Univ. of Jyväskylä, Jyväskylä, Finland*

MP 664 **Rationally Building Fungal Natural Product Libraries using Morphology selection and Environment-mimicking Culture Conditions**; Monica Ness[1, 2]; Thilini Peramuna[1]; Karen Wendt[1]; Robert Cichewicz[3]; Laura-Isobel McCall[2]; *[1]University of Oklahoma, Norman, OK; [2]San Diego State University, San Diego, CA; [3]University of Michigan, Ann Arbor, Michigan*

MP 665 **Untargeted GC-MS Analysis: Recovery of phytochemicals from Reed Canary Grass**; Roosa-Maria Liimatainen[1]; Elina Kalenius[1]; *[1]University of Jyväskylä, Jyväskylä, Finland*

MP 666 **Combining Metabologenomics and Bioactivity Screening to Discover New Anthelmintics from Fungi**; Raveena Gupta[1]; J.B. Collins[2]; Fatma A. Butun[1]; Gini Besant[1]; Maanasa Narayanamoorthy[1]; Erik Andersen[2]; Neil L. Kelleher[1]; *[1]Northwestern University, Evanston, IL; [2]Johns Hopkins University, Baltimore, MD*

MP 667 **Structural Characterization of Syanodin I using gas-phase HDbX-TIMS-ECD-MS/MS**; Miguel Santos[1]; Kevin Jeanne Dit Fouque[1]; Ukesh Karki[1]; Alain Alain Blond[2]; Severine Zirah[2]; Julian D Hegemann[3]; Prem P Chapagain[1]; Francisco Fernandez-Lima[1]; *[1]Florida International University, Miami, FL; [2]Laboratory MCAM, National Museum of Natural History, Paris Cedex 05, France; [3]Institute of Chemistry Strasse, Berlin, Germany*

MP 668 **New untargeted LC/MS/MS Assay and mass spectral / retention time libraries for natural products in food**; Uri Keshet[1]; Jeremiah D Wells[1]; Samantha R Duncan[2]; Fanzhou Kong[2]; Oliver Fiehn[1]; *[1]West Coast Metabolomics Center, UC Davis, CA; [2]UC Davis, Davis, CA*

MP 669 **Differentiation of Mitragynine Diastereomers from Kratom by Liquid Chromatography and Collision-Induced Ion Dissociation Mass Spectrometry**; William J. Crandall[1]; Cassandra L. Quave[1]; Dean P. Jones[1]; *[1]Emory University, Atlanta, GA*

MP 670 **LC/HRMS-Based Documentation of Fungal Perylenequinone Production Under Varying Growth Conditions: Insights from Isotopic Labeling Experiments**; Reema Al-Qiam[1]; Tyler N. Graf[1]; Huzefa A. Raja[1]; Cedric J. Pearce[2]; Shabnam Hematian[1]; Nicholas H. Oberlies[1]; *[1]UNCG, Greensboro, NC; [2]RTI International, Research Triangle Park, NC*

MP 671 **Unravelling antioxidant and anti-inflammatory actions of Aconitum heterophyllum plant extract: Insights from metabolomics, molecular docking, and animal studies.**; ASHWANI PUNIA[1, 2]; Rituraj Purohit[1, 2]; Yogendra Shantaram Padwad[1, 2]; Rajiv Kumar[1, 2]; *[1]CSIR-Institute of Himalayan Bioresource Technology, PALAMPUR, India; [2]Academy of Scientific and Innovative Research (AcSIR), Ghaziabad, India*

MP 672 **Lipidomics approaches to assist discovery of bioactive lipids in marine biofilms**; Sara Finnerty[1]; Yunhai Li[2]; Nicolas Touzet[1]; Brian Kelleher[3]; Shane S O'Reilly[2]; *[1]Atlantic Technological University, Sligo, Ireland; [2]Technological University Dublin, Dublin, Ireland; [3]Dublin City University, Dublin, Ireland*

MP 673 **Deprotonated glycosylated flavonoid dissociation model: a tool for charaterizing Viola yedoensis extract composition and understanding its cosmetic benefits.**; Sandra De Sousa[1]; Alexis Dubuis[1]; Samia Boudah[1]; Sreelatha Thonthula[2]; Richa Mehta[2]; Akanksha Singh[2]; Joan Eilstein[1]; Sherluck John[2]; Dhimoy Roy[3]; Steve Thomas Pannakal[2]; Jean-Claude Tabet[4, 5]; *[1]L'Oréal Research and Innovation, Aulnay-sous-Bois, France; [2]L'Oréal Research and Innovation, Bangalore, India; [3]L'Oréal Research and Innovation, Mumbai Maharashtra, India; [4]Faculty of Sciences and Engineering, Institut Parisien de Chimie Moléculaire, Sorbonne University, Paris, France; [5]Medicines and Health Technologies Department (DMTS), CEA, INRAE, MetaboHUB, Paris-Saclay University, Gif-sur-Yvette, France*

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MP 674 **Glycoproteome and Surfaceome Mapping of Epithelial-to-Mesenchymal Transition Reveals Key Ion Channel Regulation and Novel Biomarkers in Cancer Metastasis**; Xing Xu[1]; Kejun Yin[1]; Ronghu Wu[1]; *[1]Georgia Institute of Technology, Atlanta, GA*

MP 675 **Hyperplexed Analysis of Kinase Signaling Responses Combining ProKAS and TMT**; William Comstock[1]; Marcos VAS Navarro[1]; Deanna Maybee[1]; Yiseo Rho[1]; Mateusz Wagner[1]; Marcus B Smolka[1]; *[1]Cornell University, Ithaca, NY*

MP 676 **Parkinson's Disease Biomarker Discovery via LC-MS/MS characterization and quantification of alpha-**

synuclein PTMs in erythrocytes; Martin Acosta-Parra[1]; Michael Snyder[1]; *[1]Stanford University, Stanford*

MP 677 **On the Impact of Post-Translational Succination on SUMO1 Structure: A Dual Approach Combining Gas-Phase and Solution Studies**; Louis Groignet[1]; David Dellemme[1]; Quentin Duez[1]; Jean-Marie Colet[1]; Patrick Brocorens[1]; Mathieu Surin[1]; Pascal Gerbaux[1]; Julien De Winter[1]; *[1]University of Mons, Mons, Belgium*

MP 678 **Acrolein and Crotonaldehyde-Derived Hemoglobin Modifications in Oral Cancer Patients and Healthy Smokers**; Hauh-Jyun Candy Chen[1]; Kai-Ting Fu[1]; *[1]National Chung Cheng Univ., Ming-Hsiung, Chia-Yi, Taiwan*

MP 679 **Novel Parallel Accumulation with Mobility Aligned Fragmentation (PAMAF) Mode enables Proteome-Wide Succinylation Analysis with Deep Coverage and Site-Specific Characterization**; Joanna Bons[1]; Leonard Rorrer[2]; Lauren Royer[2]; Eleni Vickers[1]; Anne Silva-Barbosa[3]; Katherine Pfister[3]; Eric S Goetzman[3]; Sunder Sims-Lucas[3]; Daniel Debord[2]; Birgit Schilling[1]; *[1]Buck Institute for Research on Aging, Novato, CA; [2]MOBILion Systems, Inc., Chadds Ford, PA; [3]Department of Pediatrics, University of Pittsburgh Medical Center Children's Hospital of Pittsburgh (UPMC CHP), University of Pittsburgh, Pittsburgh, PA*

MP 680 **Development of a Platform MAM Method: Establishing System Readiness and Assay Performance Across Multiple Labs**; Li Jing[1]; Jingzhong Guo[1]; Sheila Mugabe[1]; Sameer Kumar[1]; Niomi Peckham[1]; Vishal Amancha[1]; Diane McCarthy[1]; *[1]U.S. Pharmacopeia, Clarksville, MD*

MP 681 **Phosphopeptide enrichment and online Nanoflow 2D LC/MS/MS analysis for high efficiency phosphoproteomics**; Hea Ji Lee[1]; Yeji Yang[1, 2]; Jin Young Kim[1, 3]; *[1]Korea Basic Science Institute (KBSI), Cheongju, South Korea; [2]Korea Advanced Institute for Science and Technology, Daejeon, South Korea; [3]Korea Research Institute of Bioscience and Biotechnology, Daejeon, South Korea*

MP 682 **Multi-Attribute method (MAM) compared to Conventional Methods for Assessment of PQAs of Etanercept Products**; Sheila Mugabe[1]; Jingzhong Guo[1]; Vishal Amancha[1]; Nithin Singam[1]; Sameer Kumar GS[1]; Li Jing[1]; Niomi Peckham[1]; Jarkko Huuskonen[1]; Dipankar Das[1]; Diane McCarthy[1]; *[1]United States Pharmacopeia, Rockville, MD*

MP 683 **Strategies for acquisition and processing of N-term acetylated peptides on the timsTOF Ultra 2**; Philipp Strohmidel[1]; Benoit Fatou[2]; Ganesh Balasubramanian[3]; Dijana Vitko[3]; Pierre-Olivier Schmit[2]; Virginie Redeker[4]; Carmela Giglione[4]; Thierry Meinnel[4]; *[1]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [2]Bruker France SAS, Wissembourg, France; [3]Bruker Scientific LLC, Billerica, MA; [4]Instituté Paris-Sarclay, CEA, CNRS Institute for Integrative Biology of the Cell (I2BC), Gif-sur-Yvette, France*

MP 684 **SYSTEMATIC EVALUATION OF AFFINITY ENRICHMENT METHODS FOR O-GLCNAC PROTEOMICS**; Chunyan Hou[1]; Ci Wu[1]; Junfeng Ma[1]; *[1]Georgetown University Medical Center, Washington, DC*

MP 685 **Profiling Proteome and Citrullinome of Various Lesion Types of Multiple Sclerosis Brain Tissue**; Sophia Laposchan[1, 2]; Rebecca Meelker Gonzalez[1, 2]; Erik Riedel[1, 2]; Chien-Yun Lee[1, 2]; *[1]School of Life Sciences, Technical University of Munich, Freising, Germany; [2]Young Investigator Group: Mass Spectrometry in Systems Neurosciences, CLINSPECT-M consortium, Freising, Germany*

MP 686 **Confidently detecting methylated peptides in MCF7 cells using heavy methyl SILAC and enrichment by strong cation exchange**; Jessica M. Conforti[1]; Charli S. Worth[1]; Rabin Budhathoki[1]; Joseph H. Taube[1]; Elyssia S. Gallagher[1]; *[1]Baylor University, Waco, TX*

MP 687 **Computational prediction of sequence-dependent non-consensus N-glycosylation in antibody**; Baiyu Qiu[1]; Simon Letarte[1]; *[1]Gilead Sciences Inc., Oceanside, CA*

MP 688 **High-Resolution Mapping of Post-Translational Modifications in Mammalian Tissues**; Francesca Minicozzi[1]; Maria C. Panepinto[1]; Paolo Cifani[1]; *[1]Cold Spring Harbor Laboratory, Cold Spring Harbor, NY*

MP 689 **Optimization of Histone Extraction Protocol with Low Cell Count and Fast Extraction**; Renee Dean[1]; Francisca NDL Vitorino[1]; Xingyu Liu[1]; Shri Gouri Pinjarla[1]; Benjamin A Garcia[1]; *[1]Washington University in St. Louis, University City, MO*

MP 690 **Comparison of Iodoacetamide and S-Methyl Methanethiosulfonate as Alkylating Reagent for Protein Cysteine Acylation and Nitrosylation Detection**; Jian Cai[1]; Ming Song[2]; Ming Li[2]; Michael Merchant[2]; Frederic Benz[2]; Craig McClain[2]; Jon Klein[2]; *[1]University of Louisville, Louisville, KY; [2]University of Louisville, Louisville, KY*

MP 691 **Atlas of lysine acetylation in the mouse**; Ross Soens[1, 2, 3]; Katherine A. Overmyer[1, 2, 3]; Joshua J. Coon[1, 2, 3]; *[1]University of Wisconsin-Madison, Madison, WI; [2]Morgridge Institute for Research, Madison, WI; [3]National Center for Quantitative Biology of Complex Systems, Madison, WI*

MP 692 **High Select Fe-NTA Magnetic Beads for Phosphopeptide Enrichment**; Erum Raja[1]; Leigh Foster[1]; Amarjeet Flora[1]; Bhavin Patel[1]; Ryan Bomgarden[1]; *[1]ThermoFisher Scientific, Rockford, Illinois*

MP 693 **Enrichment and Identification of Pyroglutamate-Modified Proteins Reveals Novel OGT Cleavage Substrates**; David W W Hill[1]; Daniel H Ramirez[2]; Milena Di Blasi[3]; Benjamin A Garcia[2]; *[1]Washington University in St. Louis, St. Louis, MO; [2]Washington University School of Medicine Dept. of Biochemistry and Molecular Biophysics, St. Louis, MO; [3]Southern Illinois University Edwardsville, Edwardsville, IL*

MP 694 **Identification and Quantitation of Histone Modifications using Variable Window DIA on Orbitrap and QTOF Instruments**; Emily Zahn[1]; Francisca N De Luna Vitorino[1]; Renee Dean[1]; Xingyu Liu[1]; Benjamin A Garcia[1]; *[1]Washington University School of Medicine, St. Louis, MO*

MP 695 **Improved Phosphoproteome Coverage using CHIMERYS and LPGF Protein Validation**; Philip Loziuk[1]; David Horn[2]; Pedro Navarro[3]; Kai Fritzemeier[3]; Frank Berg[3]; Waqas Nasir[3]; *[1]Thermo Fisher Scientific, Raleigh, NC; [2]Thermo Fisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific, Bremen, Germany*

MP 696 **p300 and SIRT1 function in concert to modulate acetylation, ubiquitination, and SUMOylation of the nuclear receptor RORβ**; Timothy R O'Leary[1]; Denis Shutin[1]; Dean P. Edwards[2]; Patrick R. Griffin[1]; Mi Ra Chang[1]; *[1]UF Scripps, Florida, Jupiter, FL; [2]Baylor College of Medicine, Houston, TX*

MP 697 **Infection-induced lysine lactylation enables virus immune evasion**; Matthew D Tyl[1]; Jinhang Yang[1]; Victoria U Merengwa[1]; Ileana M Cristea[1]; *[1]Princeton University, Princeton, NJ*

MP 698 **Structural Proteomics at Depth Reveals Relationships between Post-translational Modification and Conformational Change**; Edgar Manriquez-Sandoval[1]; Yilin Shen[1]; Philip To[2]; Sonja Hess[2]; Sophia Chung[2]; Stephen D Fried[1]; *[1]Johns Hopkin University, Baltimore, MD; [2]AstraZeneca, Gaithersburg, Maryland*

MP 699 **Proteomics and Phosphoproteomics of Salt-induced C3 to CAM Transition in Mesembryanthemum crystallinum**; Bowen Tan[1]; Noé Perron[2]; Qijie Guan[1]; Dan Zhu[3]; Craig Dufresne[4]; Sixue Chen[1]; *[1]University of Mississippi, University, MS; [2]University of Florida, Gainesville, Florida; [3]Qingdao Agricultural University, Qingdao, China; [4]Thermo Fisher Scientific, West Palm Beach, FL*

MP 700 **Enhanced Proteomics and Transcriptomics Reveal the Role of DHHC12 in Immune System Palmitoylation**; Hyojung Kim[1, 2]; Jiraphorn Issara-Amphorn[2, 3]; Sung Hwan Yoon[2, 3]; Aleksandra Nita-Lazar[2, 3]; Anirban Banerjee[1, 2]; *[1]Eunice Kennedy Shriver National Institute of Child Health and Human Development, Bethesda, MD; [2]National*

Institutes of Health, Bethesda, MD; [3]National Institute of Allergy and Infectious Diseases, Bethesda, MD

MP 701 **motif-x 2.0: Incorporating quantitative phosphorylation site information and other novel functionalities for better PTM motif identification and discovery**; Audrey Baker[1]; Jen Liddle[2]; Jeremy Balsbaugh[2]; Anastasios Tzingounis[1]; Daniel Schwartz[1]; *[1]Department of Physiology and Neurobiology, University of Connecticut, Storrs, Connecticut; [2]Proteomics & Metabolomics Facility, Center for Open Research Resources & Equipment, University of Connecticut, Storrs, Connecticut*

MP 702 **Optimization of Lactylation Proteomics Analysis with Orbitrap Astral**; Audrick Yang[1]; Yongji Shi[1]; Xitong Han[2]; *[1]PTM Bio LLC, Alameda, CA; [2]Dublin High School, Dublin, CA*

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MP 703 **Top-down proteomics in nanomedicine: proteoform-specific analysis of nanoparticle protein corona and its application in proteoform biomarker discovery of cancer**; Amirhossein Sadeghi[1]; Mrteza Mahmoudi[1]; Liangliang Sun[1]; *[1]Michigan State university, EAST LANSING, MI*

MP 704 **Caveat Emptor: Combined top-down/bottom-up MS analysis reveals pervasive quality control problems in commercially available proteins**; Durgalakshmi Sivasankar[1]; Md Amin Hossain[1]; Jeffrey Agar[1]; *[1]Northeastern University, Boston, MA*

MP 705 **Enhancement of proteoform sequence coverage using top-down mass spectrometry with in-source fragmentation and middle-down mass spectrometry**; Xingzhao Xiong[1]; Xiaowen Liu[1]; *[1]Tulane University, New Orleans, LA*

MP 706 **Native Top-down characterization of membrane protein-lipid interactions**; Gustavo Perrotti[1]; Sara Walters[1]; James Q. Xia[2]; Brian Fuglestad[1]; Fabio P. Gomes[1]; *[1]Virginia Commonwealth University, Richmond, VA; [2]CMP Scientific Corp, Brooklyn, NY*

MP 707 **Characterizing the H3 histone proteoforms by ultrahigh-resolution ion mobility separations with electron capture dissociation** ; Alexandre A Shvartsburg[1]; Doniesha L Perera[1]; Hayden A Thurman[1]; Muhammad Bin Zenaidee[2]; Ruth Wang[2]; Gene Hart-Smith[2]; Haifan Wu[1]; *[1]Wichita State University, Wichita, KS; [2]Macquarie University, North Ryde, Australia*

MP 708 **Are Complex-Up and Top-Down Approaches in Harmony on Ribosomal Protein PTMs and Abundances?**; Sachin Tennakoon[1]; Jared B. Shaw[1]; *[1]Department of Chemistry, University of Nebraska-Lincoln, Lincoln, NE*

MP 709 **Finding the optimal degassing condition for linear polyacrylamide coated capillaries used in capillary zone electrophoresis-mass spectrometry-based top-down proteomics**; Yifan Yue[1]; Guijie Zhu[1]; Fei Fang[1]; Guangyao Gao[1]; Liangliang Sun[1]; *[1]Michigan State University, Department of Chemistry, East Lansing, MI*

MP 710 **Top-down characterization of industrial enzymes on a timsOmni platform**; Anders MB Giessing[1]; Bruna Margues Dos Santos[1]; Christian Isak Jørgensen[1]; Christian Albers[2]; Athanasios Smyrnakis[3]; Mariangela Kosmopoulou[3]; Dimitris Papanastasiou[3]; *[1]Novonesis A/S, Kgs Lyngby, Denmark; [2]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [3]Fasmatech Science & Technology, Chalandri, Greece*

MP 711 **Chemical top-down proteomics for identifying differentially reactive proteoforms**; Teagan L Campbell[1]; Bryon S Drown[2]; *[1]Purdue University, West Lafayette, IN; [2]Purdue Univeristy, West Lafayette, IN*

MP 712 **Comprehensive Proteoform Analysis of Yeast Cells Using Sequential Extraction, Size-exclusion Chromatography Fractionation, and Capillary Electrophoresis-tandem Mass Spectrometry**; Maryam Rahimzadeh Dashtaki[1]; Liangliang Sun[2]; *[1]Michigan State University, East Lansing, MI; [2]Michigan State University Department of Chemistry, East Lansing, MI*

MP 713 **Offline tandem MSn workflows on the timsOmni platform for deep sequencing of intact proteins and mAbs**; Athanasios Smyrnakis[1]; Mariangela Kosmopoulou[1]; Anastasios Grigoriadis[1]; Florian Busch[2]; Stuart Pengelley[3]; Eduardo Carrascosa[3]; Christoph Gebhardt[3]; Amalia Apalategui[3]; Oliver Raether[3]; Dimitris Papanastasiou[1]; *[1]Fasmatech Science & Technology, Chalandri, Greece; [2]Bruker Switzerland AG, Fällanden, Switzerland; [3]Bruker Daltonics, Bremen, Germany*

MP 714 **Applying DDA-CSD-ExD on a timsOmni to the analysis of the Fab regions of antibodies originating from human serum**; Simon Ollivier[1]; Manuel R. Bauer[2]; Dina Schuster[1]; Athanasios Smyrnakis[3]; Jan Fiala[1]; Stuart Pengelley[4]; Oliver Raether[4]; Mariangela Kosmopoulou[3]; Detlev Suckau[4]; Jean-Francois Greisch[1, 2]; Dimitris Papanastasiou[3]; Albert J.R. Heck[1]; *[1]Utrecht University, Utrecht, Netherlands; [2]Bruker Switzerland AG, Fällanden, Switzerland; [3]Fasmatech Science & Technology, Chalandri, Greece; [4]Bruker Daltonics GmbH & Co. KG, Bremen, Germany*

MP 715 **State-of-the-art characterization of in vivo biotransformations of biotherapeutics on the new timsOmni platform**; Lucile Kogey-Fuchs[1, 2]; Athanasios Smyrnakis[3]; Anastasios Grigoriadis[3]; Mariangela Kosmopoulou[3]; Megan Gant[2]; Florian Busch[4]; Jonathan Dhenin[5]; Alain Krick[1]; Christine Mauriac[1]; Dimitris Papanastasiou[3]; Julia Chamot-Rooke[2]; *[1]DMPK, Sanofi R&D, Vitry-sur-Seine, France; [2]Institut Pasteur, Université Paris Cité, CNRS UAR 2024, Mass Spectrometry for Biology, Paris, France; [3]Fasmatech Science & Technology, Chalandri, Greece; [4]Bruker Switzerland AG, Fällanden, Switzerland; [5]Novartis Pharma AG, Basel, Switzerland*

MP 716 **Top-down characterization of intact adeno-associated virus (AAV) capsid protein deamidation utilizing nano spray liquid chromatography mass spectrometry (nanoLC-MS)**; Josh Smith[1]; Corentin Beaumal[1]; Aaron Richardson[1]; Felipe Guapo[1]; Sara Carillo[1]; Jonathan Bones[1, 2]; *[1]The National Institute for Bioprocessing Research and Training (NIBRT), Dublin, Ireland; [2]School of Chemical and Bioprocess Engineering, University College Dublin, Dublin, Ireland*

MP 717 **High Sensitivity Proteomic Analysis of Micropatterned Induced Pluripotent Stem Cell-Derived Cardiomyocytes**; Mallory C Wilson[1]; Mitchell Josvai[2, 3]; Janay K Walters[3]; Jodi Lawson[2, 3]; Kalina J Rossler[3]; Wendy C Crone[2, 4]; Lee L Eckhardt[3]; Ying Ge[1, 5, 6]; *[1]UW-Madison Department of Chemistry, Madison, WI; [2]UW-Madison Department of Biomedical Engineering, Madison, WI; [3]UW-Madison School of Medicine and Public Health, Madison, WI; [4]UW-Madison Department of Nuclear Engineering and Engineering Physics, Madison, WI; [5]UW-Madison Department of Cell and Regenerative Biology, Madison, WI; [6]Human Proteomics Program, University of Wisconsin-Madison, Madison, WI*

MP 718 **False Positive Assignment of Internal Fragments in Top-Down Electron-Based Dissociation of Antibodies**; Neven N. Mikawy[1, 2]; Carolina Rojas Ramírez[3]; Chad R. Weisbrod[1, 2]; Lissa C. Anderson[1, 2]; Kristina Hakansson[1, 2]; *[1]National High Magnetic Field Laboratory, Tallahassee, FL; [2]Florida State University, Tallahassee, FL; [3]Department of Pathology, University of Michigan, Ann Arbor, MI*

MP 719 **Top-Down Analysis of Fluorescent Proteins with Non-Canonical Amino Acids using Ultraviolet Photodissociation and Proton Transfer Charge Reduction**; Jessica Hellinger[1]; Andrew Gilmour[2]; Ross Thyer[2]; Jennifer S Brodbelt[1]; *[1]University of Texas - Austin, Austin, TX; [2]Rice University, Houston, TX*

MP 720 **A Gold-Standard Dataset of Carbonic Anhydrase for Future Top-Down Spectrum Deconvolution Software Programming**; Michelle Yu[1]; Novera Alam[1]; Jeffrey Agar[1]; *[1]Northeastern University, Boston, MA*

MP 721 **Overcoming challenges from internal fragmentation of modified membrane protein complexes using native top-down mass spectrometry**; Frances I Butroid[1, 2]; Corinne A Lutomski[1, 2]; Jack L Bennett[1, 2]; Tarick J El-Baba[1, 2]; Carol V

Robinson[1, 2]; *[1]Department of Chemistry, University of Oxford, Oxford, United Kingdom; [2]Kavli Institute for Nanoscience Discovery, University of Oxford, Oxford, United Kingdom*

MP 722 **Properties, Origin, and Reproducibility of Truncated Proteoforms in Recent Top-Down Proteomic Studies**; Philipp T. Kaulich[1]; James M. Fulcher[2]; Andreas Tholey[1]; *[1]Systematic Proteome Research & Bioanalytics, Institute for Experimental Medicine, University of Kiel, Kiel, Germany; [2]Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, Washington 99354*

MP 723 **Top-Down Mapping of Protein Modifications by Multimodal MS^n on the new timsOmni Platform**; Francis Berthias[1]; Nurgül Bilgin[1]; Christian Albers[2]; Athanasios Smyrnakis[3]; Mariangela Kosmopoulou[3]; Jasmin Mecinović[1]; Dimitris Papanastasiou[3]; Ole Nørregaard Jensen[1]; *[1]University of Southern Denmark, Odense M, Denmark; [2]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [3]Fasmatech Science & Technology, Chalandri, Greece*

MP 724 **Reproducible capillary electrophoresis-mass spectrometry-based top-down proteomics of complex proteomes enabled by an advanced cationic polymer coating**; Guangyao Gao[1]; Guijie Zhu[1]; Fei Fang[1]; Yifan Yue[1]; Liangliang Sun[1]; *[1]Michigan State University Department of Chemistry, East Lansing, MI*

MP 725 **Methionine Oxidation Footprinting in Intact Proteins using Top-Down Proteomics coupled with TMT-labeling**; Anju Teresa Sunny[1]; Trishika Chowdhury[1]; Kellye Cupp Sutton[1]; Si Wu[1]; *[1]The University of Alabama, Tuscaloosa, AL*

MP 726 **Quantification of attomole-level intact proteoforms using multisegmented spray-capillary CE-MS and parallel reaction monitoring**; Zhitao Zhao[1]; Kellye A. Cupp-Sutton[2]; Samin Anjum[2]; Ahmed Mohamed Amin Abdelhamed[2, 3]; Si Wu[2]; *[1]Oklahoma University, Norman, OK; [2]The University of Alabama, Tuscaloosa, AL; [3]Ain Shams University, Cairo, Egypt*

MP 727 **Enhanced proteoform identification in top-down proteomic workflows using packed emitter columns**; Andreia Filipa Ferreira De Almeida[1]; Amy K. Carfagno[2]; Jake T. Kline[2]; Jarrod Sandow[1]; Luca Fornelli[2]; *[1]IonOpticks, Melbourne, Australia; [2]University of Oklahoma, Norman, OK*

MP 728 **Enabling spatial top-down proteomics of the human cell using gas-phase fractionation and ion-ion reactions**; Jake T Kline[1]; Jingjing Huang[2]; Chirstopher Mullen[3]; Graeme C McAlister[3]; Joseph B Greer[4]; David Bergen[3]; Michael W Belford[3]; Cornelia L Boeser[3]; Vlad Zabrouskov[3]; Kenneth R Durbin[4]; Rafael D Melani[3]; Luca Fornelli[1]; *[1]University of Oklahoma, Norman, OK; [2]Thermo Fisher Scientfic, San Jose, CA; [3]Thermo Fisher Scientific, San Jose, CA; [4]Proteinaceous, Evanston, IL*

MP 729 **Top-Down Electron-Based Dissociation for Characterizing Tyrosine-O-Sulfation**; Kuan-Lu Wu[1, 2]; Neven N. Mikawy[1, 2]; Lissa C. Anderson[1, 2]; Kristina Hakansson[1, 2]; *[1]National High Magnetic Field Laboratory, Tallahassee, FL; [2]Florida State University, Tallahassee, FL*

MP 730 **SEC-complex down approaches with functional O2-affinity assay: Correlation between the higher order structure of bird hemoglobin homologues and their function**; Léa Letissier[1, 2]; Turkan Nabiyeva[1, 2]; Maïly KERVELLA[1]; François Criscuolo[1]; Fabrice Bertile[1, 2]; Christine Schaeffer[1, 2]; Sarah Cianférani[1, 2]; Oscar Hernandez Alba[1]; *[1]Institut Pluridisciplinaire Hubert Curien LSMBO, Strasbourg, France; [2]Pro FI, Infrastructure Nationale de Protéomique, Strasbourg, France*

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MP 731 **Quantifying chimeric spectra of isobaric-labelled peptides with real-time searching**; Chris McGann[1]; Michael Hoopmann[2]; Erik Bergstrom[2]; Chuwei Lin[2]; Fengchao Yu[3]; Alexey Nesvizhskii[3]; Devin Schweppe[2]; *[1]University of Washingon, Seattle, WA; [2]University of Washington, Seattle, WA; [3]University of Michigan, Ann Arbor, Michigan*

MP 732 **Synergistic Digestion of Arg-C Ultra and Lys-C in Multiplexed Proteomics**; Vyas Pujari[1, 2]; Joseph Crapse[1, 2]; Connor Nisbet[1, 2]; Chris Hosfield[3]; Mike Rosenblatt[3]; Felix Keber[1, 2]; Martin Wühr[1, 2]; *[1]Princeton University, Princeton, NJ; [2]Lewis-Sigler Institute for Integrative Genomics, Princeton University, Princeton, NJ; [3]Promega Corp, Madison, WI*

MP 733 **Accurate and Sensitive Multiplexed Quantitative Proteomics Using the DiLeu Complementary Ion Strategy**; Jingwei Zhang[1]; Zicong Wang[1]; Penghsuan Huang[1]; Lingjun Li[1]; *[1]University of Wisconsin-Madison, Madison, WI*

MP 734 **Dynamic TRPV2 ion channel proximity proteomics links calcium flux to cellular adhesion factors NCAM1 and L1CAM in neurite outgrowth**; Pamela N. Gallo[1]; Elaine Mihelc[1]; Robyn J. Eisert[2]; Gary A. Bradshaw[2]; Marian Kalocsay[3]; Vera Moiseenkova-Bell[1]; *[1]University of Pennsylvania, Perelman School of Medicine, Philadelphia, PA; [2]Harvard Medical School, Boston, MA; [3]MD Anderson Cancer Center, Houston, TX*

MP 735 **Automating Stable Isotope Standards and Capture by Anti-Peptide Antibodies (SISCAPA®) assay on the Biomek i7 Hybrid Workstation for AEMS analysis**; Maxim Zhgamadze[1]; Bart Van Puyvelde[2]; Sudha Savant[3]; Christie Hunter[4]; Esthelle Paul Hoedt[1]; Yang Oliver Wang[1]; Qin Fu[1]; Sarah Gomes De Oliveira[3]; Partha Banerjee[3]; Jennifer E Van Eyk[1]; *[1]Smidt Heart Institute, Los Angeles, CA; [2]Ghent University, Ghent, Belgium; [3]Beckman Coulter Life Sciences, Indianapolis, IN; [4]Sciex, Redwood City, CA*

MP 736 **Time-resolved absolute protein quantification in different subcellular fractions: a mass-spectrometry based approach to investigate Bacillus subtilis as industrial model**; Francesca Grilli[1, 2]; Dörte Becher[1]; Jan Maarten Van Dijl[2]; Sandra Maaß[1]; *[1]University of Greifswald, Department of Microbial Proteomics, Greifswald, Germany; [2]University Medical Center Groningen, Department Medical Microbiology and Infection Prevention, Groningen, Netherlands*

MP 737 **Testing popular proteomics sample preparation techniques across two large cohorts of new users over a two year period**; Brett Phinney[1]; Michael Krawitzky[2]; Michelle Salemi[3]; Lauren Dixon[3]; Gabriela Grigorean[3]; *[1]Univeristy of CA, Davis, Davis, CA; [2]Bruker Corporation, San Francisco, CA; [3]UC Davis, Davis, CA*

MP 738 **Antigen-Induced Proteome Alteration During Phagocytosis in Macrophages**; Wing Yin Wu[1]; Clarence T. T. Wong[1]; Zhongping Yao[1]; *[1]The Hong Kong Polytechnic University, Hong Kong, Hong Kong*

MP 739 **Label-free quantitative proteomics with high precision and accuracy, driven by ultra-high-sensitivity MS/MS**; Ihor Batruch[1]; Patrick Pribil[1]; *[1]SCIEX, Concord, ON*

MP 740 **Sensitive and accurate proteome profiling of embryogenesis using Real-Time Search and TMTproC quantification**; Alex Johnson[1]; Jingjing Huang[2]; Argit Marishta[1]; Edward Cruz[1]; Andrea Mariossi[1]; William Barshop[2]; Jesse Canterbury[2]; Rafael Melani[2]; David Bergen[2]; Vlad Zabrouskov[2]; Michael S. Levine[1]; Eric Wieschaus[1]; Graeme McAlister[2]; Martin Wühr[1]; *[1]Princeton University, Princeton, NJ; [2]Thermo Fisher Scientific, San Jose, CA*

MP 741 **Moving Towards a Proteomics Blood-Based Diagnosis of Alzheimer's Disease Using Human Brain Tissue, CSF, and Plasma Samples by nanoLC-FAIMS-MS/MS**; Andrew I. Bennett[1]; Cristian D. Gutierrez-Reyes[1]; Vishal Sandilya[1]; Sherifdeen Onigbinde[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX*

MP 742 **Characterizing 32-plex TMTpro Reagents for High-Throughput Quantitative Proteomics on Orbitrap Platforms**; Dustin Frost[1]; Frank Berg[2]; Kai Fritzemeier[2]; Pedro Navarro[2]; David Horn[3]; Ryan Bomgarden[1]; *[1]Thermo Fisher Scientific, Rockford, IL; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [3]Thermo Fisher Scientific, San Jose, CA*

MP 743 **Quantitative Accuracy and Quality of Complex Proteome Analysis: Orbitrap Astral vs. Hybrid and other Tribrid Systems**; Leila Afjehi[1, 2]; Alina Siegl[1, 2]; Marcel Kwiatkowski[3]; *[1]University of Vienna, Vienna, Austria; [2]Mass spectrometry Unit, Research Support Facilities, Vienna, Austria; [3]University of Innsbruck, Innsbruck, Austria*

MP 744 **A Streamlined Thermal Proteome Profiling Workflow in a Core Facility Using label-free DIA and Mass Dynamics**; Danielle Hanke[1]; Xiaojing Yuan[2]; Jason Rogalski[2]; Brent D.G. Page[1]; *[1]Faculty of Pharmaceutical Sciences, UBC, Vancouver, BC; [2]UBC Proteomics and Metabolomics Core Facility, Vancouver, BC*

MP 745 **TRMU Confers Resistance of Melanoma Cells to Vemurafenib through Modulating Mitochondrial tRNA Modifications**; Shiyuan Guo[1]; Tianyu F. Qi[1]; Yinsheng Wang[1]; *[1]University of California, Riverside, Riverside, CA*

MP 746 **Improved accuracy and identification in label-free quantitative proteomics with a novel ion source and separation cartridge with integrated replaceable emitters**; Martins Jansons[1]; Joshua Silveira[2]; Katherine Walker[2]; Cornelia Boeser[2]; Eloy R. Wouters[3]; Amirmansoor Hakimi[2]; *[1]Thermo Fisher Scientific, Vilnius, Lithuania; [2]Thermo Fisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific, San Jose, California*

MP 747 **Deeper Proteome Profiling with Higher Throughput via Optimized Ion Processing on a Modified Orbitrap Astral Mass Spectrometer**; Ulises Hernandez Guzman[1]; Ivo Alexander Hendriks[1]; Martin Rykær[1]; Hamish Stewart[2]; Yannick Mueller[2]; Immo Colonius[2]; Tabiwang Arrey[2]; Eugen Damoc[2]; Christian Hock[2]; Jesper V. Olsen[1]; *[1]Novo Nordisk Foundation Center for Protein Research, University of Copenhagen, Denmark; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

MP 748 **Enhancing the resolving power on a novel Orbitrap Astral instrument for TMT35plex applications**; Julia Kraegenbring[1]; Martin Zeller[2]; Bernard Delanghe[2]; Christopher Rathje[2]; Eduard Denisov[2]; Robert Ostermann[2]; Florian Bonn[2]; Alexander Wagner[2]; Dustin Frost[3]; Ryan Bomgarden[3]; Eugen Damoc[2]; Johannes Petzoldt[2]; Christian Hock[2]; Hamish Stewart[2]; *[1]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [2]Thermo Fisher Scientific, Bremen, Germany; [3]Thermo Fisher Scientific, Rockford, IL*

MP 749 **An Automated, Deep-Profiling Approach to Accelerate Target Identification for Molecular Glue Degraders Using TMTpro 32-plex**; Xudong Wang[1]; Katie May[1]; Despina Kapsitidou[2]; Vaik Strande[2]; Reinaldo Almeida[2]; Debora Bonenfant[2]; *[1]Monte Rosa Therapeutics, Boston, MA; [2]Monte Rosa Therapeutics, Basel, Switzerland*

MP 750 **Amyotrophic Lateral Sclerosis-Associated Mutants of UBQLN2 Alter Protein Homeostasis through Aberrant Interactions with TRIM9 and TRIM26**; Xingyuan Chen[1]; Zhongwen Cao[1]; Yinsheng Wang[1]; *[1]University of California, Riverside, Riverside, CA*

MP 751 **Improved Absolute Quantification of Human Kv7.2/7.3 Expressed in HEK293 Cells with Detergents or Rapid Digest in Two-Step Digestion Approach**; Rainbow WP Kwan[1]; Stephanie Lee[1]; Giselle Klynsoon[2]; Amy Wong[3]; Luis Sojo[1]; *[1]Xenon Pharmaceuticals, Burnaby, BC; [2]The University of Victoria, Victoria, British Columbia; [3]The University of British Columbia, Vancouver, British Columbia*

MP 752 **Multiplexed Data-independent Acquisition-based Proteomics Enabled by TMTpro Complementary Ions**; Zicong Wang[1]; Peng-Kai Liu[2]; Haiyan Lu[1]; Lingjun Li[1, 3]; *[1]School of Pharmacy, University of Wisconsin-Madison, Madison, WI; [2]Biophysics Graduate Program, University of Wisconsin-Madison, Madison, WI; [3]Department of Chemistry, University of Wisconsin–Madison, Madison, WI*

MP 753 **A new labeling reagent with 32 isobaric tags for quantitative proteomics**; Wenbo Cui[1, 2]; Ruixin Tian[1, 2]; Guixue Hou[1, 2]; Jin Zi[1, 2]; Shuwei Li[3]; Siqi Liu[1, 2]; *[1]College of Life Sciences, University of Chinese Academy of Sciences, Beijing, China; [2]BGI-Shenzhen, Shenzhen, China; [3]Nanjing Apollomics Biotech Inc, Nanjing, China*

MP 754 **METTL1 Interacts with XPO5 to Modulate Pre-miRNA Export**; Zhongwen Cao[1]; Xingyuan Chen[1]; Yinsheng Wang[1]; *[1]University of California, Riverside, Riverside, CA*

MP 755 **UNTARGETED AND TARGETED PROTEOMICS REVEAL THE ANTI-INFLAMMATORY POTENTIAL OF A NOVEL NRF2-ACTIVATOR IN AN ULCERATIVE COLITIS MODEL**; Alessandra Anna Altomare[1]; Giulio Fumagalli[1]; Lara Davani[1]; Emanuele Salina[1]; Rosanna Di Paola[2]; Clelia Mariangiola Luisa Dallanoce[1]; Marina Carini[1]; Daniela Impellizzeri[2]; Giancarlo Aldini[1]; *[1]University of Milan, Milano, Italy; [2]University of Messina, Messina, Italy*

MP 756 **More from less: Assessing and adapting key parameters for low-input LC-MS measurements**; Denise Jansen[1, 2, 3]; Martin Schneider[1]; Barbara Helm[2, 3]; Ursula Klingmüller[2, 3, 4]; Dominic Helm[1, 4]; *[1]Proteomics Core Facility, German Cancer Research Center (DKFZ), Heidelberg, Germany; [2]Division Systems Biology of Signal Transduction, German Cancer Research Center (DKFZ), Heidelberg, Germany, Heidelberg, Germany; [3]German Center for Lung Research (DZL) and Translational Lung Research Center Heidelberg (TRLC), Heidelberg, Germany, Heidelberg, Germany; [4]Liver Systems Medicine against Cancer (LiSyM-Krebs), Germany, Heidelberg, Germany*

MP 757 **Quantifying intact RAS proteins from cancer cell lines using a novel multiplexed proteoform reaction monitoring (PfRM) assay**; Alyssa A Williams[1]; Jake T. Kline[1]; Matthew T. Robey[2]; Grace M Scheidemantle[3]; Robert A. D'Ippolito[3]; Peter Frank[3]; Dominic Esposito[3]; Ken Durbin[2]; Caroline DeHart[3]; Luca Fornelli[4]; *[1]University of Oklahoma, Norman, OK; [2]Proteinaceous, Evanston, IL; [3]Frederick National Laboratory for Cancer Research, Frederick, MD; [4]Oklahoma University, Norman, OK*

SYSTEMS BIOLOGY
758-764

MP 758 **A proteocistromic atlas of human transcription factors**; Markku Varjosalo; *HiLIFE, University of Helsinki, Helsinki, Finland*

MP 759 **PeptideAtlases of Arabidopsis and Maize for Plant Proteome Discoveries and community resources for MS-based plant proteome data; novel biological insights**; Klaas j. Van Wijk[1]; Eric Deutsch[2]; Tami Leppert[2]; Zhi Sun[2]; Luis Mendoza[2]; Qi Sun[1]; Stephane Bentolila[1]; *[1]Cornell University, Ithaca, NY; [2]Institute for Systems Biology, Seattle, WA*

MP 760 **Using single-cell proteomics by MS to disentangle human blood stem cell differentiation**; Benjamin Furtwängler[1, 2, 3]; Üresin Nil[1, 2, 3]; Sabrina Richter[4]; Mikkel Bruhn Schuster[2]; Despoina Barmpouri[2]; Henrietta Holze[1, 2]; Anne Wenzel[2]; Kirsten Grønbæk[2, 5]; Kim Theilgaard-Mönch[2, 3, 5]; Fabian Theis[4]; Erwin Schoof[1]; Bo Porse[2, 3, 5]; *[1]DTU, Lyngby, Denmark; [2]University of Copenhagen, Copenhagen, Denmark; [3]Finsen Laboratory, Copenhagen, Denmark; [4]Helmholtz Munich, Munich, Germany; [5]Copenhagen University Hospital, Copenhagen, Denmark*

MP 761 **The RSV-inducible Interactome of Interferon Regulatory Factor-1 Using Immunoprecipitation-Mass Spectrometry**; Robert L. Gearhart[1]; Xiaofang Xu[2]; Ying Ge[1, 3, 4]; Allan R. Brasier[2, 5]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [2]Department of Medicine, University of Wisconsin-Madison, Madison, WI; [3]Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI; [4]Human Proteomics Program, University of Wisconsin-Madison, Madison, WI; [5]Institute for Clinical and Translational Research, University of Wisconsin-Madison, Madison, WI*

MP 762 **Quantification of cell-type specific protein dynamics in Drosophila embryos**; Argit Marishta[1]; Edward Cruz[1]; Alex Johnson[1]; Martin Wühr[1, 2]; Eric Wieschaus[1]; *[1]Princeton University, Princeton, NJ; [2]Lewis-Sigler Institute for Integrative Genomics, Princeton University, Princeton, NJ*

MP 763 **TimsTof DIA PASEF label-free proteomic profiling of human dendritic cells unveils the landscape of signaling pathways triggered by IFN-α/γ**; Cristina C Clement[1];

Rajesh K. Soni[2]; Laura Santambrogio[1]; *[1]Weill Cornell Medicine, New York, NY; [2]Proteomics and Macromolecular Crystallography Shared, Herbert Irving Comprehensive Cancer Center, Columbia University Irving Medical Center Resource, New York, New York*

MP 764 **Ubiquitinomics and targeted proteomics reveals de-ubiquitination dynamics by the Hao-Fountain protein Ubiquitin-Specific Protease 7 (USP7) and its role in proteostasis**; Jeroen AA Demmers; *Erasmus University Medical Center, Rotterdam, Netherlands*

TUESDAY POSTERS

TUESDAY POSTERS

Set-up for all Monday posters
6:30 - 9:00 am

ALL POSTERS PRESENT

10:30 - 12:00 pm AND 1:00 - 2:30 pm

Remove all Monday posters
5:00 - 8:00 pm

Antibodies & Antibody Drug Conjugates II 001-038
Antidoping, Cannabis, and Opioid Detection 039-046
Art, Archaeology & Paleontology 047-051
Artificial Intelligence in MS Instrumentation and Applications II 052-069
Biomarkers: Discovery II 070-113
Cancer Research II 114-143
Clinical Analysis II 144-171
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Environmental: Pharmaceuticals and Pesticides 286-309
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Fundamentals: Molecular Modeling / Quantum Mechanical Calculations 337-340
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Metabolomics: General 546-586
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Peptides: PTM Identification 624-644
Process Development MS 645-656
Proteins: Complexes/Non-covalent Interactions 657-691
Proteomics: Intact Proteins and Top Down Analysis II 692-719
Proteomics: Quantitative II 720-742
Viruses and Virus-Like Particles 743-766

ANTIBODIES & ANTIBODY DRUG CONJUGATES II
001-038

TP 001 **Couple PTCR in RP LC-MS for Therapeutic Antibody Characterization**; Aaron J Cazy[1]; Zhongping Liao[1]; *[1]Eli Lilly and Company, Indianapolis, IN*

TP 002 **Mass spectrometry imaging of antibody-drug conjugates and free payload in xenograft tissue from dosed mice**; Sarah Vickers[1]; Emma K. Sisley[2]; Oliver Hale[1]; Peter D. E. Macey[1]; Andreas Danhorn[3]; Richard J. A. Goodwin[3]; Helen Cooper[1]; *[1]University of Birmingham, Birmingham, United Kingdom; [2]OMass Therapeutics, Oxford, United Kingdom; [3]AstraZeneca, Cambridge, United Kingdom*

TP 003 **Analysis of Free Drug Content in Antibody-Drug Conjugate Using 2D-LC/Q-TOF/MS**; Yulan Bian[1]; Andreas Mielcarek[2]; *[1]Agilent Technologies, Singapore, Singapore; [2]Agilent Technologies, Inc., Waldbronn, Germany*

TP 004 **The Missing Step to Perform MAM in QC**; Julien Bourquin[1]; Mélanie Jakobczyk[1]; Véronique Karawa[1]; Alice Duperrex[1]; Amarande Murisier[1]; Rayane Mohamed[1]; Diego Bertaccini[1]; *[1]EMD Serono, Corsier-sur-Vevey, Switzerland*

TP 005 **Hot de novo Antibody Sequencing: one protease, one run, massively redundant reads covering all hypervariable regions**; Tatiana M Shamorkina[1]; Tereza Kadavá[1]; Laura Perez Paneda[1]; Sibylle M. Heidelberger[2]; Patrick Pribil[3]; Joost Snijder[1]; Albert J.R... Heck[1]; Steven M Yannone[4]; *[1]Utrecht University, Utrecht, Netherlands; [2]SCIEX, Alderley Park, United Kingdom; [3]SCIEX, Concord, L4K; [4]CinderBio, San Leandro, CA*

TP 006 **Assessment of Nonreduced IgG2 Disulfide Structure by 213 nm Ultraviolet Photodissociation**; Michael B Lanzillotti[1]; Hao Zhang[1]; *[1]Amgen, Inc., Cambridge, MA*

TP 007 **LC-MRM Method Development and Bioanalysis Strategy to Accurately Quantitate an Antibody Therapeutic with Deamidation Liability**; Radek Abarca[1]; Yihan Li[1]; Hetal Sarvaiya[1]; *[1]AbbVie, South San Francisco, CA*

TP 008 **Characterization of photo stressed Antibody Drug Conjugates by LCMS to understand degradation liabilities**; Robert Tchelepi[1]; Kevin Lindquist[1]; Jieyu Zhou[1]; Mohan Srinivasan[1]; Sachin Shivatare[1]; Steven R Cottle[2]; Abraham H Abouzeid[2]; Jianyu Zhu[1]; Yvonne Mak[1]; Gregg Czerwieniec[1]; *[1]Eli Lilly and Company, South San Francisco, CA; [2]Eli Lilly and Company, Indianapolis, IN*

TP 009 **Nano-flow pressure mobilization for icIEF fractionation and online MS detection: sharpening protein heterogeneity analysis**; She Lin Chan[1]; Teresa Kwok[1]; Tao Bo[1]; Tiemin Huang[1]; Niusheng Xu[1]; *[1]Advanced Electrophoresis Solutions, Cambridge, Ontario*

TP 010 **A Sample Prep Approach Yielding 100% Denovo Sequence Coverage**; Gabrielle Rizzo[1]; Elizabeth Dhummakupt[1]; Edward Randal Hofmann[2]; Conor Jenkins[1]; *[1]DEVCOM Chemical Biological Center, Aberdeen Proving Ground, MD; [2]Excet A Precise Systems Company, Edgewood, MD*

TP 011 **Enhanced sensitivity of intact LCMS approaches to expand the capability of biotherapeutic analysis with a novel QTOF**; Haichuan Liu[1]; Zoe Zhang[1]; Elliott Jones[1]; *[1]SCIEX, Redwood City, CA*

TP 012 **High-throughput protein quality attribute monitoring during biotherapeutics development by MALDI-MS**; Christopher Lößner[1]; Mario Valkai[1, 2]; Marianne Scheffold[1]; Arndt Asperger[3]; Göran Hübner[1]; *[1]Boehringer Ingelheim Pharma, Development CMC Biologicals, Mass Spectrometry and Characterisation, Biberach an der Riss, Germany; [2]Roche Pharma Research and Early Development, Large Molecule Research, Mass Spectrometry, Penzberg, Germany; [3]Bruker Daltonics GmbH & Co. KG, Bremen, Germany*

TP 013 **Towards long acting and potent peptide therapeutics: Cyclic Ion mobility-Mass Spectrometry reveals conformational stability of novel heterodimeric Fc-peptide fusions**; Esther Martin[1]; Monika Papworth[1]; Isabelle Sermadiras[1]; Judy Paterson[1]; Nathalie Barrett[1]; Marcin

Wolny[1]; Andrew Buchanan[1]; *[1]AstraZeneca, Cambridge, United Kingdom*

TP 014 **A novel high throughput quantitation method for an antibody drug conjugate with a β-glucuronidase cleavable linker** ; Xiaoying Zhou[1]; Zhengquan Zhang[1]; Yarong Qu[1]; Ling Xin[1]; Ganyuan Xiao[1]; Yingdong Lu[1]; Mao Yin[1]; Ling Xu[1]; *[1]PrimeLink Therapeutics, Suzhou, China*

TP 015 **A Novel Proteogenomic/de Novo Sequencing Platform for Selective Anti-Idiotype Antibody Discovery**; Teresa Nunez De Villavicencio Diaz[1]; Chelsea Reitzel[1]; Thierry Le Bihan[1]; Bin Ma[1]; *[1]Rapid Novor Inc, Kitchener, ON*

TP 016 **Beyond ELISA: A Mass Spectrometric Platform for Universal and Specific Detection of Therapeutic Antibodies in Clinical Samples**; Chelsea Reitzel[1]; Teresa Nunez De Villavicencio Diaz[1]; Emiliya Kari[1]; Thierry Le Bihan[1]; Bin Ma[1]; *[1]Rapid Novor Inc, Kitchener, ON*

TP 017 **A Novel Multidimensional Liquid Chromatography Workflow with In-Loop Enzymatic Digests of Multiple Heart-Cuts for Fast&Flexible Characterization of Biotherapeutic Protein Variants**; Kilian Mayr[1]; Thomas Weindl[1]; Achim Gärtner[1]; Julien Camperi[2]; Thomas Maetzke[3]; Markus Förster[4]; Thomas Nachtigall[4]; Frank Steiner[4]; Annette Vogt[1]; Fabian Hosp[1]; Michael Molhoj[5]; *[1]Roche, Pharma Research and Early Development (pRED), Penzberg, Germany; [2]Genentech, South San Francisco, CA; [3]HPLConsult GmbH, Pfeffingen, Switzerland; [4]Thermo Fisher Scientific GmbH, Dreieich, Germany; [5]Immatics Biotechnologies GmbH, Munich, Germany*

TP 018 **An LCMS method for routine detection and quantitation of host cell proteins in monoclonal antibody products using data-independent acquisition**; Sahana Mollah[1]; Remco Van Soest[1]; Patrick Pribil[2]; *[1]SCIEX, Redwood City, CA; [2]SCIEX, Concord, ON*

TP 019 **Investigating residual trace metals in recombinant monoclonal antibodies to facilitate drug development with LC-UV-ICPMS-HRMS**; Xueqing Zhao[1]; Jikang Wu[1]; Yu Zhang[1]; Hongxia Wang[1]; Haibo Qiu[1]; Ning Li[1]; *[1]Regeneron, Tarrytown, NY*

TP 020 **Rapid Antibody Sequencing via Microdroplet Trypsin Digestion in a Jet Stream Source**; Mengyuan Xiao[1]; Yongqing Yang[1]; Jim Lau[2]; Michael D Knierman[2]; Xi Qiu[2]; Hui Zhao[2]; Karen Luo[2]; Harsha Gunawardena[3]; Hao Chen[1]; *[1]New Jersey Institute of Technology, Newark, NJ; [2]Agilent Technologies, Wilmington, DE; [3]Janssen Pharmaceuticals, Spring House, PA*

TP 021 **Ultimate Exploration of the LLOQ of Exatecan, a Common Antibody Drug Conjugate (ADC) Payload**; Feixue Wang[1]; Sisi Xu[1]; Peiyun An[1]; Jinlian Lu[1]; Zhiyu Li[1]; Lili Xing[1]; Yi Tao[1]; Liang Shen[1]; *[1]WuXi AppTec, Shanghai, China*

TP 022 **Bioanalytical Strategy for Quantitative Conjugated Payloads of Antibody-Drug Conjugates (ADCs) with Cleavable Linker**; Li Qu[1]; Kaiyu Liu[1]; Hongmei Wang[1]; Zhiyu Li[1]; Lili Xing[1]; Yi Tao[1]; Liang Shen[1]; *[1]WuXi AppTec, Shanghai, China*

TP 023 **Top-down sequencing of bispecific antibodies by electron capture dissociation on a timsOmni platform**; Iuliia Stroganova[1]; Simon Ollivier[1]; Jean-Francois Greisch[1, 2]; Athanasios Smyrnakis[3]; Mariangela Kosmopoulou[3]; Detlev Suckau[4]; Dimitris Papanastasiou[3]; Albert J.R. Heck[1]; *[1]Utrecht University, Utrecht, Netherlands; [2]Bruker Switzerland AG, Fällanden, Switzerland; [3]Fasmatech Science & Technology, Chalandri, Greece; [4]Bruker Daltonics GmbH & Co. KG, Bremen, Germany*

TP 024 **Case study of inter-laboratory multi-attribute method (MAM) data comparison in Japan using NIST mAb**; Ayako Kurimoto[1]; K Ilker Sen[1]; *[1]Protein Metrics, LLC, Boston, MA*

TP 025 **Spectral Deconvolution for Rapid Analysis and Processing of Immunoglobulin-Based Drugs by MS (RaPiD-mAb-MS)**; John S. Chlystek[1, 2]; Austin Z. Salome[1, 2]; Alayna M. George Thompson[3]; Malika P. Godamudunge[3]; Craig D. Wenger[1]; Keaton L. Mertz[1, 2]; Alexander S. Hebert[1, 2]; Scott T. Quarmby[1, 2]; Joshua J. Coon[1, 2, 4, 5]; *[1]University of Wisconsin Madison, Madison, WI; [2]National Center for Quantitative Biology of Complex Systems, Madison, WI; [3]AbbVie, Inc., North Chicago, IL; [4]Morgridge Institute for Research, Madison, WI; [5]CeleramAb Inc., Middleton, WI*

TP 026 **Optimization of sample preparation for Dissulfide bond mapping by nLC-MS/MS of monoclonal antibodies**; Rodrigo S C Brant[1]; Kelly C Machado[1]; Hulyana Brum[1]; Anna Erika V De Araújo[2]; Iaralice M De Souza[2]; Thiago B Bandini[1]; Michel Batista[1]; *[1]Fiocruz, Curitiba, Brazil; [2]Biomanguinhos, Rio de Janeiro, Brazil*

TP 027 **High Throughput Peptide Mapping Pipeline to Support Early PTM Liability Assessments of Biologics**; John Patrick[1]; Steven Pomerantz[1]; Richard Huang[1]; Steve Jacobs[1]; *[1]Johnson and Johnson Innovative Medicine, Spring House, PA*

TP 028 **Rapid monitoring of mAb aggregates during the purification process development of therapeutic mAbs using a modified Orbitrap Hybrid MS**; Reiko Kiyonami[1]; Ying Chen[2]; Nicole Zehethofer[3]; Catharina Crone[3]; Al De Leon[2]; Heiner Koch[3]; Min Du[1]; *[1]Thermo Fisher Scientific, Lexington, MA; [2]Thermo Fisher Scientific, Bedford, MA; [3]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

TP 029 **Monitoring and characterization of glycation in a biotherapeutics degradation study using icIEF-UV/MS and LC-MS approaches**; Haichuan Liu[1]; Baiba Cabovska[1]; Scott Mark[1]; Zoe Zhang[1]; *[1]SCIEX, Redwood City, CA*

TP 030 **Alternating icIEF-UV/MS and LC-MS configurations to achieve charge heterogeneity analysis and comprehensive characterization of biotherapeutics**; Paula Orens[1]; Scott Mark[1]; Haichuan Liu[1]; Zoe Zhang[1]; Elliott Jones[1]; *[1]SCIEX, Redwood City, CA*

TP 031 **Analysis of an Antibody-Drug Conjugate on a Novel Benchtop MALDI-TOF/TOF Platform**; Laxmi Sinduri Vuppala[1]; Sergei Dikler[1]; *[1]Bruker Scientific LLC, Billerica, MA*

TP 032 **High-Sensitivity Host Cell Protein (HCP) Analysis on a Modified Hybrid Quadrupole-Orbitrap Mass Spectrometer with Optimized Sample Preparation**; Xiaoxi Zhang[1]; Reiko Kiyonami[2]; Jae Choi[3]; Bhavin Patel[3]; Cong Wang[4]; Peter Krueger[4]; Heiner Koch[4]; Min Du[5]; *[1]ThermoFisher Scientific, Shanghai, China; [2]Thermo Fisher Scientific, Lexington, MA; [3]Thermo Fisher Scientific, Rockford, IL; [4]Thermo Fisher Scientific, Bremen, Germany; [5]ThermoFisher Scientific, Lexington, MA*

TP 033 **Bioanalytical Strategy for Payloads of Antibody Drug Conjugates (ADCs) with LC-MS Platform**; Zhiren Yu[1]; Hefeng Zhang[1]; Wenhan Zhang[1]; Hongfang Cui[1]; Hongmei Wang[1]; Zhiyu Li[1]; Lili Xing[1]; Yi Tao[1]; Liang Shen[1]; *[1]WuXi AppTec, Shanghai, China*

TP 034 **Capillary electrophoresis-mass spectrometry employing CMP Scientific ECE-001 CE and EMASS-II Ion source for intact analysis of novel molecular format biotherapeutics**; Nancy Fernandes; *Lonza, Portsmouth, NH*

TP 035 **Comprehensive LC-MS Analytical Assays for Antibody-Oligonucleotide Conjugate (AOC) and siRNA Linker-Payload Characterization**; Samantha Ippoliti[1]; Brad Williams[1]; Ying Qing Yu[1]; Connor Brandenburg[2]; Tara McCulloch[2]; Michelle Chen[3]; Sophia Kenrick[3]; *[1]Waters Corporation, Milford, MA; [2]Takeda Development Center Americas, Inc, San Diego, California; [3]Waters Corporation, Goleta, California*

TP 036 **Analysis of Bispecific and Multispecific Antibody Therapeutics using Native Mass Spectrometry on a Modified Hybrid Orbitrap Mass Spectrometer**; Corentin Beaumal[1]; Lisa Füssl[1]; Sara Carillo[1]; Kai Scheffler[2]; Cong Wang[3]; Heiner Koch[3]; Kelly Broster[4]; Jonathan Bones[1, 5]; *[1]Nat'l Inst. for Bioprocessing Research & Training, Dublin, Ireland; [2]Thermo Fisher Scientific, Germering, Germany; [3]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [4]Thermo Fisher Scientific, Hemel Hempstead, United Kingdom; [5]University College Dublin, Belfield, Ireland*

TP 037 **Optimizing LC-MS/MS Peptide Mapping: Alternative Enzymatic Digestion Approaches for New Molecular Formats**; Benedict Dirnberger[1]; Francesca Ferlenghi[1];

Vesela Yokoya Encheva[1]; Robert Barton[1]; Matthew Edgeworth[1]; Karina Bora[1]; James Graham[1]; *[1]Lonza Biologics plc, Slough, United Kingdom*

TP 038 **Multi-attribute analysis of cysteine-linked ADC under native conditions by using a flexible online multiple heart-cutting 2D-LC-HRAM mass spectrometry**; Xuepu Li[1]; Xiaoxi Zhang[1]; Min Du[2]; Frank Steiner[3]; *[1]Thermo Fisher Scientific, Shanghai, China; [2]Thermo Fisher Scientific, Boston, MA; [3]Thermo Fisher Scientific, Germering, Germany*

ANTIDOPING, CANNABIS, AND OPIOID DETECTION

039-046

TP 039 **Untargeted steroids metabolism: methylclostebol**; Gianluca Barone[1,2]; Lukas Corbinian Harps[3]; Lingyu Liu[3]; Maria Kristina Parr[3]; Xavier De La Torre[1]; Francesco Botrè[1]; *[1]Laboratorio Antidoping FMSI, Rome, Italy; [2]University of Rome Tor Vergata, Rome, Italy; [3]Institute of Pharmacy, Freie Universität Berlin, Berlin, Germany*

TP 040 **In vitro metabolism study of novel synthetic cannabinoid ADB-FUBIATA and its co-existence with ethanol**; Xiaolong Hou[1]; Chenyu Xue[2]; Shiyang Qin[2]; Zhenjun Jia[1]; Ying Zhang[2]; *[1]People's Public Security University of China, Beijing, China; [2]Forensic Science Service of Beijing Public Security Bureau, Key Laboratory of Forensic Toxicology, Ministry of Public Security, Beijing, China*

TP 041 **Analysis of cannabinoid-containing fluids in illicit vaping cartridges using a sequential TOF MS, DDA-MS/MS and DIA-MS/MS method**; Molly F. Millea[1]; Alan Barnes[2]; Emily G. Armitage[2]; Chloe Hutton[2]; Simon Ashton[2]; Oliver B. Sutcliffe[1]; Neil J. Loftus[2]; *[1]MANchester DRug Analysis and Knowledge Exchange (MANDRAKE), Manchester Metropolitan University, Manchester, United Kingdom; [2]Shimadzu Corporation, Manchester, United Kingdom*

TP 042 **Fentanyl extraction and analysis in soil using automated QuEChERS**; Jonathan Rochon[1]; Mégane Moreau[2]; Sarah Demers[2]; Serge Auger[2]; Pierre Picard[2]; Jean Lacoursière[2]; *[1]Phytronix Technologies Inc., Québec, QC; [2]Phytronix Technologies, Quebec City, QC*

TP 043 **Suspect Screening and Spatial Analysis of New Psychoactive Substances and Abused Drugs in Wastewater Using Liquid Chromatography-High Resolution Mass Spectrometry**; Pao-Chi Liao[1]; Yuan-Chih Chen[1]; Jen-Yi Hsu[1]; Yung-Chieh Lin[1]; Chiau-Jun Chu[2]; Yen-Ping Lin[2]; Yun-Ju Tsai[2]; Man-Ni Zhuang[1]; *[1]National Cheng Kung University, Tainan, Taiwan; [2]Public Health Bureau, Tainan City Government, Tainan, Taiwan*

TP 044 **Quantification and Confirmation of Tranexamic Acid in Equine Plasma by LC-MS/MS**; Elizabeth Malozzi[1,2]; Youwen You[1,2]; Mary A. Robinson[1,2]; *[1]University of Pennsylvania School of Veterinary Medicine, Kennett Square, PA; [2]Pennsylvania Equine Toxicology and Research Laboratory, West Chester, PA*

TP 045 **A Headspace GC-MS/MS Methodology for the Detection of Oxygen-carrying PFAS in Equine Serum**; Leif K. McGoldrick[1,2]; Fuyu Guan[1,2]; Mary A. Robinson[1,2]; *[1]University of Pennsylvania School of Veterinary Medicine, Kennett Square, PA; [2]Pennsylvania Equine Toxicology and Research Laboratory, West Chester, PA*

TP 046 **Determination of Cobalt Concentration in Whole Equine Blood via Inductively Coupled Plasma Mass Spectrometry**; Benjamin J Burris[1]; Delaney K Ferguson[1]; Soobeng Tan[1]; Jeffrey Lakritz[2]; Teresa A Burns[2]; Ramiro E Toribio[2]; *[1]Ohio Department of Agriculture, Reynoldsburg, OH; [2]The Ohio State University College of Veterinary Medicine, Columbus, OH*

ART, ARCHAEOLOGY & PALEONTOLOGY

047-051

TP 047 **Breathing Art: A volatolomic study of The Night Watch by Rembrandt**; Alba Alvarez[1]; Lisette Vos[1]; Théo-Fany Lange[1]; Esther Van Duijn[1]; Katrien Keune[1]; *[1]Rijksmuseum, Amsterdam, Netherlands*

TP 048 **Application of nano-ESI and Paper Spray Ionization to Collagen in Archaeological Materials**; Samantha Kirgesner[1]; Rebekah E Strong[1]; Alberto J Taurozzi[2]; Mark Hubbe[1]; Amanda M Agnew[1]; Abraham K. Badu-Tawiah[1]; *[1]Ohio State University, Columbus, OH; [2]University of Copenhagen, Copenhagen, Denmark*

TP 049 **Evidence for Endogenous Collagen in Jurassic Crocodilian Bone**; Joseph Hubbard[1]; Joscelyn Harris[1]; Steven Robinson[2]; Krzystof Pawlak[2]; Stephen Taylor[1]; *[1]University of Liverpool, Liverpool, United Kingdom; [2]Materials Innovation Factory,, University of Liverpool, United Kingdom*

TP 050 **Species Identification of Carved Artifacts Using Zooarchaeology Mass Spectrometry (ZooMS) With Matrix Assisted Laser Desorption Ionization Time OF Flight (MALDI-TOF)**; Tori Lugiano; *Saint Joseph's University, Philadelphia*

TP 051 **Dye analysis of 16th century tapestry fibers by LC-MS**; Marek Smoluch[1]; Przemyslaw Mielczarek[1,2]; *[1]AGH University, Kraków, Poland; [2]Laboratory of Proteomics and Mass Spectrometry, Maj Institute of Pharmacology, Polish Academy of Sciences, Krakow, Poland*

ARTIFICIAL INTELLIGENCE IN MS INSTRUMENTATION AND APPLICATIONS II

052-069

TP 052 **Machine Learning-Enhanced MALDI Imaging Mass Spectrometry of N-Glycans for Hepatocellular Carcinoma Classification and Heterogeneity Analysis**; Muhammed F Bayram[1]; Jade K Macdonald[1]; Andrew DelaCourt[1]; Peggi M Angel[1]; Richard R Drake[1]; Paul Monga[2]; Amit Singal[3]; Anand S Mehta[1]; *[1]Medical University of South Carolina, Pharmacology & Immunology, Charleston, SC; [2]University of Pittsburgh, Pharmacology and Chemical Biology, Pittsburgh, PA; [3]University of Texas Southwestern Medical Center, Dallas, TX*

TP 053 **Large Language Model-Driven AI Agents for Automated Workflows on a Chip-based nanoESI-MS/MS Platform with Real-Time Quality Control**; Sanjay Iyer[1]; David Foreman[1]; Matthew Muhoberac[1]; Jordan Fritz[1]; Thomas Lubinsky[1]; Caitlin Randolph[1]; Gaurav Chopra[1,2,3,4,5,6,7]; *[1]Purdue University, West Lafayette, IN; [2]Department of Computer Science, Purdue University, West Lafayette, IN; [3]Purdue Institute for Drug Discovery, West Lafayette, IN; [4]Regenstrief Center for Healthcare Engineering, West Lafayette, IN; [5]Purdue Institute for Cancer Research, West Lafayette, IN; [6]Purdue Institute for Inflammation, Immunology, and Infectious Disease, West Lafayette, IN; [7]Purdue Institute for Integrative Neuroscience, West Lafayette, IN*

TP 054 **DeepLaM: A Deep Learning-Assisted Lactylprotein Mining Strategy for Potential Pan-cancer Biomarker Discovery**; Tianze Ling[1,2]; Siyuan Chen[3]; Cheng Chang[2]; *[1]Tsinghua University, Beijing, China; [2]National Center for Protein Sciences (Beijing), Beijing, China; [3]Nanjing University Of Aeronautics And Astronautics, Nanjing, China*

TP 055 **Surrogate optimization for supercritical fluid extraction – supercritical fluid chromatography-tandem mass spectrometry method development**; Niray Bhakta[1]; Jaivardhan Sood[1]; Yujing Yang[1]; Destini Black[1]; Jay Rosenberger[1]; Victoria Chen[1]; Kevin A Schug[1]; *[1]The University of Texas at Arlington, Arlington, TX*

TP 056 **Software-aided approach designed to analyze and predict cleavage sites for peptides**; Paula Cifuentes[1,2]; Ramon Adalia[2,3]; Ismael Zamora[4]; Lisa O'Callaghan[5]; Richard Gundersdorf[5]; *[1]Universitat Pompeu Fabra (UPF), Barcelona, Spain; [2]Lead Molecular Design, SL, Sant Cugat del Vallès, Spain; [3]Universitat Autònoma de Barcelona, Cerdanyola del Vallès, Spain; [4]Mass Analytica, Sant Cugat del Valles, Spain; [5]Merck, West Point, PA*

TP 057 **AI-Driven Visual Proteomics for Blood-Based Alzheimer's Disease Biomarker Discovery by LC-MS/MS and Deep Neural Networks**; Qingyang Xiao[1]; Vishal

Sandilya[2]; Yehia Mechref[2]; Haixu Tang[1]; *[1]Indiana University, Bloomington, IN; [2]Texas Tech University, Lubbock, TX*

TP 058 **AI-Designed LC-MS Methods for Metabolomics: A Comparative Study of Metabolic Profiles from Escherichia coli Grown in Nutrient-Rich vs Minimal Media**; Tara Harvey[1]; Philip Mach[1]; Kes Luchini[1]; Emilio S. Rivera[1]; Chi Yen Tseng[1]; Jessica A. Salguero[1]; Salvator Palmisano[1]; Joshua Breidenbach[1]; Zachary Sasiene[1]; Ethan M. McBride[1]; Brett Blackwell[1]; Madison Grace Thornhill[1]; Trevor Glaros[1]; *[1]Los Alamos National Lab, Los Alamos, NM*

TP 059 **Dynamically Adjusted Instrument Settling Delay Prior to Data Acquisition**; Haopeng Wang[1]; Behrooz Zekavat[1]; Laura L Pollum[1]; Huy Nguyen[1]; Patrick M Batoon[1]; *[1]Agilent Technologies Inc, Santa Clara, CA*

TP 060 **Optimizing Spectronaut's AI-Based Peptide Property Predictors for Immunopeptidomics Applications**; Alexandros Pachos[1]; An-phi Nguyen[1]; Ignacio Jauregui Novo[2]; George Rosenberger[3]; Sandra Schär[1]; Liliana Malinovska[1]; Oliver M. Bernhardt[1]; Marco Tognetti[1]; Sebastian Müller[1]; Roland Bruderer[1]; Tejas Gandhi[1]; Dennis Trede[4]; Lukas Reiter[1]; *[1]Biognosys AG, Schlieren, Switzerland; [2]Mestrelab Research S.L., Santiago de Compostela, Spain; [3]Bruker Switzerland AG, Fällanden, Switzerland; [4]Bruker Daltonics GmbH & Co. KG, Bremen, Germany*

TP 061 **Unleash the power of Hybrid-DIA data analysis with AI-driven software for Biomarker Discovery and Validation in Translational Research**; Qing Zhang[1]; Zia Rahman[1]; Ulises H. Guzman[2]; Jesper V. Olsen[2]; Baozhen Shan[1]; Yue Xuan[3]; *[1]Bioinformatics Solutions Inc, Waterloo, ON; [2]Novo Nordisk Foundation Center for Protein Research, University of Copenhagen, Denmark; [3]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

TP 062 **A de novo peptide sequencing workflow for identifying all possible classes of neoantigens and their sources of origin**; Ngoc Hieu Tran[1]; Lei Xin[1]; Baozhen Shan[1]; *[1]Bioinformatics Solutions Inc, Waterloo, ON*

TP 063 **Exploring the Future of MS: AI-Guided Design of MALDI Matrices using Theoretical and Empirical Insights**; Carlos A. Padilla[1]; Luis M. Díaz-Sánchez[1, 2]; Emmanuel Campo[3]; Cristian Blanco-Tirado[1]; Aldo F. Combariza[3]; Marianny Y. Combariza[1]; *[1]Universidad Industrial de Santander, Bucaramanga, Colombia; [2]Universidad de Pamplona, Pamplona, Colombia; [3]Universidad de Sucre, Sincelejo, Colombia*

TP 064 **AI driven quantitative metabolomics analysis for bioprocess optimization in microalgae fermentation**; Bokkyoo Jun[1]; Durga Devi Khanal[1]; Frank Xu[1]; Yao Lu[1]; Wilson Yan[1]; Jack Howland[2]; Jennifer M. Campbell[2]; *[1]dsm-firmenich, Columbia, MD; [2]Matterworks, Somerville, MA*

TP 065 **Enhanced Identity Spectrum Search with AI/ML Confidence Scoring for HRAM Data**; Gábor Zsemlye[1]; Juraj Lutišan[1]; Maria Falaq[2]; Rajesh Jha[2]; Samuel Benkovič[1]; Marynka Ulaszewska[3]; Tim Stratton[4]; Michal Raab[1]; *[1]Thermo Fisher Scientific, Bratislava, Slovakia; [2]Thermo Fisher Scientific, Bangalore, India; [3]Thermo Fisher Scientific, Milano, Italy; [4]Thermo Fisher Scientific, Austin, TX*

TP 066 **Retention Time Alignment via Deep Learning-based Change Detection in DIA-Based Proteomics**; Hojin Yoo[1]; Beomjun Park[1]; Namgil Lee[1, 2]; Heejung Yang[1, 2]; *[1]Bionsight, Inc., Chuncheon, South Korea; [2]Kangwon National University, Chuncheon, South Korea*

TP 067 **Leveraging spectral foundation models to transform raw mass spectrometry data into predictive biology**; Gabriel Asher[1]; Devesh Shah[1]; Lea Amar[1]; Niall O'Connor[1]; Timothy Kassis[1]; Jack Geremia[1]; *[1]Matterworks, Somerville, MA*

TP 068 **Harnessing Machine Learning for the Virtual Screening of Natural Compounds (Ceratonia Siliquia) for EGFR and HER2 Inhibition in Colorectal Cancer**; Ramakwala Christinah Chokwe[1]; Deli-Bright Nii Tettey Oku[1]; Yannick Nuapia[2]; *[1]University of South Africa, Johannesburg, South Africa; [2]University of Limpopo, Polokwane, South Africa*

TP 069 **Convolutional Neural Network with Transfer Learning Approach for Accelerated Quantitative Mass Spectrometry Imaging by IR-MALDESI**; Russell R. Kibbe[1]; Emily C. Hector[2]; David C Muddiman[1]; *[1]Biological Imaging Laboratory for Disease and Exposure Research (BILDER), Department of Chemistry, North Carolina State University, Raleigh, North Carolina; [2]Department of Statistics, North Carolina State University, Raleigh, North Carolina*

BIOMARKERS: DISCOVERY II
070-113

TP 070 **Analytical Considerations for Biomarker Analysis from Plasma Samples for Large Cohort and Clinical Exploratory Studies**; Danielle Gutierrez[1]; Jessica Moore[1]; Jaison I Arivalagan[1]; Tiffany Louie[1]; Kyra Richardson[1]; Alejandra Stihel[1]; Dragana Noe[1]; Don Skifter[1]; *[1]Discovery Life Sciences, Huntsville, AL*

TP 071 **Proteogenomic Characterization of High-Grade Gliomas in Indian Population Reveals Novel Mutational Signatures and Distinct Molecular Subtypes**; Sanjeeva Srivastava[1]; Ayushi Verma[2]; Srikanth S. Manda[3]; Avinash Singh[2]; Rohit Mishra[4]; Chinmay Koppal[5]; Prerana Jha[6]; R Venkataramanan[7]; Epari Sridhar[8]; Prashant Aggarwal[9]; *[1]IIT Bombay, Mumbai, India; [2]Indian Institute of Technology Bombay, Mumbai, India; [3]Nucleome Informatics Pvt. Ltd, Hyderabad, India; [4]Queensland University of Technology, Brisbane, Australia; [5]Indian Institute of Technology Bombay, Mumbai, India; [6]Bencos Research Solutions Pvt.ltd., Delhi, India; [7]Karkinos Healthcare, Mumbai, India; [8]Advanced Centre for Treatment Research and Education in Cancer, Tata Memorial Centre, Mumbai, India; [9]Datar Cancer Genetics, Mumbai, India*

TP 072 **Serum Proteomic Profiling of Recurrent Tuberculosis: Insights into Molecular Mechanisms and Biomarker Discovery**; Sanjeeva Srivastava[1]; Ayush Bhattacharya[2]; Debarghya Pratim Gupta[3]; Sonya Krishnan[4]; Gautam Sharma[3]; Divya Nair[2]; Amita Gupta[5]; Vidya Mave[5]; Rajesh Karyakarte[4]; Sanjay Gaikwad[4]; Vandana Kulkarni[4]; Mandar Paradkar[4]; *[1]IIT Bombay, Mumbai, India; [2]Indian Institute of Technology Bombay, Mumbai, India; [3]Indian Institute of Technology Bombay, Mumbai, India; [4]Johns Hopkin University, Baltimore, MD; [5]Johns Hopkins University, Baltimore, MD*

TP 073 **Spatially Resolved Multimodal Single Cell Analysis of Proteomic and Metabolomic Changes Associated with Senescence in Idiopathic Pulmonary Fibrotic Lungs**; Rashmi Kumar[1]; Yumi Kwon[2]; Lorena Rosas[3]; Kevin J Zemaitis[1]; Ana Mora[3]; Mauricio Rojas[3]; Ljiljana Paša Tolić1[2]; *[1]Pacific Northwest National Lab, Richland, WA; [2]Pacific Northwest National Laboratory, Richland, Washington; [3]Ohio State University, Columbus, OH*

TP 074 **Proteomic Analysis of Secreted Proteins from Human Oligodendrocyte Precursor Cells (OPCs) to Identify Potential Pharmacodynamic (PD) Biomarkers for GPR17**; Maryam Nikpayam[1]; Luna Zhang[2]; Bekim Bajrami[2]; *[1]Oregon State University, Corvallis, OR; [2]Biogen, Cambridge, MA*

TP 075 **Identification of Potential Protein Biomarkers for Diagnosing Bacterial Exacerbation in Chronic Obstructive Pulmonary Disease (COPD) using Longitudinal Clinical Proteomics**; Chao Xue[1]; Erfei Shang[1]; Xiaoyu Zhu[1]; Sanjay Sethi[1]; Jun Qu[1]; *[1]University at Buffalo, Buffalo, NY*

TP 076 **In-depth, Quantitative Characterization of Key Regulators and Predictive Biomarkers for CAR T-cell Therapy Induced Toxicities in a Clinical Cohort**; Min Ma[1]; Maosheng Wei[1]; Erfei Shang[1]; Ming Zhang[1]; Xiaoyu Zhu[1]; Davila Marco[2]; Megan Herr[2]; Jun Qu[1]; *[1]University at Buffalo, Buffalo, NY; [2]Roswell Park Comprehensive Cancer Center, Buffalo, NY*

TP 077 **Identification of androgen-regulated exosomal proteins and metabolites from prostate cancer cells**; Joshitha Bhaskar[1]; Priya Thapliyal[1]; Adaikkalam Vellaichamy[1]; *[1]Centre for Biotechnology, Anna University, Chennai, India*

TP 078 **Probing the efficacy of Polygonatum odoratum in alleviating type 2 diabetes through gut microbiome and untargeted metabolomics**; XUEWEI YE[1, 2]; Kefei Wu[3]; Siyi Qiam[3]; Langyu Xu[3]; Yingxin Cen[3]; Jiahui Ni[3]; Andy Lui[2]; Lanjuan Li[3]; Sheng Zhang[2]; Wei Liu[4]; *[1]Key Laboratory of Artificial Organs and Computational Medicine of Zhejiang Province, Shulan International Medical College, Zhejiang Shuren University, Hangzhou, China; [2]Proteomics and Metabolomics Facility, Cornell University, Ithaca, NY; [3]Key Laboratory of Artificial Organs and Computational Medicine of Zhejiang Province, Shulan International Medical College, Zhejiang Shuren University, Hangzhou, China; [4]nstitute of Plant Protection and Microbiology, Zhejiang Academy of Agricultural Sciences, Hangzhou, China*

TP 079 **Identification of salivary biomarkers and enriched domain/motif families for early-detection and lymph node invasion in OSCC patients of Indian population**; Avinash Singh[1]; Pratibha Sharma[2]; Subash BV[3]; Seema Patil[3]; Richa Vaish[4]; Sudhir Nair[5]; Sanjeeva Srivastava[2]; *[1]IIT Bombay, Powai, India; [2]Indian Institute of Technology Bombay, Mumbai, India; [3]D.A. Pandu Memorial R.V. Dental College, Bangalore, India; [4]Tata Memorial Hospital, Mumbai, India; [5]Advance Centre for Treatment Research & Education in Cancer, Mumbai, India*

TP 080 **Large-Scale Plasma metabolomics uncovers metabolites associated with ovarian malignancy**; Melanie Weigert[1]; Niklas Thompson[2]; Calla O'Connor[1]; Hardik Shah[2]; Ernst Lengyel[1]; *[1]Department of Obstertrics and Gynecology/Section of Gynecologic Oncology, The University of Chicago, Chicago, Illinois; [2]Metabolomics Platform, University of Chicago Comprehensive Cancer Center, Chicago, Illinois*

TP 081 **Identification of Flavor Specific E-cigarette Constituents via Untargeted Mass Spectrometry for Blinded Detection of E-cigarette Flavor Use in Human Urine**; Tatiana Rodriguez[1]; Drew Jones[1]; Yik Siu[1]; *[1]NYU Langone, New York City, NY*

TP 082 **GlycoTyper™ - a novel liquid-biopsy platform for high-throughput, high-sensitivity targeted glycoproteomics, exemplified be differentiating Systemic Lupus Erythematosus and Lupus Nephritis**; Gray Huffman[1]; Grace Grimsley[1]; Aaron Angerstein[2]; Tamara Nowling[3]; Steve Castellino[1]; Klaus Lindpaintner[4]; *[1]Bruker Scientific LLC, Billerica, MA; [2]Medical University of South Carolina, Medicine, Charleston, SC; [3]Medical University of South Carolina, Pharmacology & Immunology, Charleston, South Carolina; [4]Bruker, Concord, NH*

TP 083 **Applying deep, unbiased plasma proteomics to understand dementia classification, cognitive decline and pTau-217 biology in a 1,786 sample study**; Harendra Guturu[1]; Xiaoyuan Zhou[1]; Alexey Stukalov[1]; Matthijs De Geus[2]; Hiroko Dodge[1]; Pia Kivisakk[2]; Sudeshna Das[2]; Brad Hyman[2]; Serafim Batzoglou[1]; Omid C Farokhzad[1]; Steven E Arnold[2]; Asim Siddiqui[1]; *[1]Seer, Redwood City, CA; [2]Massachusetts General Hospital, Boston, MA*

TP 084 **A Quality Management System Dashboard for Bruker's new GlycoTyper™ Targeted High-Throughput Glycoproteomics Platform**; Grace Grimsley[1]; Gray Huffman[1]; Klaus Lindpaintner[2]; Steve Castellino[1]; *[1]Bruker Scientific LLC, Billerica, MA; [2]Bruker, Concord, NH*

TP 085 **Low-Abundance Serum Protein Biomarkers for HCC in Patients with Liver Cirrhosis**; Habtom W Ressom[1]; Muhammad Salman Sajid[1]; Rency S Varghese[1]; *[1]Georgetown University, Lombardi Cancer Center, Washington, DC*

TP 086 **Multi-omics profiling of sarcoma patients serum identified new putative circulating biomarkers for soft-tissue sarcoma diagnosis**; Elettra Barberis[1]; Veronica De Giorgis[2]; Marco Ghirimoldi[2]; Elia Amede[2]; Maria Rescigno[3]; Marcello Manfredi[2, 4]; *[1]ISALIT - University of Piemonte Orientale, Novara, Italy; [2]Department of Translational Medicine, University of Piemonte Orientale, Novara, Italy, Novara, Italy; [3]Humanitas University, Rozzano, Italy; [4]IRCCS Policlinico San Donato, Institute of Molecular and Translational Cardiology, Milan, Italy*

TP 087 **Enhancing biopsy interpretation for kidney allograft dysfunction by biopsy-based proteomics and AI-assisted biomarker discovery and pathway analysis**; Fei Fang[1]; Tiffany Wei[2]; Kyla Frenia[3]; Parmjeet Randhawa[4]; Kevin (Kunhong) Xiao[2]; *[1]Department of Pharmacology and Chemical Biology, University of Pittsburgh, Pittsburgh, PA; [2]AHNCI, Pittsburgh, PA; [3]Department of Bioengineering, Swanson School of Engineering, University of Pittsburgh, Pittsburgh, PA; [4]6Department of Pathology, The Thomas E Starzl Transplantation Institute, University of Pittsburgh, Pittsburgh, Pittsburgh, PA*

TP 088 **Comparison of Membrane Protein Coverage Using Different Bottom-Up Proteomics Digestion Techniques**; Kenneth B Tomkovich[1]; Reihaneh Safavisohi[1]; *[1]Seton Hall University, South Orange, NJ*

TP 089 **Proteomic atlas of peritoneal tissue: a "soil sampling" technique for the metastatic seed**; Qiangmin Zhang[1]; Christopher Sherry[1]; David Bartlett[1]; Patrick Wagner[1]; Kevin (Kunhong) Xiao[1]; *[1]AHNCI, Pittsburgh, PA*

TP 090 **Optimization of dried blood spot proteomics for plasma biomarker analysis**; Morgan Fair[1]; Anirudh A Kashyap[1]; Liang Zhao[1]; Raghothama Chaerkady[1]; Qing Wang[1]; *[1]Complete Omics Inc., Baltimore, MD*

TP 091 **Discovering novel biomarkers in small-volume tear samples for dry eye disease using a machine learning-based proteomics approach**; Kyla Frenia[1]; Leanne T. Labriola[2]; Kevin (Kunhong) Xiao[3]; *[1]Department of Bioengineering, Swanson School of Engineering, University of Pittsburgh, Pittsburgh, PA; [2]Retina Department, Sewickley Eye Group, Sewickley, PA; [3]AHNCI, Pittsburgh, PA*

TP 092 **Defining the True Tear Proteome: An Integrative Experimental and Bioinformatics Analysis**; James Xiao[1]; Kyla Frenia[2]; Maria Beatty[1]; Julia Gelman[1]; Veena Raiji[3]; Leanne T. Labriola[1]; *[1]Retina Department, Sewickley Eye Group, Sewickley, PA; [2]Department of Bioengineering, Swanson School of Engineering, University of Pittsburgh, Pittsburgh, PA; [3]Department of Ophthalmology, Rush University Medical Center, Chicago, IL*

TP 093 **Comparison of Volatile Organic Compounds in the Lung Microenvironment and Exhaled Breath in Early-Stage Lung Cancer**; Kristian J. Kiland[1]; Scott A. Borden[1]; Crista Bartolomeu[1]; Lucas Martins[1]; Deborah Estevam[1]; Abigail Walker[1]; Heather Lam[1]; Khushi Bimbrahw[1]; Michael Brown[1]; Stephen Lam[1, 2]; Renelle Myers[1, 2]; *[1]British Columbia Cancer Research Institute, Vancouver, BC; [2]The University of British Columbia, Vancouver, British Columbia*

TP 094 **Development of red blood cells and plasma-based diagnostic lipid biomarker panel for Parkinson's disease**; Fathima Shaima MuhammedNazaar[1]; Anne Roberts[1]; Malcolm Horne[2]; Stephan Klatt[3]; Chris Fowler[2]; Colin L Master[2]; James Doecke[4]; Blaine R. Roberts[1]; *[1]Department of Biochemistry and Department of Neurology, Emory University, Atlanta, GA; [2]The Florey Institute of Neuroscience and Mental Health, The University of Melbourne, Parkville, Australia; [3]Institute for Vascular signaling, University of Frankfurt-Goethe University, Frankfort, Germany; [4]CSIRO Health and Biosecurity, Herston, Australia*

TP 095 **Mass spectrometry-based proteomic analysis of extracellular vesicles derived from glioblastoma and healthy brain cells**; Kristen Hope Hutson[1]; Guoting Qin[2]; Jennifer Copeland[3]; Huamin Cai[3]; Stan Stearns[3]; Chengzhi Cai[2]; Gergana Nestorova[1]; *[1]Louisiana Tech University, Ruston, LA; [2]University of Houston, Houston, TX; [3]VICI Valco Instruments, Houston, TX*

TP 096 **Using LC-TIMS-PASEF 4D Lipidomics for Enhanced Plasma Biomarker Discovery**; Steph Collins[1]; Lilu Guo[1]; Bailin Zhang[1]; *[1]Sanofi, Cambridge, MA*

TP 097 **Differential responses to chemotherapy in triple negative breast cancer defined by in situ FFPE protein digestion**; Francis Scott Heinemann[1]; Paul Gershon[2]; *[1]Hoag*

Memorial Hospital Presbyterian, Newport Beach, CA; [2]UC-Irvine, Irvine, CA

TP 098 **Identifying Putative Urinary Biomarkers of Renal Scar-Associated Marker Proteins (SCAMPs) Following Resolution of Pyelonephritis**; John Froehlich[1]; Shannon E. DiMartino[2]; Kyle L. Katamba[2]; Rosalyn M. Adam[2, 3]; Xin Wang[4]; Juan De Dios Ruiz-Rosado[4]; Brian Becknell[4]; Richard S Lee[2, 3]; *[1]Boston children's hospital, Boston, MA; [2]Children's Hospital Boston, Boston, MA; [3]Harvard Medical School, Boston, Massachusetts; [4]Kidney and Urinary Tract Center, Abigail Wexner Research Institute, Nationwide Children's Hospital, Columbus, Ohio*

TP 099 **Targeted Quantitative Serum Proteomics Analysis in donors with Breast cancer (BC) and matched controls**; Brian T. Pentecost[1]; Victor T. Njoku[1]; Kaya R Johnson[1]; Sumona Mondal[2]; Claudia Gaither[3, 4]; Adeline Shanker[3]; Robert Popp[3]; Christoph H. Borchers[5, 6, 7, 8]; Costel C. Darie[1]; *[1]Biochemistry & Proteomics Laboratories, Department of Chemistry & Biochemistry, Clarkson University, Potsdam, NY 13699-5810; [2]Department of Mathematics and Statistics, Clarkson University, Potsdam, NY 13699-5810; [3]MRM Proteomics Inc, Montreal, Quebec; [4]Département de biomédecine vétérinaire, Faculté de médecine vétérinaire, Université de Montréal, Montreal, Saint-Hyacinthe, QC J2S 2M2; [5]Segal Cancer Proteomics Centre, Lady Davis Institute, Jewish General Hospital, McGill University, Montreal, QC H3T 1E2; [6]Gerald Bronfman Department of Oncology, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC H3T 1E2; [7]Division of Experimental Medicine, McGill University, Montreal, QC H4A 3J1; [8]Department of Pathology, McGill University, Montréal, QC H3A 2B4*

TP 100 **A comprehensive study of sera from women with breast cancer and age-matched controls to identify potential protein biomarkers**; Hailey A Morrissiey[1]; Danielle Whitham[1]; Pathea S Bruno[1]; Brian T. Pentecost[1]; Costel C. Darie[1]; *[1]Clarkson University, Potsdam, NY*

TP 101 **Simultaneous Extraction and Integrative Proteomics, Metabolomics, and Lipidomics Analyses for Serum Biomarker Discovery and Validation in Alzheimer's Disease**; Ching-Yuan Yang[1]; Haiyan Lu[2]; Michael Rosenblat[3]; Zicong Wang[2]; Lingjun Li[2, 4]; *[1]Biophysics Graduate Program, University of Wisconsin-Madison, Madison, WI; [2]School of Pharmacy, University of Wisconsin-Madison, Madison, WI; [3]Promega Corporation, Madison, WI; [4]Department of Chemistry, University of Wisconsin-Madison, Madison, WI*

TP 102 **Development of an Immunoprecipitation Mass Spectrometry method for Tau Peptides in Plasma for Alzheimer's Disease Diagnosis**; Alexandra Izydorczak[1]; Xuemei Zeng[2]; Thomas K Karikari[1]; *[1]University of Pittsburgh, Pittsburgh, PA; [2]University of Pittsburgh Medical Center, Pittsburgh, PA*

TP 103 **The Senescence-Associated Interferon Response: A Potential Target for Therapeutic Interventions Aimed at Mitigating Inflammaging**; Mansi Shrivastava[1]; Reema Banerjee[1]; Thedoe Nyunt[1, 2]; Bradley Olinger[1]; Linna Cui[1]; Ceereena Ubaida-Mohien[1]; Alexey Lyashkov[1]; Amit Dey[1]; Dimitrios Tsitsipatis[1]; Martina Rossi[1]; Myriam Gorospe[1]; Nathan Basisty[1]; *[1]NIA, NIH, Baltimore, MD; [2]The Mount Sinai Hospital, New York City, New York*

TP 104 **Separation and identification of Sphingolipids produced by Bacteroidota using HPLC/high resolution mass spectrometry with Ion mobil**; Sheher Banu Mohsin[1]; Yolanda Huang[2]; Jeremy P Koelmel[3]; Krystal Pollitt[4]; *[1]Agilent Technologies, Wood Dale, IL; [2]University at Buffalo, Buffalo, NY; [3]Yale University, New Haven, CT; [4]Yale University, West Haven, CT*

TP 105 **Enhanced biomarker discovery in blood plasma through a unique single-particle workflow for deeper proteome coverage**; Measho H Abreha[1]; Zehan Hu[2]; Katrin Hartinger[2]; Roland Bruderer[3]; Nils Kulak[2]; *[1]PreOmics, Martinsried, Germany; [2]PreOmics GmbH, Martinsried, Germany; [3]Biognosys, Schlieren, Switzerland*

TP 106 **Multi-omic analysis of Hirschsprung's disease in three mouse models by LC-MS/MS**; Oriana Zambito[1, 2]; Nejia Lassoued[2, 3]; Rodolphe Soret[2, 3]; Nicolas Pilon[2, 3]; Lekha Sleno[1, 2]; *[1]University of Quebec in Montreal (UQAM), Chemistry department, Montreal, QC; [2]CERMO-FC, Centre d'Excellence de Recherche sur les Maladies Orphelines-Fondation Courtois, Montreal, QC; [3]University of Quebec in Montreal (UQAM), Biology Department, Montreal, QC*

TP 107 **Investigating proteome variations in vitreous humor from patients affected by ocular diseases**; Maggy Lepine[1]; Sebastien Methot[2]; Ali Dirani[2]; Lekha Sleno[1]; *[1]Université du Québec à Montréal, Chemistry department/CERMO-FC/PROTEO, Montreal, QC; [2]Centre de recherche du CHU de Québec-Université Laval, Quebec, QC*

TP 108 **Novel, specific protein structural biomarkers for Alzheimer's Disease and Dementia with Lewy Bodies**; Anna Pagotto[1]; Luise Nagel[2]; Jan-Philipp Quast[1]; Wilma D J Van De Berg[3]; Juliette Van Alphen[3]; Charlotte E Teunissen[3]; Afina Willemina Evelien Lemstra[3]; Natalie De Souza[1, 4]; Andreas Beyer[2]; Paola Picotti[1]; *[1]ETH Zurich, Zurich, Switzerland; [2]University of Cologne, Cologne, Germany; [3]Amsterdam UMC, Amsterdam, Netherlands; [4]University of Zurich, Zurich, Switzerland*

TP 109 **Glycosaminoglycans isomers profile for the incidence of colorectal cancer in patients with inflammatory bowel disease**; Mariusz Grzegorz Fleszar[1]; Paulina Fortuna[1]; Małgorzata Krzystek-Korpacka[2]; Iwona Bednarz-Misa[2]; Gabriela Maciejewska[1]; Anna Kłopot[2]; Łukasz Lewandowski[2]; Radosław Kempiński[3]; Wojciech Pisarek[3]; Ewelina Frejlich[4]; Przemysław Dzierżek[4]; Julia Rudno-Rudzińska[4]; Katarzyna Neubauer[3]; *[1]Omics Research Center, Wroclaw Medical University, Wroclaw, Poland; [2]Department of Biochemistry and Immunochemistry, Wroclaw Medical University, Wroclaw, Poland; [3]Department of Gastroenterology and Hepatology, Wroclaw Medical University, Wroclaw, Poland; [4]Oncological Surgery Clinic, Wroclaw Medical University, Wroclaw, Poland*

TP 110 **Nanoparticle-based proteomics by mass spectrometry in plasma samples from Huntington's disease cohort**; Samira Vautrin[1]; Oliver Kardell[1]; Mari Aaltonen[1]; Doris Staudt[1]; Johannes Trefz[1]; Carleen Kluger[1]; Andreas Tebbe[1]; Christoph Schaab[1]; Jim Rosinski[2]; *[1]EVOTEC, Munich, Germany; [2]CHDI management, New York, NY*

TP 111 **Unique Correlations Between Cytokines and Lipid Inflammatory Biomarkers in the Stratum Corneum of Cancer Patients With Immune-Related Cutaneous Adverse Events**; Evgeny Berdyshev[1]; Elena Goleva[1]; Taras Lyubchenko[1]; Irina Bronova[1]; Olivia Xiao[1]; Anna Sofia Bronoff[1]; Kadin Sorenson[1]; Jeff Kern[1]; Mario Lacouture[2]; Donald YM Leung[1]; *[1]National Jewish Health, Denver, CO; [2]New York University Langone Hospital, New York, NY*

TP 112 **Biomarkers of Iron-induced Glycation in Human Cells**; Brynmar G Degenhardt[1]; Cole Babcock[1, 2]; Bradley Scott[1]; Makan Golizeh[1]; *[1]Concordia University Edmonton, Edmonton, AB; [2]Babcock Synthetics ltd., Wainwright, AB*

TP 113 **SARS-CoV-2 severity biomarkers identified via quantitative proteomics in lung, brain, liver, and heart from a small cohort of COVID-19 autopsies**; Emma K. Luhmann[1]; Roberth Anthony Rojas Chavez[2]; Kiran Nazarali[3]; Ellen M. Upton[1]; Hanxi Xiao[3]; Ryan K. Betters[1]; Marco M. Hefti[1]; Jishnu Das[3]; Lilliana Radoshevich[2]; *[1]The University of Iowa, Iowa City, IA; [2]National Jewish Health, Denver, CO; [3]University of Pittsburgh, Pittsburgh, PA*

CANCER RESEARCH II
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TP 114 **A Molecular Array for 10-second Diagnosis of Common Spinal Tumour Types with Picosecond Infrared Laser Mass Spectrometry**; Alexa Fiorante[1]; Michael Woolman[1]; David Munoz[1, 2]; Taira Kiyota[3]; Lan Anna Ye[4]; Yasamine Farahmand[4]; Darah Vlaminck[1]; Francis Talbot[4]; Sunit Das[1,

[2]; Sorcha Kellett[2]; Christine Giuffrida[2]; Gelareh Zadeh[1, 4]; Howard Ginsberg[1, 2]; Ahmed Aman[1, 3]; Arash Zarrine-Afsar[1, 4]; *[1]University of Toronto, Toronto, ON; [2]Unity Health Toronto, Toronto, ON; [3]Ontario Institute for Cancer Research, Toronto, ON; [4]Princess Margaret Cancer Center, Toronto, ON*

TP 115 **Comprehensive Multi-Omics Profiling of Bladder Cancer Evolution: Insights from Proteomics, Metabolomics and Mutational Analyses**; Sung Yun Jung[1]; Sangkyou Lee[2]; Paweł Kuś[3]; Jolanta Bondaruk[2]; June Goo Lee[2]; Roman Jaksik[3]; Nagireddy Putluri[1]; Khanh N. Dinh[4]; David Cogdell[2]; Huiqin Chen[2]; Yishan Wang[2]; Jiansong Chen[2]; Neema Nevai[2]; Colin Dinney[2]; Cathy Mendelsohn[4]; David McConkey[5]; Richard R. Behringer[2]; Charles C. Guo[2]; Peng Wei[2]; Marek Kimmel[6]; Bogdan Czerniak[2]; *[1]Baylor College of Medicine, Houston, TX; [2]MD Anderson Cancer Center, Houston, TX; [3]Silesian University of Technology, Gliwice, Poland; [4]Columbia University, New York City, NY; [5]Johns Hopkins, Baltimore, MD; [6]Rice University, Houston, TX*

TP 116 **Combined Click probe-Seq and LC-MS2 Method for Genome-wide DNA Damage Induced by Catechol Estrogens Reveals Endogenous Genotoxicity Beyond Receptor-mediated Signaling**; Shu-Hui Chen[1]; Quynh-Trang Do[1]; *[1]National Cheng Kung University, Tainan, Taiwan*

TP 117 **Proteogenomic Analysis of Uterine Leiomyosarcoma in a Prior Benign Myomectomy Site from an Adolescent Patient**; Satishkumar Ranganathan Ganakammal[1]; Pang-ning Teng[2]; Tamara Abulez[2]; Julie Oliver[2]; Brian L. Hood[2]; Kelly A. Conrads[2]; Jeremy Loffredo[2]; Katlin N. Wilson[2]; Tracy J. Litzi[2]; Marshé Edwards[2]; Victoria Olowu[2]; Glenn Gist[2]; Dave Mitchell[2]; Kathrine Zhou[2]; Matthew D. Wilkerson[3]; Clifton L. Dalgard[3]; Shaoqiu He[3]; Liqun Jiang[3]; Emanuel F. Petricoin[4]; Kathleen M. Darcy[2]; Christopher M. Tarney[2]; Larry Maxwell[1]; Thomas P. Conrads[1]; Nicholas W. Bateman[2]; *[1]Women's Health Integrated Research Center, Annandale, VA; [2]Gynecologic Cancer Center of Excellence and the Women's Health Integrated Research Center, Annandale, VA; [3]The American Genome Center, Department of Anatomy Physiology and Genetics, Uniformed Services University of the Health Sciences, Bethesda, MD, United States, Bethesda, MD; [4]Center for Applied Proteomics and Molecular Medicine, George Mason University, Manassas, VA*

TP 118 **Lipidomic and metabolomic analysis of single patient-derived glioblastoma neurospheres**; Cyrene Catenza[1]; Won Shik Choi[2]; Seth Peyton[2]; Roseline Godbout[2, 3]; Liang Li[1, 4]; *[1]University of Alberta, Faculty of Science, Chemistry Department, Edmonton, AB; [2]University of Alberta, Faculty of Medicine & Dentistry, Oncology Department, Edmonton, AB; [3]Cross Cancer Institute, Edmonton, AB; [4]The Metabolomics Innovation Centre (TMIC), University of Alberta, Edmonton, AB*

TP 119 **Response Marker Enrichment Analysis links mass spectrometry-based cancer proteomics to the antiproliferative impact of pharmacological and genetic perturbations**; Luke Higgins[1]; Pedro Maria Izquierdo Casado[1]; Federico Pedicona[1, 2]; Nadia Nishat[1]; Suhana Yasmin[1]; Pedro Rodriguez Cutillas[1, 2]; *[1]Barts Cancer Institute, Queen Mary University of London, London, United Kingdom; [2]Kinomica Ltd., London, United Kingdom*

TP 120 **Comprehensive Profiling of Bladder Cancer: Altered Fatty acid metabolism in Smokers**; Abu Hena Mostafa Kamal[1]; Vasanta Putluri[2]; Chandra Shekar R Ambati[2]; Chandra Sekhar Amara[3]; Mohammed Khurshidul Hassan[3]; Pooja Popli[4]; Danthasinghe Waduge Badrajee Piyarathna[3]; Tanja Gangnus[3]; Erin H Seeley[5]; Xuefeng Liu[6]; Natalie R. Gassman[7]; Roni J Bollag[8]; Krishna Parsawar[9]; Martha K Terris[8]; Livia S Eberlin[10]; Ramakrishna Kommagani[4]; Seth P Lerner[11]; Chad Creighton[12]; Yair Lotan[13]; Nagireddy Putluri[3]; *[1]Baylor College of Medicine, Houston, TX; [2]Advanced Technology Core, Dan L Duncan Comprehensive Cancer Center, Baylor College of Medicine, Houston, Texas, United States., Houston, TX; [3]Department of Molecular and Cell Biology, Baylor College of Medicine, Houston, Texas, United States., Houston, TX; [4]Dept. of Pathology and Immunology, Baylor College of Medicine, Houston, Texas, United States., Houston, TX; [5]Department of Chemistry, University of Texas at Austin, Austin, Texas, United States., Austin, TX; [6]Department of Pathology, The Ohio State University, Columbus, Ohio, United States., Columbus, Ohio; [7]Department of Pharmacology and Toxicology, Heersink School of Medicine, The University of Alabama at Birmingham, Birmingham, Alabama, United States., Birmingham, AL; [8]Georgia Cancer Center, Augusta University, Augusta, Georgia, United States., Augusta, Georgia; [9]Analytical and Biological Mass Spectrometry Core Facility, The University of Arizona, Tuscon, AZ, United States, Tucson, AR; [10]Department of Surgery, Baylor College of Medicine, Houston, Texas, United States., Houston, TX; [11]Scott Department of Urology, Baylor College of Medicine, Houston, Texas, United States., Houston, TX; [12]Department of Medicine, Dan L. Duncan Comprehensive Cancer Center Division of Biostatistics, Baylor College of Medicine, Houston, Texas, United States., Houston, TX; [13]Department of Urology, University of Texas Southwestern, Dallas, Texas, United States., Dallas, TX*

TP 121 **An Online Two-Dimensional Approach to Characterizing the Charge-Based Heterogeneity of Recombinant Monoclonal Antibodies Using a 2D-CEX–AEX–MS Workflow**; Anurag Singh Rathore[1]; KUNAL KRISHNA[1]; Vadiraja Bhat[2]; Sunil Kumar[1]; Vineela Peruri[1]; *[1]IIT Delhi, Delhi, India; [2]Agilent Technologies, BENGALURU, India*

TP 122 **Titer and charge-based heterogeneity multiattribute monitoring of mAbs in cell culture harvest using 2D ProA CEX MS**; Anurag Singh Rathore[1]; KUNAL KRISHNA[1]; Vadiraja Bhat[2]; Sunil Kumar[1]; Deepika Sarin[1]; *[1]IIT Delhi, Delhi, India; [2]Agilent Technologies, BENGALURU, India*

TP 123 **Machine Learning-Enhanced Extraction of Protein Signatures of Renal Cell Carcinoma from Proteomics Data**; Hongyi Liu[1]; Zhuo Ma[2]; Mamie Lih[1]; Lijun Chen[1]; Yingwei Hu[1]; Yuefan Wang[1]; Zhenyu Sun[1]; Yuanyu Huang[1]; Yuanwei Xu[1]; Hui Zhang[1]; *[1]Johns Hopkins School of Medicine, Baltimore, MD; [2]Johns Hopkin University, Baltimore, MD*

TP 124 **Proteome Changes Correlating with Neoadjuvant Chemotherapy Response and Residual Disease in Advanced Ovarian Cancers**; Nicholas W. Bateman[1]; Amma Asare[2]; Sean Cronin[1]; Jonathan Ogata[1]; Tamara Abulez[1]; Brian L. Hood[1]; Kelly A. Conrads[1]; Jun Yao[2]; Joseph Celestino[2]; Nicole Fleming[2]; Sara Corvigno[2]; Sanghoon Lee[2]; Christopher M. Tarney[1]; Kathleen M. Darcy[1]; Neil Phippen[1]; Thomas P. Conrads[3]; Larry Maxwell[3]; Anil Sood[2]; *[1]Gynecologic Cancer Center of Excellence, Annandale, Virginia; [2]MD Anderson Cancer Center, Houston, Texas; [3]Women's Health Integrated Research Center, Annandale, Virginia*

TP 125 **Serum Metabolic Fingerprints Reveal Lung Adenocarcinoma Progression Using Nanoparticle-Enhanced Laser desorption/Ionization Mass Spectrometry**; Shouzhi Yang[1]; Lin Huang[1]; Qian Kun[1]; *[1]Shanghai Jiaotong University, Shanghai, China*

TP 126 **Deciphering Proteomic Alterations in hABCB1-Mediated Multidrug Resistance in Lung Cancer**; Geul Bang[1]; Eun Hee Han[2]; *[1]Korea Basic Science Institute, Cheongju, South Korea; [2]Korea Basic Science Institute, Cheongju, South Korea*

TP 127 **Characterization and Classification of Human Renal Cell Carcinomas Through Lipid Imaging by Mass Spectrometry (LIMS)**; Ibai Calvo[1, 2]; Beatriz Suarez[1, 2]; Olatz Fresnedo[3]; Alberto Saiz[4]; Lorena Mosteiro[5, 6]; Jose Ignacio Lopez[5, 6]; Gorka Larrinaga[2, 3, 5]; Jose Andres Fernandez[1]; *[1]Department of Physical Chemistry, Faculty of Science and Technology, University of the Basque Country, Leioa, Spain; [2]Department of Nursing, Faculty of Medicine and Nursing, University of the Basque Country, Leioa, Spain; [3]Department of Physiology, Faculty of Medicine and Nursing, University of* *the Basque Country, Leioa, Spain; [4]Department of Pathology, Galdakao-Usansolo University Hospital, Galdakao, Spain; [5]Biobizkaia Health Research Institute, Barakaldo, Spain; [6]Department of Pathology, Cruces University Hospital, Barakaldo, Spain*

TP 128 **Quantitative spatial proteomics analysis of the nucleolus reveals a Ras-mediated, CK2-dependent mechanism to drive ribosome biogenesis in cancer**; Emilie L Alard[1, 2]; Faraz K Mardakheh[1, 2]; *[1]Barts Cancer Institute, Queen Mary University of London, London, United Kingdom; [2]Department of Biochemistry, University of Oxford, Oxford, United Kingdom*

TP 129 **Profiling the lipidome of adrenal cancer tissues using fast LC-MS methodologies**; Sheba Jarvis[1]; Lee A Gethings[2]; Anthony Midey[3]; Elizabeth Want[1]; Charlotte Bevan[1]; *[1]Imperial College London, London, United Kingdom; [2]Waters, Wilmslow, United Kingdom; [3]Waters Corporation, Milford, MA*

TP 130 **Decoding the Biology of a Rare Brain Tumor: Integrative Proteogenomic and Metabolomic Profiling of Oligodendroglioma**; Bianca Janine Kuhn[1]; Natalie M Clark[1]; C Williams[1]; Jackson White[1]; Joe D Allen[1]; Karl R Clauser[1]; Pinar Eser[1]; Adam C Resnick[2]; Mateusz P Koptyra[2]; Komal Rathi[2]; Shuangcheng Wu[3]; Pei Wang[4]; Francesca Petralia[4]; Weiping Ma[4]; Hui Zhang[5]; Yingwei Hu[5]; Brock Greene[6]; Samuel McBrayer[3]; Shankha Satpathy[1]; Steven A. Carr[1]; DR Mani[1]; Michael A. Gillette[1]; Children's Brain Tumor Network[7]; Philadelphia Coalition For A Cure[2]; Oligo Nation[6]; Clinical Proteomic Tumor Analysis Consortium[8]; *[1]Broad Institute of MIT and Harvard, Cambridge, MA; [2]Children's Hospital of Philadelphia, Philadelphia, Pennsylvania, United States, Philadelphia, PA; [3]University of Texas Southwestern Medical Center, Dallas, TX; [4]Icahn School of Medicine at Mount Sinai, New York City, NY; [5]Johns Hopkins University School of Medicine, Baltimore, Maryland; [6]Oligo Nation, Sebastopol, CA; [7]Children's Brain Tumor Network, US, US; [8]Clinical Proteomic Tumor Analysis Consortium (CPTAC), US, US*

TP 131 **Proteomic Analysis Unveils Divergent Functions of Cohesin Paralogs STAG1 and STAG2**; Shannon Marshall[1]; Caroline Clarke[2]; Hyojin Kim[2]; Giuditta Illuzzi[2]; David Fisher[2]; Ben Pullman[1]; Ted Hong[3]; Steven Criscione[3]; Emanuela Cuomo[2]; Matthew Glover[1]; Sonja Hess[1]; *[1]AstraZeneca, Gaithersburg, MD; [2]AstraZeneca, Cambridge, United Kingdom; [3]AstraZeneca, Waltham, MA*

TP 132 **Development of a multiplexed proteomics assay for patient selection for HER2 antibody-drug conjugant therapies**; Kristine A Tsantilas[1]; Jeffrey R Whiteaker[1]; Lei Zhao[1]; Regine M Schoenherr[1]; Uliana J Voytovich[1]; Richard G Ivey[1]; ChenWei Lin[1]; Zhangfang Guo[2]; Cynthia X Ma[2]; Amanda G Paulovich[1]; *[1]Fred Hutchinson Cancer Center, Seattle, WA; [2]Washington University in St. Louis School of Medicine, St. Louis, MO*

TP 133 **MutaQuant: development of a highly multiplexed MRM assay to quantify the mutation rate in 1000 cancer related proteins**; Vincent Richard[1, 2, 3]; Foroughsadat Absar[2]; Timon Geib[2]; Constantinos Blidjios[2]; Laleh E Ghahnavieh[4]; Pradyumn Maheshwari[4]; Ruhi Jaiswal[4]; Yassene Mohammed[3, 5]; Christoph H. Borchers[2, 3, 4, 6, 7, 8]; *[1]Segal Cancer Center, Lady David Institute, McGill University, Montreal, QC; [2]McGill University - Lady Davis Institute, Montréal, QC; [3]Segal Cancer Proteomics Centre, Jewish General Hospital, Montreal, QC; [4]MRM Proteomics Inc, Montreal, Quebec; [5]Leiden University Medical Center, Leiden, Netherlands; [6]Gerald Bronfman Department of Oncology, Montreal, QC; [7]Division of Experimental Medicine, McGill University, Montreal, QC; [8]Department of Pathology, McGill University, Montreal, QC*

TP 134 **Erlotinib Bioactivation: Reactive Intermediates Characterization by LC-MS/MS and Implications for Drug-Induced Organ Toxicity**; Adnan A Kadi[1]; Mohamed W. Attwa[1]; Ali S. Abdelhameed[1]; Haitham AlRabiah[1]; *[1]King Saud University, Riyadh, Saudi Arabia*

TP 135 **Quantitative Proteomics of Silva Patterns and the Tumor Microenvironment in Cervical Adenocarcinomas**; Jonathan Ogata[1, 2]; Sarah M. Drayer[1]; Sean Cronin[1]; Jordyn Tumas[1]; Saeid Movahedi-Lankarani[1]; Tamara Abulez[1, 2]; Kelly A. Conrads[1, 2]; Brian L. Hood[1, 2]; Jordan Driscoll[1, 2]; Kathleen M. Darcy[1, 2]; Christopher M. Tarney[1]; G. Larry Maxwell[2]; Thomas P. Conrads[2, 3]; Nicholas W. Bateman[1, 2, 3]; Neil T. Phippen[1]; *[1]Gynecologic Cancer Center of Excellence and the Women's Health Integrated Research Center, Annandale, VA; [2]The Henry M. Jackson Foundation for the Advancement of Military Medicine Inc., Bethesda, Maryland; [3]Women's Health Integrated Research Center, Women's Service Line, Inova Health System, Falls Church, Virginia*

TP 136 **Comprehensive Multiomics Characterization of Gastric Cancer with Proteogenomic Insights**; Yuefan Wang[1]; Lindsey Kathleen Olsen[2]; Hui Zhang[1]; Bing Zhang[2]; CPTAC Consortium[3]; *[1]Johns Hopkins University, Baltimore, MD; [2]Baylor College of Medicine, Houston, TX; [3]NIH, BETHESDA, MD*

TP 137 **Comprehensive Surfaceome Profiling of Osteosarcoma Alterations Using WGA-HRP and DIA-PASEF**; Snehal Ganjave[1]; Kevin Leung[1]; Trenton Peters-clarke[1]; Leanne Sayles[1]; E. Alejandro Sweet-Cordero[1]; Jim Wells[1]; *[1]University of California San Francisco, San Francisco, CA*

TP 138 **Spatial Proteomics Identifies Inflammation-Related Protein Changes in Gastric Neuroendocrine Carcinomas**; Jiyoung Yu[1]; Bokyung Kim[2]; Bokyung Ahn[3]; Chang Seok Ko[4]; Jihyeon Kim[2]; Minjoong Kim[5]; Yelin Lee[5]; Seung-Mo Hong[3]; Beom-Su Kim[6]; Kyunggon Kim[1, 2]; *[1]Clinical Proteomics Core Lab, Convergence Research Center, Asan Medical Center, Songpa-gu, South Korea; [2]Department of Digital Medicine, BK21 Project, University of Ulsan College of Medicine, A, Songpa-gu, South Korea; [3]Department of Pathology, Asan Medical Center, University of Ulsan College of Medicine, Songpa-gu, South Korea; [4]Division of gastrointestinal surgery, Department of surgery, Asan Institute for Life Sciences, Asan Medical Center, Songpa-gu, South Korea; [5]Department of Digital Medicine, BK21 Project, University of Ulsan College of Medicine, Songpa-gu, South Korea; [6]Department of Gastrointestinal Surgery, Asan Medical Center, University of Ulsan College of Medicine, Songpa-gu, South Korea*

TP 139 **Mass Spectrometry-based metabolomics and lipidomics to determine the impact of PIKfyve inhibition in pancreatic cancer cell metabolism**; Caleb Cheng[1]; Li Zhang[1]; Pietro Morlacchi[2]; Peter Sajjakulnukit[1]; Jasmine Wisniewski[1]; Sydney Peters[1]; Rüya Pakkan[1]; Yuanyuan Qiao[1]; Arul M. Chinnaiyan[1, 3]; Costas A. Lyssiotis[1]; *[1]University of Michigan, Ann Arbor, MI; [2]Agilent Technologies, Lexington, MA; [3]Howard Hughes Medical Institute, Chevy Chase, Maryland*

TP 140 **Membrane proteomic analysis revealed resistant mechanisms of epidermal growth factor receptor tyrosine kinase inhibitors in lung cancer cells**; Yu-Teng Zheng[1]; Chia-Li Han[2]; *[1]National Taiwan University, Taipei, Taiwan; [2]Taipei Medical University, Taipei, Taiwan*

TP 141 **AKT Isoform-Specific Regulation of Hepatic Eicosanoid Metabolism in PTEN-Deficient Liver Disease and HCC Progression**; Mario M Alba[1, 2]; Ielyzaveta Slarve[1]; Qi Tang[1]; Dante Dikemen[1]; Taojian Tu[1]; Jared Khan[1]; Yiren Zhou[1]; Yunyi Jia[1]; Aditi Datta[1]; Brandon Ebright[1]; Yushan Wang[1]; Zixin Zong[1]; Elizabeth Elton[1, 3]; Francisca NDL Vitorino[4]; Handan Hong[1]; Pranav Pammidimukkala[1]; Guo Zhang[1]; Lina He[1]; Phillip Nguyen[1]; Ethan Canfield[3]; Ebony Flowers[1]; Whitaker Cohn[1, 5]; Karam Ashouri[6]; Anastasia Martynova[6]; Christina Nakhoul[6]; Jonathan E Katz[1, 3]; Anthony El-Khoueiry[6]; Benjamin A Garcia[4]; Julian Whitelegge[5]; Stan Louie[1]; Bangyan Stiles[1]; *[1]USC, Los Angeles, CA; [2]Cedars Sinai Medical Center, Los Angeles, CA; [3]Ellison Medical Institute, Los Angeles, CA; [4]Washington University in St. Louis, University City, MO; [5]UCLA, Los Angeles, CA; [6]Keck School of Medicine, Norris Comprehensive Cancer Center of USC, Los Angeles, CA*

TP 142 **Lipid Alterations Across Seven Pancreatic Ductal Adenocarcinoma-Related Cohorts Using RP-UHPLC/MS**; Zuzana Lasko[1]; Ondrej Peterka[1]; Robert Jirasko[1]; Lenka Dubska[1]; Anna Taylor[1]; Tomas Hajek[1]; Beatrice Mohelnikova-Duchonova[2]; Martin Lovecek[2]; Bohuslav Melichar[2]; Petr Karasek[3]; Jan Trna[3]; Ondrej Urban[2]; Petra Vyhnalek[4]; Ondrej Kuda[5]; Roman Hrstka[3]; Michal Holcapek[1]; *[1]University of Pardubice, Pardubice, Czech Republic; [2]University Hospital Olomouc, Olomouc, Czech Republic; [3]Masaryk Memorial Cancer Institute, Brno, Czech Republic; [4]Regional Hospital Pardubice, Pardubice, Czech Republic; [5]Institute of Physiology of the Czech Academy of Sciences, Prague, Czech Republic*

TP 143 **Ensuring High Quality Data from Fresh Frozen Tissue Samples with Robust, Scalable, and Comprehensive Protein Analysis Sample Preparation Workflows**; Debadeep Bhattacharyya[1]; Sameer Vasantgadkar[1]; Lia Abarzua[1]; Ulrich Thomann[1]; Eugenio Daviso[1]; Patrick McCarthy[1]; *[1]Covaris, Woburn, MA*

CLINICAL ANALYSIS II
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TP 144 **Development and validation of a UPLC–MS/MS method for the quantification of cabotegravir, lenacapavir, and rilpivirine in seminal plasma**; Noah C. Neverette[1]; Raymond E. West[1]; Patrick J. Oberly[1]; Thomas D. Nolin[1]; Aaron S. Devanathan[1]; *[1]Center for Clinical Pharmaceutical Sciences, Department of Pharmacy and Therapeutics, School of Pharmacy, University of Pittsburgh, Pittsburgh, PA*

TP 145 **Development and validation of a candidate reference method for PTH 1-84 by LC-MS/MS**; Ruichen Liu[1]; Xuzhe Pei[1]; Chao Huang[1]; Xianglong Zhao[1]; Bingjie Liu[1]; *[1]Shanghai AB Sciex Analytical Instrument Trading Co., Ltd., Beijing, China*

TP 146 **Determination of five peptide antibiotics in plasma using rapid magnetic beads method in couple with liquid chromatography-tandem mass spectrometry**; Dan Liu[1]; Fengmei Hu[1]; Chao Huang[1]; Xianglong Zhao[1]; Bingjie Liu[1]; *[1]SCIEX, Shanghai, China*

TP 147 **Measurement of 7 critical PFAS compounds from human serum utilizing dispersive in-pipette SPE sample prep prior to LC-MS/MS Analysis**; Hugh Cramer[1]; M. James Ross[1]; Olga Shimelis[1]; *[1]MilliporeSigma, Bellefonte, PA*

TP 148 **MALDI glycotyping of E. coli and Shigella spp O-antigens**; Shogo Urakami[1]; Hiroshi Hinou[2]; *[1]Hokkaido University, Sapporo, Japan; [2]Hokkaido University, Sapporo, Japan*

TP 149 **High-throughput quantitative targeted lipidomics revealed common lipid signatures in mice and human plasma samples after anaesthetization**; Yuanyuan Ji[1]; Yun Li[2]; Sheng Feng[3]; Robert H. Christensen[3]; Junfang Wu[2]; Jace W. Jones[1]; *[1]University of Maryland, School of Pharmacy, Department of Pharmaceutical Sciences, Baltimore, MD; [2]University of Maryland, School of Medicine, Department of Anesthesiology, Shock, Trauma and Anesthesiology Research (STAR) Center, Baltimore, MD; [3]University of Maryland, School of Medicine, Department of Pathology, Baltimore, MD*

TP 150 **Fast and Efficient LC-MS/MS Analysis of 34 PFAS Analytes in Serum for Clinical Research**; Shahana Huq[1]; Stephanie J. Marine[2]; *[1]Phenomenex, Torrance, CA; [2]Phenomenex, Torrance, California*

TP 151 **Development and Utilization of a Quantitative PIKfyve Substrate and Metabolite Assay**; Xiaohui Yu[1]; Dante Dikeman[1]; Isaac Asante[1]; Whitaker Cohn[1]; Stan Louie[1]; *[1]University of Southern California, Los Angeles, CA*

TP 152 **Utilization of Isobaric Peptide Probes for the Early Prediction of Severe Acute Pancreatitis using Mass Spectrometry**; Sophie Miller[1]; Jackson Fischer[1]; Ella Warner[1]; Ruth M Speidel[1]; Georgios Papachristou[2]; Peter Lee[2]; Abraham Badu-Tawiah[1]; *[1]Ohio State University, Columbus, OH; [2]Wexner Medical Center Ohio State University, Columbus, OH*

TP 153 **Analysis of urinary sugars by GC-MS for the study of gut permeability**; Anna M. Caldwell[1]; Aaron S. Bancil[1]; Megan Rossi[1]; Kevin Whelan[1]; Ana Rodriguez-Mateos[1]; John M Halket[1]; *[1]Department of Nutritional Sciences, King's College London, London, United Kingdom*

TP 154 **Application of Magnetic Beads in Automated Sample Preparation for Simultaneous Extraction of 24 Steroids in Serum by LC-MS/MS**; Pengyun Liu[1]; Zhouyang Kang[1]; Hehuan Liu[1]; Xiaofen Yuan[1]; Weijia Wu[1, 2]; Huafen Liu[1]; *[1]Calibra Scientific, Inc., Hangzhou, China; [2]3P BioSolutions Inc., Woodbridge, VA*

TP 155 **Refined SPE-HPLC-MS/MS Method for Investigating Exposure Levels and Correlations of Legacy Perfluoroalkyl Substances in a Korean Cohort**; Ji-Hyeon Cha[1]; Young-Heun Jung[1]; Seung Min Chung[2]; Ju-Hyun Kim[1]; *[1]Yeungnam University, Gyeongsan-si, South Korea; [2]Yeungnam University, Daegu, South Korea*

TP 156 **Application of a HRMS polarity switching method for targeted quantitation and unknown screening for drugs of abuse in urine**; Emily G Armitage[1]; Alan Barnes[1]; Simon Ashton[1]; Chloe Hutton[1]; Lucy Murfitt[2]; Ellen Rumsby[2]; Neil J Loftus[1]; *[1]Shimadzu Corporation, Manchester, United Kingdom; [2]Northern Care Alliance NHS Foundation Trust, Salford, United Kingdom*

TP 157 **TDM of immunosuppressant in whole blood in 8 seconds using LDTD-MS/MS**; Jean Lacoursière[1]; Jonathan Rochon[1]; Mégane Moreau[1]; Sarah Demers[1]; Serge Auger[1]; Pierre Picard[1]; *[1]Phytronix Technologies, Quebec, QC*

TP 158 **Sample Cleanup Approaches for the Analysis of A Multi-Class Drugs of Abuse Panel in Breast Milk**; Kyle Dukes[1]; Sohel Rana[2]; Lee Williams[2]; *[1]Biotage, Charlotte, NC; [2]Biotage LLC, Charlotte, NC*

TP 159 **Accurate assessment of endogenous large molecules by LC-MS/MS bioanalysis from FFPE tissues with spatial resolution**; Soumya Kandi[1]; Qin C Ji[1]; Bit Na Kang[2]; Edyta Jarmulkowicz[3]; Amanda Krempley[3]; Jan Schejbal[4]; Lori Duggan[2]; Yingli Yang[2]; Susan Westmoreland[2]; Lucy A Phillips[2]; Marianna Kleyman[2]; Shashikanth Gannu[1]; Mary J Saltarelli[5]; Mario Richter[6]; Gary J Jenkins[1]; *[1]AbbVie, QTAS, North Chicago, IL; [2]AbbVie: Bioresearch Center, Discovery Immunology, Worcester, MA; [3]AbbVie, PCS, North Chicago, IL; [4]AbbVie: Bioresearch Center: QTAS, Worcester, MA; [5]AbbVie, QTAS, South San Francisco, CA; [6]AbbVie, QTAS, Ludwigshafen, Germany*

TP 160 **Analysis of Lipid Biomarkers in Pancreatic Cyst Fluid by Targeted and Untargeted LC-MS/MS**; Li Zhang[1]; Hong Sun Kim[2]; Timothy Frankel[3]; Costas Lyssiotis[1]; Jiaqi Shi[2]; *[1]Department of Molecular & Integrative Physiology, University of Michigan, Ann Arbor, MI; [2]Department of Pathology & Clinical Labs, University of Michigan, Ann Arbor, MI; [3]Department of Surgery, University of Michigan, Ann Arbor, MI*

TP 161 **Rapid Detection, Subtyping, and Intraoperative Tumor Margin Assessment of Lung Cancer Using MasSpec Pen Technology**; Yasmin Shanneik[1]; Alberto Antonicelli[2]; Maheshwari Ramineni[3]; Bryan M. Burt[2]; Livia S. Eberlin[1]; *[1]Department of Surgery, Baylor College of Medicine, Houston, Texas; [2]Department of Surgery, University of California-Los Angeles, Los Angeles, California; [3]Department of Pathology, Baylor College of Medicine, Houston, Texas*

TP 162 **Comprehensive Evaluation of Sample Preparation Strategies for Blood Proteomics: Achieving the Largest MS-Based Blood Proteome to Date**; Zhenyu Sun[1]; T. Mamie Lih[1]; Yuefan Wang[2]; Yuanyu Huang[1]; Lijun Chen[1]; Hui Zhang[1]; *[1]Johns Hopkin University, Baltimore, MD; [2]Johns Hopkins University, Baltimore, MD*

TP 163 **Point-of-care testing of drugs and toxicant with miniature mass spectrometer**; Nan Zhang[1]; Junhan Wu[2]; Wenpeng Zhang[3]; Jiexun Bu[1]; Zheng Ouyang[3]; *[1]PURSPEC Technology (Beijing) Ltd., Beijing, China; [2]PURSPEC Technology (China) Ltd., Suzhou, China; [3]Department of Precision Instrument, Tsinghua University, Beijing, China*

TP 164 **Performance and Application of Vitamin D Calibration/Verification Linearity Material Across the Clinical Laboratory**; Cole Bedeaux[1]; Jessica Pawlak[1]; *[1]LGC Clinical Diagnostics, Cumberland Foreside, ME, ME*

TP 165 **Quantitation of Nicotin, Cotinin and 3-OH-trans-cotinin in urine using LC-MS/MS with a dilute-and-shoot method approach**; Dennis JA Van Den Heuvel[1]; Tom Stokhof De Jong[1]; Jacob Diepenbroek[1]; Pascal Mannaert[1]; *[1]Shimadzu Benelux, 's-Hertogenbosch, Netherlands*

TP 166 **Advancing Clinical Diagnostics through Integration of Proteomics and Data Science at a Danish Hospital**; Annelaura Bach Nielsen[1,2]; Christine Rasmussen[3]; Lylia Drici[2]; Maud Ottenheijm[2,3]; Lasse Fjordside[4]; Helene Mens[4]; Anne-Mette Lebech[4,5]; Shaodong Wei[6]; Jesper Brix Petersen[6]; Jens Helby Petersen[6]; Andreas Glenthøj[6]; Matthias Mann[2,7]; Nicolai Jacob Wewer Albrechtsen[2,3,5,8]; *[1]Department of Clinical Biochemistry, Copenhagen University Hospital, Bispebjerg and Frederiksberg Hospital, Copenhagen, Denmark, Copenhagen NV, Denmark; [2]Novo Nordisk Foundation Center for Protein Research, University of Copenhagen, Denmark; [3]Department of Clinical Biochemistry, Copenhagen University Hospital, Bispebjerg and Frederiksberg Hospital, Copenhagen, Denmark; [4]Department of Infectious Diseases, Copenhagen University Hospital Rigshospitalet, Copenhagen, Denmark; [5]Department of Clinical Medicine, Faculty of Health and Medical Sciences, University of Copenhagen, Copenhagen, Denmark; [6]Danish Red Blood Cell Centre, Department of Haematology, Copenhagen University Hospital Rigshospitalet, Copenhagen, Denmark; [7]Department of Proteomics and Signal Transduction, Max Planck Institute of Biochemistry, Munich, Germany; [8]Copenhagen Center for Translational Research, Copenhagen University Hospital - Bispebjerg and Frederiksberg, Copenhagen NV, Denmark*

TP 167 **Development of an LC/MS based bacteria culture media metabolomics analysis approach for malodor evaluation**; Egodage Udeesha Inoshi De Silva[1]; Jianchuan Wen[1]; Yuyu Sun[1]; Pengyuan Liu[1]; *[1]University of Massachusetts, Lowell, Lowell, MA*

TP 168 **A Comparison of Sample Preparation Techniques for Drugs of Abuse in Oral Fluids**; Jared Burkhart[1]; Samantha Herbick[1]; *[1]Restek Corporation, BELLEFONTE, PA*

TP 169 **Novel machine vision-based tool for assessment of sample quality of dried blood spot DBS samples for LC/MS analysis**; Tomasz Bienkowski[1,2]; Michał Czubenko[3]; Dawid Masłowski[3]; Rafał Okuński[3]; Anna Kołodyńska[2]; Konrad Kowalski[2]; *[1]MS Ekspert Sp. z o.o., Gdańsk, Poland; [2]Masdiag Sp. z o.o., Warszawa, Poland; [3]Intema sp. z o.o., Gdańsk, Poland*

TP 170 **Next generation antithrombin testing by mass spectrometry for precision diagnosis of antithrombin deficiency**; Renee Ruhaak[1]; Mirjam Kruijt[1]; Niek Kijk In De Vegte[1]; Michelle Van Der Helm[1]; Eugenia De La Morena-Barrio[2]; Zsuzsanna Bereczky[3]; Javier Corral - De La Calle[2]; Christa Cobbaert[1]; *[1]Leiden University Medical Center, Leiden, Netherlands; [2]Servicio de Hematología, Hospital Universitario Morales Meseguer, Centro Regional de Hemodonación, Universidad de Murcia, IMIB-Pascual Parrilla, CIBERER-ISCIII, Murcia, Spain; [3]Division of Clinical Laboratory Science, Department of Laboratory Medicine, Faculty of Medicine, University of Debrecen, Debrecen, Hungary*

TP 171 **LC-MS/MS Method Development for the Measurement of Trimethylamine-N-Oxide (TMAO) in Sickle Cell Disease in a Clinical Laboratory**; Thando Gcingca[1]; Ning Pan Bernhardt[2]; Caroline Nottingham[1]; *[1]National Institute of Health, Bethesda, MD; [2]NIH, Bethesda, MD*

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TP 172 **Quantitative Neuropeptidomics with Multiplexed DIA-MS: Unveiling Feeding Regulation in Cancer borealis via mdDiLeu Labeling**; Lauren Fields[1]; Peng-Kai Liu[1]; Tina C. Dang[1]; Angel E. Ibarra[1]; Zicong Wang[1]; Lingjun Li[1]; *[1]University of Wisconsin-Madison, Madison, WI*

TP 173 **Proteomic Analysis Uncovers Region-Specific Renal Aging Processes in Macaca mulatta**; Christina D King[1]; Jordan B Burton[1]; George Schaaf[2]; Stephan Kritchevsky[2]; J. Mark Cline[2]; Jamie N Justice[2,3]; Eric S Goetzman[4]; Sunder Sims-Lucas[4]; Ellen E Quillen[2]; Birgit Schilling[1]; *[1]Buck Institute for Research on Aging, Novato, CA; [2]Wake Forest School of Medicine, Winston-Salem, NC; [3]XPRIZE Foundation, Culver City, CA; [4]Children's Hospital of Pittsburgh of UPMC, University of Pittsburgh, Pittsburgh, PA*

TP 174 **Development and Application of a Stability-Based Proteomics Method using a Data Independent Acquisition Strategy**; Natalie M. Labbe[1]; Meghan Virani[1]; Michael C. Fitzgerald[1]; *[1]Duke University, Durham, NC*

TP 175 **Enhanced Ocean Metaproteomic Profiling with Orbitrap Astral in Data Independent Acquisition**; Kushani Attanayake[1]; Yunyun Zhu[1]; Joel Bucci[1]; Lichun Zhang[2]; Mak Saito[3]; Jacob Waldbauer[2]; *[1]Thermo Fisher Scientific, Lexington, MA; [2]Department of the Geophysical Sciences, University of Chicago, Chicago, IL; [3]Marine Chemistry & Geochemistry, Woods Hole Oceanographic Institution, Woods Hole, MA*

TP 176 **Integrating Robotic Automation and DIA Acquisition in CETSA-MS for Enhanced Throughput, Coverage, and Efficiency**; Renze Ma; *AbbVie, Inc., North Chicago, IL*

TP 177 **Staggered Window Data Independent Acquisition with Variable Window Sizes May Improve LC-MS Proteomic Coverage on Orbitrap Mass Spectrometers**; Quentin D Bethune[1]; Shiri Meira[1]; Gautham V Sridharan[1]; *[1]Alnylam Pharmaceuticals, Cambridge, MA*

TP 178 **Evaluation of the false discovery rate in library-free search by DIA-NN using human in vitro proteome**; Kongxin Gu[1]; Naoki Goshima[2]; Takeshi Masuda[1,3]; Shingo Ito[1]; Sumio Ohtsuki[1]; *[1]Kumamoto University, Kumamoto, Japan; [2]ProteoBridge Corporation, Tokyo, Japan; [3]Keio University, Tsuruoka, Japan*

TP 179 **Comparison of fast scanning data dependent and data independent acquisition methods for a multi-OMIC cancer study using high-speed chromatography**; Lee A Gethings[1]; Martin Palmer[1]; Nyasha C Munjoma[1]; Jason Wildgoose[1]; Richard Lock[1]; James Langridge[1]; *[1]Waters Corporation, Wilmslow, United Kingdom*

TP 180 **DIA analysis on the Orbitrap Astral combined with PTMScan enrichment provides an expanded global view of protein post translational modifications**; Mukesh Kumar[1]; Anthony P. Possemato[1]; Barry M. Zee[1]; Jian Min Ren[1]; Alissa Nelson[1]; Jeffrey C. Silva[1]; Brett Larsen[2]; Tonya Pekar Hart[3]; Matthew P. Stokes[1]; Sean A Beausoleil[1]; *[1]Cell Signaling Technology, Danvers, MA; [2]Thermo Fisher Scientific, Toronto, Ontario; [3]Thermo Fisher Scientific, San Jose, California*

TP 181 **Quantitative proteomics using high-sensitivity data-independent acquisition**; Ihor Batruch[1]; Patrick Pribil[1]; *[1]SCIEX, Concord, ON*

TP 182 **Redefining Targeted Activity-based Protein Profiling (ABPP) depth by Stellar Mass Spectrometer**; Abootaleb Sedighi[1]; Bilal Saqib[1]; Balmiki Kumar[1]; Timothy B. Wright[1]; Naman H. Patel[1]; Graham Simpson[2]; Mark Bell[2]; Albert Arul[3]; Scott M. Peterman[4]; Brett Larsen[5]; Elvin D. De Araujo[1]; Patrick T. Gunning[2]; *[1]University of Toronto, Mississauga, ON; [2]University of Glasgow, Glasgow, United Kingdom; [3]Thermo Fisher Scientific, Somerset, NJ; [4]Thermo Fisher Scientific, San Jose, CA; [5]Thermo Fisher Scientific, Mississauga, ON*

TP 183 **More for Less; A memory and runtime efficient library free workflow for a significantly improved analysis of immunopeptidomics in Spectronaut**; Oliver M Bernhardt[1]; Grzegorz Skoraczyński[1]; Monika Pepelnjak[1]; Anamarija Pfeiffer[1]; Maik Mueller[1]; Tejas Gandhi[1]; Lukas Reiter[1]; *[1]Biognosys AG, Schlieren, Switzerland*

TP 184 **The Proteome Atlas – Deep Proteomic Characterization of More Than 120 Frequently Used Model Cell Lines**;

Johanna Wallner[1, 2]; Janine Sequeira[1]; Theresa Keil[1]; Alexander Betz[1]; Johannes Krumm[1]; Christin Zasada[1]; Jan Muntel[1]; Hannes Hahne[1]; *[1]OmicScouts GmbH, Freising, Germany; [2]Technical University of Munich, Garching, Germany*

TP 185 **An integrated analysis of global proteome, phosphoproteome and secretome reveals BFT-Associated differences in Bacteroides fragilis Strains**; Sinae Lee[1, 2, 3, 4]; Eunmi Chu[4, 5]; Hong-Beom Park[2, 3]; Gyuri Park[2, 3, 6]; Hyeon Chang Lee[2, 3, 6]; Eunseo Kim[2, 3, 5]; Minhyeok Kang[2, 3, 6]; Soeun Yun[2, 3, 5]; Jin Lee[2, 3, 5]; Jinki Yeom[4, 5]; Dohyun Han[2, 3, 7]; *[1]Interdisciplinary Program in Cancer Biology, Department of Biomedical Sciences, Seoul National University, Seoul, South Korea; [2]Department of Transdisciplinary Medicine, Seoul National University Hospital, Seoul, South Korea, Seoul, South Korea; [3]Proteomics Core Facility, Biomedical Research Institute, Seoul National University Hospital, Seoul, South Korea; [4]Cancer Research Institute, Seoul National University college of medicine, Seoul, South Korea; [5]Department of Biomedical Science, College of Medicine, Seoul National University, Seoul, South Korea; [6]Molecular Medicine and Biopharmaceutical Sciences, WCU Graduate School of Convergence Science and Technology Seoul National University, Seoul, South Korea; [7]Department of Medicine, Seoul National University College of Medicine, Seoul, South Korea*

TP 186 **Maximizing the ion-usage of timsTOF acquisitions through segmented ion mobility elution and curved diagonal-PASEF methods boosts the analytical performance**; Christopher Below[1]; Bettina Streckenbach[2]; Stephanie Kaspar-Schoenefeld[3]; Florian Krohs[3]; Chris David Goessling[3]; Oliver Raether[3]; Roland Bruderer[1]; Lukas Reiter[1]; *[1]Biognosys, Schlieren, Switzerland; [2]Biognosys AG, Schlieren, Switzerland; [3]Bruker Daltonics GmbH & Co.KG, Bremen, Germany*

TP 187 **Advancements in ZT Scan data independent acquisition (DIA) on a novel QTOF system**; Anjali Chelur[1]; Gordana Ivosev[1]; Hieu Cuong Le[1]; Wen Jin[1]; Nic Bloomfield[1]; *[1]SCIEX, Concord, ON*

TP 188 **Timsbuktoolkit: Open-source platform for on-demand interactive peptide search on timsTOF DIA data**; J. Sebastian Paez[1]; Sander Willems[2]; Andrea Gutierrez[1]; Daniele Canzani[1]; Alexander J. Federation[1]; Lindsay K Pino[1]; William E. Fondrie[1]; *[1]Talus Bioscience, Seattle, WA; [2]Bruker Daltonics GmbH & Co.KG, Bremen, Germany*

TP 189 **Enhanced proteomic profiling of Mu-Opioid Receptor Interactions in Alcohol Addiction using DDA and DIA based Mass Spectrometry**; Meera Asokan[1]; Luis A Natividad[2]; *[1]University of Texas Austin, Austin, TX; [2]University of Texas at Austin, Austin, TX*

TP 190 **Refined Library Searching Increases Proteome Coverage in diaPASEF Small Sample Amounts**; Joshua Charkow[1]; Mahmoudreza Ghaznavi[1]; Brendon Seale[2]; Anne-Claude Gingras[1, 2]; Hannes Röst[1]; *[1]University of Toronto, Toronto, ON; [2]Lunenfeld-Tanenbaum Research Institute, Toronto, ON*

TP 191 **Diagonal-PASEF enables robust and high-throughput proteomic profiling of samples of varying complexities**; Dain Ryan Brademan[1]; Angelina Mullarkey[1]; Emily Blythe[2]; Ruth Huttenhain[1]; *[1]Stanford University, Stanford, CA; [2]University of California San Francisco, San Francisco, CA*

TP 192 **Benchmarking diagonal-PASEF data acquisition for high-throughput proteomics applications**; Shourjo Ghose[1]; Stephanie Kaspar-Schoenefeld[2]; Christopher Below[3]; Oliver M. Bernhardt[4]; Tejas Gandhi[4]; Jonathan R Krieger[5]; Roland Bruderer[4]; Lukas Reiter[4]; Markus Lubeck[6]; *[1]Bruker Scientific, Billerica, MA; [2]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [3]Biognosys, Zurich, Switzerland; [4]Biognosys AG, Schlieren, Switzerland; [5]Bruker Ltd., Milton, ON; [6]Bruker, Bremen, Germany*

TP 193 **DIA for the masses: strategies for implementation in unit resolution**; Deanna L Plubell[1]; Christine C. Wu[1]; Bo Wen[1]; Fengchao Yu[2]; Philip M. Remes[3]; Lilian R Heil[3]; Alexey I. Nesvizhskii[4]; Michael J MacCoss[1]; *[1]University of Washington, Seattle, WA; [2]University of Michigan, Ann Arbor, Michigan; [3]Thermo Fisher Scientific, San Jose, CA; [4]University of Michigan, Ann Arbor, MI*

TP 194 **Proteomic Landscape of HPV-Associated Cervical Cancer Reveals Significant Perturbations in EMT, Focal Adhesion, and Immune Pathways**; Amrita Mukherjee[1]; Avinash Singh[1]; Sanjeeva Srivastava[1]; *[1]IIT Bombay, Powai, India*

TP 195 **A phosphoproteomic turnover atlas across 15 mouse tissues established by DIA**; Wenxue Li[1]; Abhijit Dasgupta[2]; Ka Yang[2]; Shisheng Wang[3]; Nisha Hemandhar-Kumar[4]; Surendhar R. Chepyala[2]; Jay M. Yarbro[2]; Zhenyi Hu[1]; Barbora Salovska[1]; Eugenio F. Fornasiero[4]; Junmin Peng[2]; Yansheng Liu[1]; *[1]Yale University, New Haven, CT; [2]St. Jude Children's Research Hospital, Memphis, TN; [3]Sichuan University, Chengdu, China; [4]University Medical Center Göttingen, Göttingen, Germany*

TP 196 **An Automated High Throughput Label-free DIA Platform to Accelerate Target Identification for Molecular Glue Degraders**; Despina Kapsitidou[1]; Vaik Strande[1]; Aurelie Dubois[1]; Laura Schwander[1]; Arnaud Osmont[1]; Xudong Wang[2]; Debora Bonenfant[1]; Reinaldo Almeida[1]; *[1]Monte Rosa Therapeutics, Basel, Switzerland; [2]Monte Rosa Therapeutics, Boston, MA*

TP 197 **Assessment of a narrow-window dia-PASEF method for high-throughput proteomics**; Stephanie Kaspar-Schoenefeld[1]; Jonathan R Krieger[2]; Savannah Snyder[3]; Markus Lubeck[4]; *[1]Bruker Daltonics GmbH & Co.KG, Bremen, Germany; [2]Bruker Ltd., Milton, ON; [3]Bruker Daltonics, Billerica, MA; [4]Bruker Daltonics GmbH & Co. KG, Bremen, Germany*

TP 198 **Extending LOD/LOQ Estimation and Quantitative Benchmarking for High-Throughput Proteomics**; Lindsay K Pino[1]; Seth Just[2]; Daniele Canzani[1]; Jack Penny[3]; Ben Collins[3]; Sebastian J. Paez[1]; Michael Riffle[4]; Michael J. MacCoss[4]; William E. Fondrie[1]; Alexander J. Federation[1]; *[1]Talus Bioscience, Seattle, WA; [2]Seer, Inc, Redwood City, CA; [3]Queen's University Belfast, Belfast, United Kingdom; [4]University of Washington, Seattle, WA*

TP 199 **Quantifying the ~75-95% of Peptides in DIA-MS Files that have been Historically Ignored, Despite their Value**; Gautam Saxena[1]; Qin Fu[2]; Aleksandra Binek[2]; Jennifer Van Eyk[2]; *[1]GoldenHaystack Lab, Bethesda, MD; [2]Cedars Sinai Medical Center, Los Angeles, CA*

TP 200 **Comparing Study-Specific Data-Independent Acquisition Libraries to In Silica produced Data-Independent Acquisition Libraries for Proteomics Analysis**; Mynaja Ferguson[1]; Rachel Muriph[1]; Jason J. Evans[1]; *[1]University of Massachusetts Boston, Boston, MA*

TP 201 **diaPASEF analysis of adult Nrf2 and αB-crystallin mutant zebrafish lenses under oxidative stress**; Sarah Zelle[1]; Hassane S. Mchaourab[1]; Kevin L. Schey[1]; *[1]Vanderbilt University, Nashville, TN*

TP 202 **Optimizing Selectivity and Ion Utilization for Trapped Ion Mobility Spectrometry for Enhanced DIA Performance**; Markus Lubeck[1]; Andreas Schmidt[1]; Stephanie Kaspar-Schoenefeld[2]; Matt Albano[3]; Dijana Vitko[3]; Matthew Willetts[3]; Daniel Hornburg[4]; *[1]Bruker Daltonics GmbH & Co.KG, Bremen, Germany; [2]Bruker Daltonics GmbH & Co.KG, Bremen, Germany; [3]Bruker Daltonics GmbH & Co. KG, Billerica, MA; [4]Bruker Daltonics GmbH & Co. KG, San Francisco, CA*

TP 203 **Development and benchmarking of a novel mass tag for improving depth and throughput of plexDIA experiments**; Sarah N Sipe[1]; Madeline J Yeh[1]; Harrison Specht[1]; Nikolai Slavov[1, 2]; *[1]Parallel Squared Technology Institute, Watertown, MA; [2]Northeastern University, Boston, MA*

TP 204 **Assessing The Performance of Data Independent Acquisition (DIA) On Microbial Community Proteomics**; Samantha A. Obermiller[1]; Victoria N. Prozapas[2]; Paul D.

Piehowski[1]; Aivett Bilbao[1]; Geremy C. Clair[2]; Mary S. Lipton[3]; Isaac Kwame Attah[2]; *[1]Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, Washington 99354; [2]Pacific Northwest National Laboratory (PNNL), Richland, WA; [3]PNNL, Richland, WA*

TP 205 **Analysis of diaPASEF data using FragPipe computational platform**; Kai Li[1]; Guo Ci Teo[1]; Kevin L. Yang[1]; Fengchao Yu[1]; Alexey I. Nesvizhskii[1]; *[1]University of Michigan, Ann Arbor, Michigan*

TP 206 **Utilising data-independent acquisition mass spectrometry (DIA-MS) to enable rapid, in depth profiling of the human secretome**; Chloe Tayler; *GSK, Stevenage, United Kingdom*

TP 207 **Evaluation of ZTScan DIA for the diagnosis of bloodstream infections**; Julie Flecheux[1]; Agnès Dupas[1]; Chloé Desbiolles[2]; Roxane Prat[2]; Ihor Batruch[3]; Jean-Baptiste Vincendet[4]; Kristina Jurcic[5]; François Vandenesch[2]; Jérôme Lemoine[1]; *[1]1. University Claude Bernard Lyon1, ISA, UMR5280, CNRS, Villeurbanne, France; [2]2. Institute of Infectious Diseases, Hôpital de la Croix-Rousse, HCL, Lyon, France; [3]SCIEX, Concord, L4K; [4]SCIEX, Alderley Park, United Kingdom; [5]Bioinformatics Solutions Inc., Waterloo, N2J*

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TP 209 **Innovative Application of ICP-MS Technology in Discovery and Early Development of Radioligand Therapeutics**; Daniel Wall[1]; Vipin Jain[1]; Francesca Ferri[1]; Peter Wipfli[1]; Jennifer Cunliffe[1]; *[1]Novartis, Cambridge, MA*

TP 210 **Integration of High-Throughput, Microflow LC-High-Resolution Mass Spectrometry (HT-µfLC-HRMS) in Early Discovery Bioanalysis**; Brendon Kapinos[1]; Jamie Tourville[1]; Hannah Moulton[1]; Christopher Healy[1]; Matthew Troutman[1]; Steve Ainley[2]; Wayne Lootsma[2]; *[1]Pfizer, Groton, CT; [2]Sound Analytics, Deep River, CT*

TP 211 **nMS as a tool for affinity selection mass spectrometry screening (ASMS) method development and validation**; Wenyi Hua[1]; Prem Patel[2]; Ian McCombes Tolis[1]; Xidong Feng[1]; *[1]Pfizer Inc., Groton, CT; [2]Net2Source, Somerset, New Jersey*

TP 212 **An LC-MS/MS Method for Separation and Quantification of Chiral Molecules**; Xu Zhang[1]; Lingyan Hua[1]; Dan Li[1]; Jinlian Lu[1]; Zhiyu Li[1]; Lili Xing[1]; Yi Tao[1]; Liang Shen[1]; *[1]WuXi AppTec, Shanghai, China*

TP 213 **Development of a High-throughput and Cost-effective Method for Experimental Polar Surface Area Measurement with Ultra-Performance Convergence Chromatography Tandem Mass Spectrometry**; Li Qu[1]; Yongjing He[1]; Lizhi Guo[1]; Hongmei Wang[1]; Zhiyu Li[1]; Lili Xing[1]; Yi Tao[1]; Liang Shen[1]; *[1]WuXi AppTec, Shanghai, China*

TP 214 **Evaluating Whole Blood Stability of Lipid Nanoparticles Using LC-MS for Accurate Pharmacokinetic Profiling**; Erika Van Andel[1]; Kellen DeLaney[1]; Ling Morgan[1]; Kelin Wang[1]; *[1]Moderna Tx, Cambridge, MA*

TP 215 **Development of a combined proteomic-machine learning platform for the identification of new therapeutical approaches**; Vittoria F Borrini[1]; Shahzaib Khoso[2]; Denise Marradi[2]; Valeria Caneparo[2]; Francesco Dondero[1]; Marcello Manfredi[2]; *[1]University of Piemonte Orientale, Alessandria, Italy; [2]University of Piemonte Orientale, Novara, Italy*

TP 216 **DEVELOPMENT OF 'PVCap-co-Aam' POLYMERIC MATRIX FOR EFFICIENT BIOANALYSIS: A COST-EFFECTIVE APPROACH FOR ANALYTE EXTRACTION, STABILITY, AND STORAGE FROM BIOLOGICAL SAMPLE**; Nasir Khan[1]; Pinaki Sengupta[1]; Akshay Srivastava[1]; *[1]National Institute of Pharmaceutical Education and Research, Ahmedabad (NIPER-A),, Gandhinagar, India*

TP 217 **Polyethylene glycol (PEG)-8k and PEG-20k quantitation in plasma from a preclinical porcine model of lethal hemorrhagic shock**; Maria Lasaosa[1]; Martin J Mangino[2]; Melissa Morgan[2]; Laerissa Reveill[2]; Matthew S Halquist[1]; *[1]Virginia Commowealth University, Richmond, VA; [2]Virginia Commonwealth University, Richmond, VA*

TP 218 **Developing a Robust Pipeline for Identifying Druggable Aspects of Proteins Implicated in Brain Research Using Mass Spectrometry Data**; Sanjeeva Srivastava[1]; Ankit Halder[2]; Deeptarup Biswas[2]; Sabyasachi Samantaray[2]; Sahil Barbade[2]; Aditya Gupta[2]; *[1]IIT Bombay, Mumbai, India; [2]Indian Institute of Technology Bombay, Mumbai, India*

TP 219 **A Robust Method for Detection of Covalent Drugs in Mouse Blood**; Xiaodie Zhu[1]; Li Gao[1]; Yanfu Ren[1]; Zhiyu Li[2]; Lili Xing[2]; Yi Tao[2]; Liang Shen[2]; *[1]WuXi AppTec (Suzhou), Suzhou, China; [2]WuXi AppTec, Shanghai, China*

TP 220 **Inhibition of carboxylesterase activity in rodent plasma: Implications for the clinical interpretation of chlorogenic acid pharmacokinetics**; Hye-Jin Jo[1]; Min-Gyu Kim[1]; Yeon-Su Jang[1]; Ju-Hyun Kim[1]; *[1]Yeungnam University, Gyeongsan-si, South Korea*

TP 221 **Screening Novel Potentially Antiviral Peptides and Evaluating Host Environment-mediated Breakdown**; Joshua D Breidenbach[1]; Shepard Moore[1]; Alba Montoya[1]; Brian Jun[1]; Jennifer Harris[1]; Jurgen Schmidt[1]; Brett R. Blackwell[1]; Madison Grace Thornhill[1]; Trevor G. Glaros[1]; Tyler Reddy[1]; Karissa Sanbonmatsu[1]; *[1]Los Alamos National Laboratory, Los Alamos, NM*

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TP 222 **Challenges with the Bioanalysis of esterase Pro-drugs and their Active Pharmaceutical Ingredients**; Khyati S Shah; *Glaxosmithkline, Collegeville, PA,19426*

TP 223 **Disulfide bond stability – a critical factor for PK and PD profiles of insulins**; Christian Cramer[1]; Jeppe Sturis[1]; Hans Helleberg[1]; Christian Lehn Brand[1]; František Hubálek[1]; *[1]Novo Nordisk A/S, Maaloev, Denmark*

TP 224 **Quantification of Free, Encapsulated, and Total Doxorubicin in Dog Plasma by LC-MS/MS: Using a Stabilizer to Enhance Liposome Stability**; Wangwei Guo[1]; Gongming Luo[2]; Xiaoying Jin[3]; Lan Li[4]; *[1]WuXi AppTec, Suzhou, China; [2]WuXi AppTec, Chengdu, China; [3]WuXi AppTec (Suzhou), Suzhou, China; [4]WuXi AppTec, Shanghai, China*

TP 225 **Optimizing an immunoprecipitation mass-spectrometry workflow for enrichment of surface proteins: applications to surrogate CAR-T cells**; Nicolle Serrano; *Novartis, Cambridge, MA*

TP 226 **A High-throughput Targeted Mass Spectrometry Assay for Covalent Library Screening**; Yanyan Qu[1]; Yuhong Fang[1]; Christopher A. LeClair[1]; Dingyin Tao[1]; *[1]National Center for Advancing Translational Sciences (NCATS), Rockville, MD*

TP 227 **ThermoTargetMiner: a thermal proteome solubility database for identification of protein targets of novel agents against lung cancer**; Hezheng Lyu[1]; Hassan Gharibi[1]; Bohdana Sokolova[1]; Anna Voiland[2]; Brady Nilsson[1]; Zhaowei Meng[1]; Massimiliano Gaetani[1]; Amir Ata Saei[1]; Roman A. Zubarev[1]; *[1]Karolinska Institutet, Solna, Sweden; [2]The French National Institute for Industrial Environment and Risks (Ineris), Verneuil-en-Halatte, France*

TP 228 **COOKIE-Pro: Covalent Inhibitor Binding Kinetics Profiling on the Proteome Scale**; Hanfeng Lin[1]; Jin Wang[1]; *[1]Baylor College of Medicine, Houston, TX*

TP 229 **Ligand Identification for orphan GPCRs using affinity selection mass spectrometry**; Thuy Duong Nguyen[1]; Haruka Sakai[1]; Hiroki Tanabe[1]; Naoko Nomura[1]; Masaharu Nakayama[1]; Naoki Tarui[1]; *[1]SEEDSUPPLY INC., 26-1, Muraoka-Higashi 2-Chome Fujisawa, Kanagawa 251-0012, Japan*

TP 230 **Differentiating isomeric pneumococcal polysaccharides by using partial chemical degradation followed by mass spectrometry**; Jeremy Manheim[1]; Mingxiang Lin[1]; John Kong[1]; Mirlinda Biba[1]; *[1]Merck, Rahway, NJ*

TP 231 **Using Novel RNases to Measure 5' Cap and Poly(A) Tail Modifications during Oligonucleotide Mapping LC-MS of mRNA**; Bala Addepalli[1]; Tatiana Johnston[2]; Catalin E Doneanu[2]; Alexandre Gomes[2]; Christian Reidy[2]; Ying Qing Yu[2]; Matthew Lauber[2]; *[1]Waters Corp, Milford , MA; [2]Waters Corporation, Milford, MA*

TP 232 **Calculating Extinction Coefficients for Antibodies, Linker-Payloads, and ADCs Using LC-MRM and Nanodrop UV280, Streamlines Pre-Clinical R&D Characterization for Antibody-Drug Conjugates**; Dominick Yeo[1]; Jesus Aguilar[1]; Robyn Barfield[1]; Maxine Bauzon[1]; Allison Benger[1]; Xiao Cai[1]; James Cassidy[1]; Stepan Chuprakov[1]; Penelope Drake[1]; Ryan Kim[1]; Thomas Linz[1]; Kevin Nganga[1]; Alyssa Occiano[1]; Ayodele Ogunkoya[1]; Dharmaraj Samuel[1]; Ana Santandreu[1]; Matthew Smith[1]; Adam Tencer[1]; Tiffany Unsulangi[1]; Jia Yang[1]; Anna Zawadzka[1]; Fangjiu Zhang[1]; *[1]Catalent Pharma Solutions, Emeryville, CA*

TP 233 **Screening and Identification of Traditional Chinese Medicine Compounds as inhibitors of SARS-CoV-2 3CL Protease Using C18 plates and MALDI-TOF-MS**; Chia-Hsin Lee[1]; Chao-Jung Chen[1]; *[1]China Medical University, Taichung, Taiwan*

TP 234 **Multiplexed Cellular Protein Binding Assays of Lanthanide-Labelled Ligands by ICP-MS**; Samuel Barritt[1]; Shimin Wang[1]; Scott Tria[1]; Jon Goodwin[1]; Nick Pullen[1]; Wendy Picariello[2]; MaryRose Steed[2]; Terryl Fritz[2]; Can C Ozbal[2]; *[1]Artbio, Cambridge, MA; [2]Momentum Biotechnologies, Billerica, MA*

TP 235 **Unveiling Structural Complexity: 2D-LC-MS Applications for mAb-like Biotherapeutic Modalities**; Olivia K. Huffman[1]; Koyuki Takenaka[1]; Joomi Ahn[1]; *[1]Eli Lilly & Co, San Diego*

TP 236 **Comprehensive Investigation on Degradation Pathways of Docetaxel and the Protective Role of Carvacrol Oil for Enhanced Stability and Therapeutic Potential**; GOGIKAR SHIVA KUMAR; *National Institute of Pharmaceutical Education And Research (NIPER) University in Hyderabad, Telangana, Hyderabad, India*

TP 237 **Development of a High-Throughput Drug Discovery Assay Combining DESI-MS and MagMASS**; Gee Yin Bryan Wong[1]; Elmeri Latvanen[1]; Elizabeth Want[1]; Zoltan Takats[1]; Lauren Ford[1]; *[1]Imperial College London, London, United Kingdom*

TP 238 **Deep proteomic screening platform for targeted protein degradation drug discovery**; Jessica Wohlfahrt[1]; Martin Steger[2]; Uli Ohmayer[2]; Bachuki Shashikadze[2]; Björn Schwalb[2]; Katrin Hartinger[3]; Zuzana Demianova[3]; Garwin Pichler[3]; *[1]PreOmics, Billerica, MA; [2]NEOsphere Biotechnologies GmbH, Planegg, Germany; [3]PreOmics, Planegg/Martinsried, Germany*

TP 239 **AI-driven absolute quantification of polar metabolites for screening metabolic perturbations in pancreatic meta cells induced by incretin mimetic exposure**; Kathy Wei[1]; Baljit K. Ubhi[2]; Jack Howland[2]; Tim Riley[1]; *[1]310.ai, San Francisco, CA; [2]Matterworks, Somerville, MA*

TP 240 **LC-MALDI-MS Offline Approach for Non-traditional Biologics in the Discovery Space**; Elizabeth F Bayne[1]; Zhuo Gao[1]; Yuan Jiang[1]; Raffeal Bennett[1]; Erik L. Regalado[2]; Gregory F. Pirrone[1]; Alexey A. Makarov[1]; *[1]Merck & Co., Inc., Boston, MA; [2]Merck & Co., Inc., Rahway, NJ*

TP 241 **High-Throughput LC-MS/MS Method for the Quantification of 64 Common Cardiovascular Drugs and their Metabolites Across 10,000 Human Plasma Samples**; Isabelle St-Jean[1]; Martin Jutras[1]; Jean-Claude Tardif[2, 3, 4]; Marie-Pierre Dubé[2, 3, 4]; Grégoire Leclair[1, 5]; Simon De Denus[3, 4, 5]; *[1]Platform of Biopharmacy, Université de Montréal, Montreal, QC; [2]Faculty of Medicine, Université de Montréal, Montreal, Qc; [3]Montreal Heart Institute, Montreal, QC; [4]Université de Montréal Beaulieu-Saucier Pharmacogenomics Center, Montreal, Qc; [5]Faculty of Pharmacy, Université de Montréal, Montreal, Qc*

TP 242 **Development of a Quantitative LC-MS/MS Method for 15 Antidiabetic Compounds in Volumetric Absorptive Microsampling (VAMS) with QTRAP 6500+**; Louiza Mahrouche[1]; Martin Jutras[2]; Isabelle St-Jean[2]; Jean-Claude Tardif[3, 4, 5]; Marie-Pierre Dubé[4, 5, 6]; Grégoire Leclair[2]; *[1]Platform of Biopharmacy / Université de Montréal, Montreal, QC; [2]Platform of Biopharmacy / University of Montreal, Montreal, QC; [3]Faculty of Medicine/ Université de Montréal, Montreal, Qc; [4]Montreal Heart Institute, Montreal, QC; [5]Université de Montréal Beaulieu-Saucier Pharmacogenomics Center, Montreal, Qc; [6]Faculty of Medicine, Montreal, Qc*

TP 243 **Development of polyHis-targeting PROTAC degraders**; Dong Zhu[1]; Hui Chen[2]; Guangrong Zheng[2]; Dongwen Lv[1]; *[1]Department of Biochemistry and Structural Biology and Center for Innovative Drug Discovery, School of Medicine, University of Texas Health Science Center at San Antonio, San Antonio, TEXAS; [2]Department of Medicinal Chemistry, College of Pharmacy, University of Florida, Gainesville, Florida*

TP 244 **TACTICIAN: A Hierarchical Linear Model for Identifying Functional Hits, Target Engagement, and Combined Hits in Proteomics-Driven Drug Discovery**; Lillian T.A. Tatka[1]; Sebastian J. Paez[1]; Lindsay K. Pino[1]; Alexander J. Federation[1]; William E. Fondrie[1]; *[1]Talus Bioscience, Seattle, WA*

TP 245 **Implementation of SFC-MS/MS for Chiral Quantitation in Regulated Bioanalysis**; Zhihui Zhang; *Bristol Myers Squibb, Princeton, NJ*

TP 246 **Unveiling the Hidden: Liraglutide Oligomerization Pathways via Direct Mass Technology, Electron-Capture Dissociation, and Molecular Dynamics**; Syuan-Ting Kuo[1]; Zhenyu Xi[1]; Xiao Cong[2]; Xin Yan[1]; David H Russell[1]; *[1]Texas A&M, College Station, TX; [2]Boehringer Ingelheim, Ridgefield, CT*

TP 247 **Polyethyleneimine-Modified Spongy Monoliths for Improved Lipid Nanoparticle Characterization in Nucleic Acid Therapeutics**; Brady W Drennan[1]; Phat Dinh[1]; Rebecca L Taylor[2]; Kevin A Schug[2]; *[1]University of Texas at Arlington, Arlington, TX; [2]University of Texas at Arlington, Arlington*

TP 248 **High-Throughput Data-Independent Acquisition Mass Spectrometry Workflow for In-Depth Identification of Protein Ubiquitination Using an Orbitrap Astral Mass Spectrometer**; Kevin Yang[1]; Mukesh Kumar[2]; Alissa Nelson[2]; Kathryn Abell[2]; Anthony P. Possemato[2]; Matthew P. Stokes[2]; Sean A Beausoleil[2]; Brett Larsen[1]; Amirmansoor Hakimi[1]; Tonya Pekar Hart[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Cell Signaling Technology, Danvers, MA*

TP 249 **High-throughput PROTAC compound screening workflow for targeted protein degradation on an Orbitrap Astral mass spectrometer with accurate label-free quantitation**; Kevin Yang[1]; Hanfeng Lin[2]; Helen Sun[1]; Brett Larsen[1]; Amirmansoor Hakimi[3]; Tonya Pekar Hart[1]; Jin Wang[2]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Baylor College of Medicine, Houston, TX; [3]Thermo Fisher Scientfic, San Jose, CA*

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TP 250 **Thermal Decomposition Products of Representative Per- and Polyfluoroalkyl Substances (PFAS) Explored with Thermal Desorption and Pyrolysis Mass Spectrometry**; Katerina Litvanova[1]; Bethany Klemetsrud[1]; Alena Kubatova[1];

Feng Xiao[2]; *[1]University of North Dakota, Grand Forks, ND; [2]University of Missouri, Columbia, Missouri*

TP 251 **Environmentally Friendly Implementation of EPA 8270E by Solid-Phase Extraction and Hydrogen as Carrier Gas for GC/MS Analysis**; Arielle Cocozza; *UCT, Bristol, PA*

TP 252 **A direct in-situ MALDI-TOF MS technology for rapidly detecting and identifying biological warfare agents**; Young-Su Jeong[1]; Sang-Soo Han[1]; Young Jin Koh[1]; *[1]Agency for Defense Development, Daejeon, South Korea*

TP 253 **Intracellular metabolites of mammalian cells exposed to low concentration of persistent organic pollutants**; Sam Li; *National University of Singapore, Singapore, Singapore*

TP 254 **Analysis of Iodinated Acetic Acids by Direction Injection Liquid Chromatography Tandem Mass Spectrometry in Finished Water**; Rebecca Trenholm[1]; Brett Vanderford[1]; Eric Dickenson[1]; *[1]Southern Nevada Water Authority, Las Vegas, NV*

TP 255 **Machine learning-assisted recognition of sulfur-containing chemicals in high-resolution mass spectrometry of 30,000 mass resolution**; Brian Low[1]; Tingting Zhao[1]; Xing-Fang Li[2]; Tao Huan[1]; *[1]University of British Columbia, Vancouver, BC; [2]University of Alberta, Edmonton, AB*

TP 256 **Characterizing PFAS in cosmetic products using non-targeted acquisition**; Craig Butt[1]; Mikyanny Reyes[2]; Holly Lee[3]; Keegan Harris[4]; Amy Rand[4]; *[1]SCIEX, Framingham, MA; [2]SCIEX - Framingham, MA, Framingham, MA; [3]SCIEX, Concord, ON; [4]Carleton University, Department of Chemistry, Ottawa, ON*

TP 257 **Differentiating PFAS Isomers: A Multi-Pass Cyclic Ion Mobility Mass Spectrometry Approach for Detection, Identification, and Relative Quantitation**; Sarah Dowd[1]; Lindsay Hatch[1]; Michael McCullagh[2]; Jennifer Marciano[3]; Punam Oza[3]; *[1]Waters Corporation, Milford, MA; [2]Waters Corporation, Wilmslow, United Kingdom; [3]The Public and Environmental Health Laboratory, Suffolk County Department of Health, Hauppauge, NY*

TP 258 **Novel Breath Sampling Devices for the Detection and Quantification of Respiratory Per- and Polyfluoroalkyl Substances (PFAS)**; Elijah A Bliss[1]; Peter Stambeck[2]; Jack Henion[3]; Kara M. Joseph[1]; James Dodds[1]; Erin S. Baker[1]; *[1]University of North Carolina at Chapel Hill, Chapel Hill, NC; [2]Munkplast AB, Uppsala, Sweden; [3]Advion Interchim Scientific, Ithica, NY*

TP 259 **Non-targeted analysis of PFAS and legacy pollutants in dust using multidimensional chromatography, high-resolution mass spectrometry, and scaled mass defect plots**; David E Alonso[1]; Joe Binkley[1]; *[1]Leco Corporation, St. Joseph, MI*

TP 260 **HPLC-21T FT-ICR MS and Mass Difference Analysis for Ultra-Complex Emerging Contaminants: Expanding Molecular Coverage and Structural Insights**; Martha Liliana Chacón-Patiño[1]; Lissa C. Anderson[1, 2]; Joseph W. Frye-Jones[3]; Teja Potu[2]; Christopher Holder-Montenegro[2]; Alvaro J. Tello-Rodríguez[2]; Germain S. Vallverdu[4]; Christopher L Hendrickson[1, 2]; Nathan K. Kaiser[1]; Chad R. Weisbrod[1]; Pierre Giusti[5]; Ryan P Rodgers[1, 2]; *[1]National High Magnetic Field Laboratory, Tallahassee, FL; [2]Florida State University, Tallahassee, FL; [3]Woods Hole Oceanographic Institution (WHOI), Falmouth, MA 02543; [4]IPREM, Universite de Pau et des Pays de l'Adour, Pau, France; [5]TotalEnergies Research and Technology Gonfreville, Harfleur, France*

TP 261 **Differences in composition of organics extracted from seawater from three hydrographic regions measured using liquid chromatography and high-resolution mass spectrometry**; Amber E Birt[1]; Daniel Ammer[1]; Felix E Agblemanyo[2]; Andrew S Wozniak[2]; Amanda A Frossard[1]; *[1]University of Georgia, Athens, GA; [2]University of Delaware, School of Marine Science and Policy, Lewes, Delaware*

TP 262 **Structural Characterization of DOM using TIMS-FT ICR MS/MS and Machine Learning**; Pablo R Batista Oliveira[1, 2]; Lilian Valadares Tose[1]; Kevin Jeanne Dit Fouque[1]; Bilal Shabbir[3]; David P A Kilgour[4]; Fahad Saeed[2, 3]; Francisco Fernandez-Lima[1, 2]; *[1]Department of Chemistry and Biochemistry, Florida International University, Miami, FL; [2]Institute of Environment, Florida International University, Miami, FL; [3]School of Computing and Information Science, Florida International University, Miami, FL; [4]Vibrat-Ion Ltd, Aberystwyth, United Kingdom*

TP 263 **Current LC/MS Approaches for PFAS Analysis with Ultrashort and Long Chain Mixtures** ; Conner McHale[1]; Barry Boyes[1]; *[1]Advanced Materials Technology, Wilmington, DE*

TP 264 **Comprehensive non-targeted analysis of perfluoroalkyl substances in complex AFFF formulations and AFFF-impacted soils**; Richard E. Cochran[1]; Sarah Choyke[2]; Collin Meyers[2]; Ralf Tautenhahn[3]; *[1]Thermo Fisher Scientific, Bannockburn, IL; [2]Eurofins Environment Testing, Denver, CO; [3]Thermo Fisher Scientific, San Jose, CA*

TP 265 **Targeted Analysis of Per- and Polyfluoroalkyl Substances in Natural Water Sources of Ecuador**; Khoa Huan Nguyen[1]; Brandie M Ehrmann[1]; Valeria Ochoa-Herrera[1, 2]; *[1]University of North Carolina at Chapel Hill, Chapel Hill, NC; [2]Universidad San Francisco de Quito, Quito, Ecuador*

TP 266 **Fast quantification method for polychlorinated alkanes in oil, oilseed, and presscake samples using quadrupole Time-Of-Flight Mass Spectrometry**; Jonatan Nygren[1]; Jakob Hauns[2]; Franz Hansert[2]; Sascha Rexroth[3]; Ron Hail[4]; Sicco Brandsma[5]; Pim Leonards[5]; Jeroen Kool[1]; Alexander Schächtele[2]; *[1]Department of Chemistry and Pharmaceutical Sciences, Vrije Universiteit, Amsterdam, Netherlands; [2]European Union Reference Laboratory for PCBs and Dioxins in Feed and Food (EURL POPs), Freiburg, Germany; [3]Shimadzu Europe GmbH, Duisburg, Germany; [4]Shimadzu Deutschland GmbH, Duisburg, Germany; [5]Department of Environment and Health (E&H), Vrije Universiteit, Amsterdam, Netherlands*

TP 267 **Surface-bound disinfection byproducts from multiphase hypochlorous acid reactions with phenolic compounds found in wood smoke**; Christina Y Clarke[1]; Douglas B Collins[1]; *[1]Bucknell University, Lewisburg, PA*

TP 268 **Cyclosiloxane artifacts from GC-MS Yield False Henry's Law Constants for Nonvolatile Fluorotelomer Sulfonates**; Sophia Nelson[1]; Mitchell Kim-Fu[1]; Mohammad Azizian[1]; Jennifer Field[1]; *[1]Oregon State University, Corvallis, OR*

TP 269 **Advanced detection of PFAS in water beyond current regulations using UHPLC Trapped-Ion-Mobility QTOF MS**; David Liwara[1]; Carsten Baessmann[2]; Birgit Schneider[2]; Ilona Nordhorn[2]; Arnd Ingendoh[2]; Pim Leonards[1]; Sicco Brandsma[1]; *[1]Amsterdam Institute for Life and Environment (A-LIFE), Vrije Universiteit Amsterdam, Amsterdam, Netherlands; [2]Bruker Daltonics GmbH & Co. KG, Bremen, Germany*

TP 270 **EPA 537.1 and 533 with the Novel LCMS-8050RX: Demonstration of Instrument and Method Performance to meet PFAS regulatory levels**; Ethan R Hain[1]; Lihini Mendis[1]; Sarah A. Monti[1]; Valeria Zerda-Pinto[1]; Ruth Marfil-Vega[1]; Landon Wiest[1]; Christopher T. Gilles[1]; *[1]Shimadzu Scientific Instruments, Columbia, MD*

TP 271 **Real-time detection of PFAS for industrial applications**; Spiro Jorga[1]; Maya Abou-Ghanem[1]; Michael Groessl[2]; Veronika Pospisilova[1]; *[1]TOFWERK, Thun, Switzerland; [2]Tofwerk, Thun, Switzerland*

TP 272 **Practical approaches to address the analytical challenges of PFAS analysis by LC-MS**; Matthew James[1]; Arianne Soliven[1]; Tony Edge[1, 2]; Gemma Lo[1]; Helen Poole[1]; Geoff Faden[3]; *[1]Avantor, Theale, United Kingdom; [2]University of Liverpool, Liverpool, United Kingdom; [3]MAC-MOD Analytical, Chadds Ford, PA*

TP 273 **Improving Nontargeted Analysis of PFAS in Aqueous Environmental Samples**; Erika P Portero[1]; Lam Leung[1]; *[1]The Chemours Company, Newark, DE*

TP 274 **Detection of VOCs by Agilent 8697 Headspace with 7010D GC/MS/MS Using Hydrogen Carrier Gas**; Erinn M

O'Neill[1]; Alexis Willey[2]; *[1]Agilent Technologies, Wilmington, DE; [2]Agilent Technologies, Inc., Wilmington, Delaware*

TP 275 **Identification of Per- and Polyfluoroalkyl Substances Hotspots in Surface Water collected along the Mississippi coastline**; Isabella S Cioffi[1]; John A Bowden[2]; Lauren E Blackman[2]; Jennifer DeBose[3]; Jack P Arnold[2]; *[1]University of Florida, Gainesville, FL; [2]University of Florida, Gainesville, Florida; [3]Grand Bay National Estuarine Research Reserve, Moss Point, MS*

TP 276 **Analysis of 40 Per- and Polyfluoroalkyl Substances in Sand, Soil, Sediment, Biosolid and Fish Samples by US EPA Method 1633**; Jingcun Wu[1]; Autumn Payne[2]; Jacob Jalali[2]; *[1]PerkinElmer Inc., Woodbridge, ON; [2]PerkinElmer Inc., Shelton, CT*

TP 277 **The Influence of Mixtures on the Reactivity of Fatty Acids when Exposed to Chlorine Bleach Vapor**; Lauren Stettler[1]; Ryan Ziskin[1]; Douglas Collins[1]; *[1]Bucknell University, Lewisburg, PA*

TP 278 **Monitoring Explosive Contaminants in Cultivated Plants: Development of Rapid LC-MS/MS Techniques**; Inga Sowik[1]; Lena Ruzik[1]; *[1]Warsaw University of Technology, Warsaw, Poland*

TP 279 **Retrospective analysis of PFAS using sediment cores along the vulnerable coastline of Mississippi**; Lauren E Blackman[1]; Isabella S Cioffi[2]; Alina S Timshina[2]; Jennifer DeBose[3]; John A Bowden[2]; *[1]University of Florida, Gainesville, FL; [2]University of Florida, Gainesville, Florida; [3]Grand Bay National Estuarine Research Reserve, Moss Point, MS*

TP 280 **Optimizing complementary fluorine-based workflows: Targeted tandem mass spectrometry and total fluorine to characterize known and “total potential PFAS” in compost**; Alina Timshina[1]; Esmee Belzer[2]; Lauren E Blackman[1]; Jack P Arnold[1]; Graham Peaslee[2]; John A Bowden[1]; *[1]University of Florida, Gainesville, Florida; [2]University of Notre Dame, Notre Dame, IN*

TP 281 **Combination of bubble-based preconcentration and SALDI for rapid PFAS detection**; Chuping Lee; *Department of Chemistry, National Chung Hsing University, Taichung City, Taiwan*

TP 282 **Structural Characterization of PFAS via Oxygen Attachment Dissociation: A Complementary Approach to CID**; Hidenori Takahashi[1]; Atsuhiko Toyama[1]; *[1]Shimadzu Corporation, Kyoto, Japan*

TP 283 **Quantification of Halo ethers in water by GCMS**; Jessin Mathai[1]; Jenishia Menezes[1]; Anant Lohar[1]; Shailesh Damale[1]; *[1]Shimadzu Middle East & Africa FZE, Dubai, United Arab Emirates*

TP 284 **Comparative Analysis of Air Sampling Strategies for VOC Monitoring using TD-GCMS with chemometrics study to enhance understanding of complex samples**; Praveen Arya[1]; Saurabh Nagpal[1]; Abbey Fausett[2]; Eric Fausett[2]; Kiran Piduru[3]; *[1]Application Engineer, Agilent Technologies, Manesar, India; [2]Application Engineer, Agilent Technologies, Littlefalls, DE; [3]Market Development Specialist, Markes International, Bridgend, United Kingdom*

TP 285 **Measuring the Interfacial Chemistry of Micro- and Nano-Plastics Using Matrix Assisted Laser Desorption Ionization (MALDI) Mass Spectrometry**; Samantha Kruse[1]; Christian A. Pattyn[1]; Andre Benally[1]; Mohammad Shohel[1]; Steven Storch[1]; Jake Zenker[1]; Andres Sanchez[1]; Jess Kustas[1]; Ryan D Davis[1]; *[1]Sandia National Laboratories, Albuquerque, NM*

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TP 286 **A Government Perspective on Pesticide Surveillance and Enforcement: Food and Environmental Analysis**; Deidre Damon; *Ohio Department of Agriculture, Reynoldsburg, OH*

TP 287 **Development of a sensitive LC-MS method for the analysis of NDSRI in rasagiline pharmaceutical products**; Chanhong Min[1]; Han Bin Oh[2]; *[1]Sogang university, Seoul, South Korea; [2]Sogang University, Seoul, South Korea*

TP 288 **Fortified Sample Preparation and LC-MS/MS Enabled Methods for Comprehensive Dicamba Herbicide Analysis in Leaves, Nectar, and Pollen**; Luke M. Collier[1]; Sean Newmister[1]; Joseph Redinger[1]; Elise Kanefsky[1]; Regina Baucom[1]; David H. Sherman[1]; *[1]University of Michigan, Ann Arbor, MI*

TP 289 **Quantifying Antidepressant Medication in Wastewater Effluent Using Liquid Chromatography, Ion Mobility Spectrometry, and Mass Spectrometry Separations**; Emily K Crawford[1]; Erin S. Baker[1]; *[1]University of North Carolina at Chapel Hill, Chapel Hill, NC*

TP 290 **GC-MS/MS Pesticide Analysis of Cambodian Waters**; Reagan Guerra[1]; Melissa Lenczewski[2]; Khy Eam Eang[3]; Justin Lafser[4]; Kevin Tucker[1]; *[1]Southern Illinois University Edwardsville, Edwardsville, IL; [2]Northern Illinois University, Dekalb, IL; [3]Institute of Technology of Cambodia, Phnom Penh, Cambodia; [4]Shimadzu Scientific Instruments, Columbia, MD*

TP 291 **HPLC-MS/MS Analysis of Antibiotics and Sunscreens in International Waters**; Noah Hanratty[1]; Boonyarak Chuanchit[2]; Vanessa Tsang[3]; Reagan Guerra[1]; Nevannah Harlan[1]; Chit Wityi Oo[2]; Melissa Lenczewski[2]; Kevin Tucker[1]; *[1]Southern Illinois University Edwardsville, Edwardsville, IL; [2]Northern Illinois University, Dekalb, IL; [3]Denison University, Granville, OH*

TP 292 **Combined targeted, DIA, and imaging approach to analysis of pharmaceutical prevalence in wastewater effluent and affected plants**; Claire E. Korte[1]; Chloe I. Koons[1]; Reagan H. Guerra[1]; Noah E. Hanratty[1]; Sarah A. Monti[2]; Kevin R. Tucker[1]; *[1]Southern Illinois University Edwardsville, Edwardsville, IL; [2]Shimadzu Scientific Instruments, Columbia, MD*

TP 293 **Innovative Integration of LC-HRMS and In-Silico Libraries for Pharmacetical Metabolite Annonationand MALDI-HRMS Spatial Residue Analysis in Environmental Samples**; Jan Fučík[1]; Stanislav Fučík[2]; Jarošová Rea[3]; Sascha Rexroth[4]; Andreas Baumeister[4]; Ann-Christin Niehoff[4]; Marie Hamplová[1]; Jitka Navrkalová[1]; Helena Zlámalová Gargošová[1]; Ludmila Mravcová[1]; *[1]Institute of Chemistry and Technology of Environmental Protection, Faculty of Chemistry, Brno University of Technology, Brno, Czech Republic; [2]Faculty of Electrical Engineering and Communication, Brno University of Technology, Brno, Czech Republic; [3]Veterinary Research Institute Brno, Brno, Czech Republic; [4]Shimadzu Europe GmbH, Duisburg, Germany*

TP 294 **Validated Method for the Determination of 46 Pesticides in Surface, Subterranean, and Wastewater with No Pre-concentration**; Monique F. Dos Santos[1]; Marilia S. Cardoso[1]; Luis O Junqueira[1]; Marcos A Pudenzi[1]; Ichiro Hirano[1]; *[1]Shimadzu Brasil, Barueri, Brazil*

TP 295 **From Prescription to Pollution: The Accumulation of Antidepressants in Crawfish**; Sydney R. Worth[1]; Claire E. Korte[1]; Jillian R. Tonnies[1]; Jenna R. Williamson[1]; Jeffrey A. Licklider[1]; Cassandra E. Stirling[1]; Kevin R. Tucker[1]; *[1]Southern Illinois University Edwardsville, Edwardsville, IL*

TP 296 **Combined GC-LC-MSMS using DBDI to Analyse both GC-Labile and LC-Labile Pesticides Simultaneously**; Ciara Conway[1, 2]; Markus Weber[1, 2]; Jan-Christoph Wolf[1]; Christoph Haisch[2]; Thomas Wolf[1]; *[1]Plasmion, Augsburg, Germany; [2]Technical University of Munich, Garching, Germany*

TP 297 **Determination of Pesticides in Tap Water without Pretreatment by LC-MS/MS**; Monique F. Dos Santos[1]; Marilia S. Cardoso[1]; Luis O. Junqueira[1]; Marcos A Pudenzi[1]; Ichiro Hirano[1]; *[1]Shimadzu do Brasil, Barueri, Brazil*

TP 298 **MRM profiling and solid-phase extraction as first-pass screening to evaluate the occurrence of antibiotics and pesticides in environmental samples**; Karen Chibana Ferreira[1]; João Pedro Da Silva[1]; Eduardo L Rossini[1]; Christina R Ferreira[2]; Paulo Clairmont F. Lima Gomes[1]; *[1]Sao Paulo State University, Araraquara, Brazil; [2]Purdue Univeristy, West Lafayette, IN*

TP 299 **Rapid and Quantitative Detection of Nitrosamines in Pharmaceuticals Using Headspace-SIFT-MS**; Akeema Onalaja[1]; Finlay, Juby Mathew And William Pelet Aitcheson[2]; Juby Matthew[2]; William Pelet[2]; *[1]Syft Technologies, Anaheim, CA; [2]Syft Technologies, Inc., Anaheim, CA*

TP 300 **Antibiotic monitoring in soils from organic and intensive olive cultivars in the Mediterranean basin by LC-MS/MS**; Andrés J. Rascón[1, 2]; David Moreno-González[1, 2]; Bienvenida Gilbert-López[1, 2]; Juan F. García-Reyes[1, 2]; *[1]University of Jaen, Jaen, Spain; [2]University Institute of Research on Olive and Olive Oils (INUO), Jaen, Spain*

TP 301 **Quantitation of AcetaldehydeEthylene Oxide, 2-Chloroethanol, Ethylene Glycol, 1,4-Dioxane & Diethylene Glycolin PEG 3350 by using dynamic headspace GC-MS/MS**; Sanket Anand Chiplunkar[1]; Hemant Bhikaji Kesarkar[1]; Prashant Dattatray Hase[1]; Durvesh Prabhakar Sawant[1]; Rahul Dwivedi[1]; Satyendra Singh[2]; Mohit Sharma[2]; Jitendra Kelkar[1]; Pratap Rasam[1]; Dheeraj Handique[1]; *[1]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India; [2]Shimadzu Analytical (India) Pvt. Ltd., New Delhi, India*

TP 302 **Machine-Learning Driven Non-targeted Mass Spectrometry Approach for Pesticide Screening in Sri Lankan Drinking Water Samples**; Fiona Q Zabel[1]; Adam Graichen[2]; Rohana Chandrajith[3]; Ishara Athauda[3]; Dhananjalee Mahalekam[3]; Nishad Jayasundara[4]; Shuchi Anand[5]; Penny Vlahos[2]; *[1]University of Connecticut, Storrs, CT; [2]University of Connecticut, Storrs; [3]University of Peradeniya, Peradeniya, Sri Lanka; [4]Duke University, Durham, NC; [5]Stanford University, Stanford, CA*

TP 303 **Development of an HILIC-MS/MS method for the monitoring of polar pesticides in olive grove soils of the Mediterranean basin**; Alfonso Fernández-García[1, 2]; Andrés J. Rascón[1, 2]; Ana B. Martínez-Piernas[1, 2]; David Moreno-González[1, 2]; Bienvenida Gilbert-López[1, 2]; Juan F. García-Reyes[1, 2]; *[1]University of Jaén, Analytical Chemistry Research Group, Jaén, Spain; [2]University Research Institute for Olives Grove and Olive Oil (INUO), Jaén, Spain*

TP 304 **Regioselective gas-phase ion-molecule reactions of protonated polyfunctional aromatic compounds with 2-methoxypropene**; Razieh Zamani[1]; Annika M. Little[2]; Hilkka I. Kenttämaa[2]; *[1]Purdue University, West Lafayette, IN; [2]Purdue Univeristy, West Lafayette, IN*

TP 305 **Multi-residue Analytical Method for the Confirmation and Quantification of500+ Pesticides in Fruit and Vegetables** ; Autumn Payne[1]; Jesse Leonard[1]; Victor Cai[1]; Jacob Jalali[1]; *[1]PerkinElmer Inc., Shelton, CT*

TP 306 **In depth characterization of complex PFAS samples using rapid screening, suspect screening, and non-targeted RPLC-HRIM-MS strategies**; Emanuel Zlibut[1]; Miriam Fico[1]; Frederick G. Strathmann[1]; *[1]Mobilion Systems Inc., Chadds Ford, PA*

TP 307 **Dual ESI/APCI StayClean Ion Source LC-MS/MS for Analysis of Near 400 Polar and Non-polar Pesticide Residues in Tea**; Sheng-Suan (Victor) Cai[1]; Autumn Payne[1]; Jesse Leonard[1]; Jacob Jalali[1]; *[1]PerkinElmer US, LLC, Shelton, CT*

TP 308 **Insight into the Influence of Statins on Earthworm (Eisenia hortensis) Metabolism by GC-MS Metabolomics and MALDI Mass Spectrometry Imaging**; Violet J Marrs[1]; Kendra G Selby[2]; Kevin R. Tucker[1]; *[1]Southern Illinois University - Edwardsville, Edwardsville, IL; [2]University of Wisconsin-Madison, Madison, WI*

TP 309 **Examining the Spatial Distribution of Benzalkonium Chloride and Altered Lipid Profiles in Mouse Kidneys**; Marie Brzoska[1]; Ryan P. Seguin[1]; Vanessa Lopez[2]; Sydney Arnzen[1]; Libin Xu[1]; *[1]University of Washington, Seattle, WA; [2]University of Washington - Seattle, WA, Seattle, WA*

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TP 310 **The next frontier in extractable screening analyses: Increased identification confidence provided by a benchtop multi-reflecting time-of-flight mass spectrometer**; Rachel J Sanig[1]; Hernando J. Olivos[2]; Lee Gethings[1]; Jayne Kirk[1]; Richard Lock[1]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Waters Corp., Milford, MA*

TP 311 **Comprehensive Profiling of PFAS from Neat Fluoropolymers and Plastic Bonded ExplosivesUsing Untargeted LC-MS Analyses**; Austin R. Anderson[1]; Christopher E. Freye[1]; Brooke Baumgarten[1]; *[1]High Explosives Science and Technology Group, Los Alamos National Laboratory, Los Alamos, NM*

TP 312 **PFAS in Bottled Water: A Simple Approach Using HS-SPME GC/MS/MS for Volatile Contaminant Analysis**; Andy Sandy[1]; Dominika Gruszecka[1]; Ruth Marfil-Vega[1]; Evelyn H. Wang[1]; *[1]Shimadzu Scientific Instruments, Columbia, Maryland*

TP 313 **Material Component Libraries and Their Role in Improving Confident Identifications and Semi-quantitation in Extractable and Leachable Analysis**; Michael Rush[1]; Pramod Poudel[1]; Dmitriy Pastarnak[1]; *[1]Edwards Lifesciences, Salt Lake City, UT*

TP 314 **Determination of PFAS in Pharmaceutical Water Used for Development of Injectable Drugs Using a High Speed Triple Quadrupole**; Lucas Lima Zanin[1]; Luis Otavio Junqueira[2]; Marcos Albieiri Pudenzi[2]; Ichiro Hirano[2]; *[1]Shimadzu, Barueri, Brazil; [2]Shimadzu do Brasil, Barueri, Brazil*

TP 315 **Extractable Leachable Analysis Workflow Using MassHunter Explorer 2.0 with NIST and SIRIUS MS/MS Searching for En**; David A Weil[1]; Sierra Durham[1]; James Pyke[1]; Matthew Curtis[1]; *[1]Agilent Technologies, Santa Clara, CA*

TP 316 **Simultaneous targeted, non-targeted PFAS screening as part of extractables screening for pharmaceutical packaging, manufacturing components, and medical device by LC-HRAM-MS**; Chongming Liu[1]; Sven Hackbusch[2]; Rajesh Chennam Shetti[1]; Dujuan Lu[1]; Mark Rogers[1]; Sebastien Morin[3]; Jon Bardsley[4]; *[1]SGS North America Inc., Fairfield, NJ; [2]Thermo Fisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific, Mississauga, ON; [4]Thermo Fisher Scientific, Hemel Hempstead, United Kingdom*

TP 317 **Analysis of extractables and leachables in catheters using accurate mass libraries and high-resolution GC/MS and LC/MS**; Sofia Nieto[1]; David A Weil[1]; Matthew Curtis[1]; *[1]Agilent Technologies, Inc., Santa Clara, CA*

TP 318 **Beyond Aligners: Unmasking Hidden Extractables and Leachables in Orthodontic Devices**; Ronnel Ronnel Azizollahi[1]; Tess Foote[1]; Snehlata Oberoni[1]; Elizabeth Eve[1]; Christine Hong[1]; Ahmed Najar[2]; Sofia Nieto[3]; Kara Lynch[2]; *[1]University of California San Francisco, School of Dentistry, Department of Orthodontics, San Francisco, CA; [2]University of California San Francisco, School of Medicine, Department of Lab Medicine, San Francisco, CA; [3]Agilent Technologies, Inc., Santa Clara, CA*

TP 319 **Characterization of Extractables in Dental Bite Guards using Gas Chromatography and Time of Flight Mass Spectrometry**; Elizabeth Humston-Fulmer[1]; Joseph Binkley[1]; *[1]LECO, St. Joseph, MI*

TP 320 **PFAS Analysis in Aqueous Film-Forming Foams (AFFF) Using a High-Resolution Mass Spectrometer and Newly Integrated Software Suite**; Michael Deible[1]; Vikki Johnson[2]; Logan Miller[3]; Rachel Hale[1]; *[1]RJ Lee Group, Monroeville, PA; [2]Shimadzu Scientific Instruments, Carlsbad, CA; [3]Shimadzu Scientific Instruments, Columbia, MD*

TP 321 **Development of a Targeted LC-MS/MS Method for the Analysis of PFAS in Concrete Matrices**; Logan Miller[1]; Michael Deible[2]; Michael Baker[2]; Rachel Hale[2]; Victoria Johnson[1]; Toshiya Matsubara[1]; *[1]Shimadzu Scientific Instruments, Columbia, MD; [2]RJ Lee Group, Monroeville, PA*

TP 322 **Characterizing small quantities of a nitrogen containing compound from nylon utilizing mass spectrometry and NMR**; Kelsey Alexander[1]; JoAnn Chen[1]; Ramon Verduzco[1]; Peifeng Hu[1]; D. Paul Cole[1]; *[1]Baxter, Roun Lake, IL*

TP 323 **Getting the most out of your Extractables and Leachables LC/MS Analysis with the proposed US FDA**

CDRH CLAP Standard Set; Sierra Durham[1]; David A Weil[1]; *[1]Agilent Technologies, Santa Clara, CA*

TP 324 **Thermal Extraction and Accurate Mass to Increase the Confidence in the Extractables and Leachables Analysis of Catheters**; Matthew Curtis[1]; Sofia Nieto[1]; David A Weil[1]; *[1]Agilent Technologies, Santa Clara, CA*

TP 325 **Adverse Effects of Leachables and Contaminants on Mass Spectrometry-Based Lipidomic Analysis**; Carlos R. Canez[1]; Bowen Yang[1]; Liang Li[1]; *[1]University of Alberta, Edmonton, AB*

TP 326 **Extractable polar organosulfur species from Bennu asteroid**; Bela Reiz[1]; Robert W Hilts[1]; Chris Herd[1]; Randy M. Whittal[1]; *[1]University of Alberta, Edmonton, AB*

TP 327 **A novel untargeted liquid chromatography-high-resolution mass spectrometry method with In-Silico quantitation of Extractables & Leachables from biomanufacturing processes**; Noemi Dorival-Garcia[1]; Anna Mulligan[1, 2]; Charles Felice[3]; Ping-Ping Wang[3]; Aidan Sexton[4]; Jonathan Bones[1, 2]; *[1]The National Institute for Bioprocessing Research and Training (NIBRT), Dublin, Ireland; [2]School of Chemical and Bioprocess Engineering, University College Dublin, Dublin, Ireland; [3]Johnson and Johnson, Malvern, Pennsylvania; [4]Janssen Sciences Ireland, Cork, Ireland*

FUNDAMENTALS: ION MOLECULE, ION/ION, ION/ELECTRON INTERACTIONS

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TP 328 **High Extraction Anode Lens Voltage Increases the Electron Energy Distribution High Energy Tail in Gas Phase Ion-Electron Reactions**; Steven A. DeFiglia[1, 2, 3]; Teresa Lee[1]; Neven N. Mikawy[1, 2, 3, 4]; Carson W. Szot[1]; Kristina Hakansson[2, 3]; *[1]University of Michigan, Ann Arbor, Michigan; [2]Florida State University, Tallahassee, FL; [3]National High Magnetic Field Laboratory, Tallahassee, FL; [4]Ain Shams University, Cairo, Egypt*

TP 329 **Steric Effects in Anion Tandem Mass Spectrometry of Peptides with "Fixed" Negative Charge Tags**; Teresa Lee[1]; Steven A. DeFiglia[1, 2]; Kristina Hakansson[1, 2, 3]; *[1]University of Michigan-Ann Arbor, Ann Arbor, MI; [2]National High Magnetic Field Laboratory, Tallahassee, FL; [3]Florida State University, Tallahassee, FL*

TP 330 **Dendrimers as Molecular Containers for Gas Phase Synthesis**; Alexander M Koers[1]; Scott A. McLuckey[2]; *[1]Purdue University, West Lafayette, IN; [2]Purdue Univeristy, West Lafayette, IN*

TP 331 **A Numerical Approach for Calculating Mass Diffusivity of Molecules and ions in Gas Media Using the Two Temperature Approximation**; Farah Mubas-Sirah[1]; Wiljones Djoutsop[1]; Carlos Larriba-Andaluz[1]; *[1]Purdue Univeristy, West Lafayette, IN*

TP 332 **Evolution of an NO REMPI Laser Plasma - Comparative Study of PIC, Barnes-Hut and FMM Simulations**; Markus Hübner[1]; Walter Wißdorf[1]; Maja Hammelrath[1]; Franziska Schuler[1]; Hendrik Kersten[1]; Thorsten Benter[1]; *[1]University of Wuppertal, Wuppertal, Germany*

TP 333 **Ion Molecule Reactions of [UH]+ and U+ with Haloalkanes to Form [UHX]+ and [UXn]+ (X=Cl, Br, and I) Using PTMSn**; Justin G Terhorst[1]; Samuel Lenze[1]; Theodore A Corcovilos[1]; Michael J Van Stipdonk[1]; *[1]Duquesne University, Pittsburgh, PA*

TP 334 **Controlling the reactivity of Fe complexes on surfaces using ion soft-landing**; Raquel Cericatto Konzen[1]; Hugo Y. Samayoa-Oviedo[2]; Julia Laskin[1]; *[1]Purdue University, West Lafayette, IN; [2]Texas A&M University, College Station, TX*

TP 335 **Ozonolysis of metalated lipids: expanding the isomeric coverage of OzID**; Troy R Scoggins IV[1]; Yingchan Guo[1]; Paul Zerebinski[1]; Boone M Prentice[1]; *[1]Department of Chemistry, University of Florida, Gainesville, FL*

TP 336 **Characterization of Aromatic Imide Functionality in Protonated Analytes by Using Ion-Molecule Reactions in an LQIT Mass Spectrometer**; Michael J Rees[1]; Annika M Little[2]; Hilkka I Kenttamaa[2]; *[1]Purdue University, West Lafayette, IN; [2]Purdue Univeristy, West Lafayette, IN*

FUNDAMENTALS: MOLECULAR MODELING/QUANTUM MECHANICAL CALCULATIONS

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TP 337 **Ion Mobility Resolved Tandem Mass Spectrometry of Drug Protomers**; Amar Rai[1, 2]; Shahd Abuhelal[3]; Stefania Maneta-Stavrakaki[1]; Elizabeth Want[1]; Stephen W. Holman[4]; Andrew D. Ray[5]; Zoltan Takats[1, 2, 6]; Bela Paizs[1, 2, 6]; *[1]Faculty of Medicine, Department of Metabolism, Digestion and Reproduction, Imperial College London, London, United Kingdom; [2]The Rosalind Franklin Institute, Building R113 Rutherford Appleton Laboratory, Harwell Campus, Didcot, United Kingdom; [3]National Heart and Lung Institute, Imperial College London, London, United Kingdom; [4]Chemical Development, Pharmaceutical Technology & Development, Operations, AstraZeneca, Macclesfield, United Kingdom; [5]New Modalities & Parenteral Development, Pharmaceutical Technology & Development, Operations, AstraZeneca, Macclesfield, United Kingdom; [6]deShape Ltd., London, United Kingdom*

TP 338 **Incorporating Charge Movement within Molecular Dynamics Simulations of an Activated Non-Covalent Complex**; Toy Lemmons[1]; Joseph A. Loo[1]; Rachel R. Loo[1]; *[1]UCLA, Los Angeles, CA*

TP 339 **Exploring Liquid-Liquid Phase Separation of Dipeptides by Mass Spectrometry, Condensed-Phase Analysis, and Computational Approaches**; Jenna E Lees[1]; Nwanne Banor[1]; Daniel A Thomas[1]; *[1]University of Rhode Island Department of Chemistry, Kingston, RI*

TP 340 **Rayleigh charge-induced instability in sub-nanometer aqueous clusters charged by a trivalent metal cation and multiple hydroniu**; Styliani Consta[1]; Jihong Shi[1]; *[1]Western University, London, Ontario*

FUNDAMENTALS: NATIVE MS

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TP 341 **Conjugation of Short Chain Fatty Acids to Bicyclic-Amines for Analysis by Liquid Chromatography Tandem Mass Spectroscopy**; Reese B Berger[1]; Daniel N Darlington[1, 2]; *[1]Blood and Shock Research, US Army Institute of Surgical Research, JBSA Fort Sam Houston, TX; [2]Department of Surgery/Trauma and Emergency Surgery, San Antonio, TX*

TP 342 **Mass Spectrometry of Proteins and Protein Complexes Electrosprayed in the Presence of Common Biological Buffers Using Theta Emitters**; Erick G Baez Bolivar[1]; Scott A. McLuckey[1]; *[1]Purdue University, West Lafayette, IN*

TP 343 **Conformational Analysis of Deep Ultraviolet Laser Ablated Proteins: A Combined Circular Dichroism (CD) and Native Ion Mobility-Mass Spectrometry (IM-MS) Study**; Neda Feizi[1]; Maiah Woodring[1]; Kelcey B. Hines[2]; Bismark A. Nyaaba[1]; Jonathan Clinger[1]; Kermit K. Murray[2]; Touradj Solouki[1]; *[1]Baylor University, Waco, TX; [2]Louisiana State University, Baton Rouge, LA*

TP 344 **Interaction of substrate and inhibitors with Salmonella FraB deglycase, a drug target**; Yuan Gao[1]; Jamison Law[1]; Venkat Gopalan[1]; Vicki H Wysocki[2]; *[1]The Ohio State University, Columbus, OH; [2]Georgia Institute of Technology, Atlanta, GA*

TP 345 **Mass Spectrometry for Single Particle Imaging of Dipole Oriented Complexes (MS SPIDOC) and First Scattering Measurements of Gas-phase Protein Complexes**; Jocky Chun Kui Kung[1, 2]; Tomislav Damjanović[1, 2]; Alan Kádek[1, 3]; Thomas Kierspel[1]; Charlotte Uetrecht[1, 2]; *[1]Centre for Structural Systems Biology, Hamburg, Germany; [2]University of Lübeck, Lübeck, Germany; [3]BIOCEV, Vestec, Czech Republic*

TP 346 **Native Charge Detection Mass Spectrometry Enables Accurate Mass and Structural Measurements of Messenger RNA and Ribosomal Particles**; Raihana Afroz[1]; Kyle P. Bowen[2]; Weijing Liu[2]; Ke Ma[3]; Rosa Viner[2]; Varun Gadkari[1]; *[1]University of Minnesota, Twin Cities, Minneapolis, MN; [2]Thermo Fisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific, Sunnyvale, CA*

TP 347 **Charge Detection Mass Spectrometry Meets Cryo-EM: Insights into Proteasome Activator Complexes**; Brad Davis[1]; Anisha Haris[2]; Alexander F. A. Keszei[3]; David Bruton[2]; Kevin Giles[2]; Mohammad T. Mazhab-Jafari[3]; Siavash Vahidi[1]; *[1]University of Guelph, Guelph, ON; [2]Waters Corporation, Wilmslow, United Kingdom; [3]University of Toronto, Toronto, ON*

TP 348 **Monitoring Effects of Nonvolatile Buffers on Assembly of Protein Complexes Using Submicron Emitters and Native Mass Spectrometry**; Hanlin Ren[1]; Jennifer S Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX*

TP 349 **Examining the Structural Effects of Electrosprayed Native-Protein Ions upon Transition from Solution to the Gas Phase**; Michael S Cordes[1]; Elyssia Gallagher[1]; *[1]Baylor University, Waco, TX*

TP 350 **Native Mass Spectrometry as a Tool for Characterizing Metal Binding to Proteins**; Michael Xiao[1]; Owen Skinner[1]; *[1]Northeastern University, Boston, MA*

TP 351 **Unravelling the complexity of the early stages of Amyloid-β aggregation using Trapped Ion-Mobility Mass Spectrometry**; Andrea Istrati[1, 2]; Melissa Baerenfaenger[1, 2]; Anouk. M Rijs[1, 2]; *[1]Division of Bioanalytical Chemistry, Department of Chemistry and Pharmaceutical Sciences, AIMMS Amsterdam Institute of Molecular and Life Sciences, Vrije Universiteit Amsterdam, 1081 HV Amsterdam, The Netherlands, Amsterdam, Netherlands; [2]Centre for Analytical Sciences Amsterdam, 1098XH Amsterdam, The Netherlands, Amsterdam, Netherlands*

TP 352 **Deciphering endogenous Nicotinic Acetylcholine Receptor from Torpedo Marmorata proteoforms by Orbitrap-based Charge Detection Mass Spectrometry and Intact Mass Analysis.**; Sarah M Delaux[1, 2]; Dinesh K. Chinthapalli[3]; Tiago Moreira[3]; Korantin Le Mouël[4, 5]; Manuela Zoonens[4, 5]; Frank Sobott[3]; Sarah Cianférani[1, 2]; *[1]Laboratoire de Spetrométrie de Masse BioOrganique, IPHC UMR 7178, Université de Strasbourg, CNRS, Strasbourg, France; [2]Pro FI, Infrastructure Nationale de Protéomique, Strasbourg, France; [3]School of Molecular and Cellular Biology & Astbury Centre, University of Leeds, Leeds, United Kingdom; [4]Laboratoire de Biologie Physico-Chimique des Protéines Membranaires, CNRS, UMR 7099, Université Paris Cité, F-75005, Paris, France; [5]Institut de Biologie Physico-Chimique, Paris, France*

TP 353 **Resolving Higher Order Transthyretin Oligomers with Direct Mass Technology**; Jared Hampton[1]; Carter Lantz[1]; Robert Rider[1]; David H. Russell[1]; *[1]Texas A&M University, College Station, TX*

TP 354 **Exploring asymmetric charge partitioning in ESI-MS using hemoglobin derivatized with proline-alanine-serine (PAS) tails to mimic single subunit unfolding**; Alex Listigovers[1]; Derek J Wilson[1]; *[1]York University, Toronto, ON*

TP 355 **Characterizing Insulin Aggregation using Cyclic Ion Mobility–Mass Spectrometry**; Emmanuel Dare[1]; Kenneth W Lee[1]; *[1]Brigham Young University, Provo, UT*

TP 356 **Native mass analyses of membrane proteins with high resolution multi-turn TOF-MS system**; Yusuke Tateishi[1]; Hiroko Morinaga[1]; Hiroyuki Miura[1]; Masaru Nishiguchi[1]; Daisuke Okumura[1]; Hitomi Sawai[2]; Michiko Tajiri[3]; Terukazu Nogi[3]; Satoko Akashi[3]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]Nagasaki University, Nagasaki, Japan; [3]Yokohama City university, Yokohama, Japan*

TP 357 **Native mass spectrometry provides insights for identification and characterization of ligand binding to human serum albumin**; Yifan Liu[1]; Owen Skinner[2]; *[1]Northeastern University, Quincy, MA; [2]Northeastern University, Boston, MA*

TP 358 **Automated buffer-exchange of native proteins in salty matrices for on-line MS analyses**; Rachel Koerber[1]; Mason Chilmonczyk[2]; Carter Asef[2]; Jim Filippini[2]; Susan Abbatiello[1]; Catherine Tremblay[1]; Lindsay J Morrison[1]; Nick Tomczyk[3]; *[1]Waters Corp., Milford, MA; [2]Andson Biotech Inc., Atlanta, GA; [3]Waters Corp, Wilmslow, United Kingdom*

TP 359 **Reduction of disulfide bonds in lysozyme monitored by ion mobility-mass spectrometry**; Sarah O'Keefe[1]; David E. Clemmer[2]; Anthony Pestritto[2]; *[1]Indiana University, Bloomington, IN; [2]Indiana University Bloomington, Bloomington, IN*

TP 360 **Characterizing bortezomib's effect on the structure and dynamics of the human 20S proteasome using vT-ESI-IMS-MS**; Colin R Johnson[1]; Lucas W. Henderson[2]; Edie M. Sharon[2]; David E. Clemmer[2]; *[1]Indiana University, Bloomington, IN; [2]Indiana University Bloomington, Bloomington, IN*

TP 361 **Native Charge Detection Mass Spectrometry for Biopharma**; Tian Tian[1]; Anisha Haris[2]; Iain D G Campuzano[3]; Nastaran N Tajoddin[4]; Daniela Salas Acosta[4]; Elizabeth Hecht[1]; David Bruton[2]; Keith Richardson[2]; Kevin Giles[2]; *[1]Amgen, South San Francisco, CA; [2]Waters Corporation, Wilmslow, United Kingdom; [3]Amgen Inc., Thousand Oaks, CA; [4]Amgen, Burnaby*

TP 362 **Structural mass spectrometry and gas-phase fluorescence spectroscopy demystify the metal-mediated early oligomerization and emergent ligand-transporter dynamics of GLP-1 receptor agonists**; Si Huang[1]; Yuye Zhou[1]; Tinyi Lui[1, 2]; Ri Wu[1]; Renato Zenobi[1]; *[1]ETH Zürich, Zürich, Switzerland; [2]The Chinese University of Hong Kong, Hong Kong, China*

GLYCOPROTEINS II
363-387

TP 363 **Comprehensive Target Analysis of Glycopeptides using LC-FAIMS-MS/MS-PRM Strategies**; Cristian D Gutierrez Reyes[1]; Sherifdeen B Onigbinde[1]; Moyinoluwa Adeniyi[1]; Joy O Solomon[1]; Oluwatosin E Daramola[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX*

TP 364 **Unveiling the Accurate Site-specific N- and O-Glycosylation of Hyperglycosylated Erythropoietin Protein Therapeutics**; Shuye Wu[1]; Jihong Lu[1]; Nafisa Tursumamat[1]; Qiannan Liu[1]; Yanlin Bian[1]; Joshua Klein[2]; Joseph Zaia[2]; Cheng Lin[2]; Jianwei Zhu[1]; Juan Wei[1]; *[1]Shanghai Jiao Tong University, Shanghai, China; [2]Boston University Chobanian & Avedisian School of Medicine, Boston, MA*

TP 365 **Can a HILIC retention model for N-glycans be developed that applies to multiple stationary phases?**; Mya M Brown[1]; Ngan Hoang Kim Thai[1]; Ron Orlando[1]; *[1]University of Georgia, Athens, GA*

TP 366 **An automated pipeline for glycoprotein characterization by integrating glycomics and glycoproteomics analysis**; Weiping Sun[1]; Zheng Chen[1]; Xiyue Zhang[1]; Shuyang Zhang[1]; Linting Li[1]; Baozhen Shan[1]; Wenting Li[1]; *[1]Bioinformatics Solutions Inc., Waterloo, ON*

TP 367 **Mapping the Monocyte Senescence Surfaceome and Surface Interactome Using Glycoprotein Cell-Surface Capture DIA-MS: Unlocking New Targets for Senotherapeutic Intervention**; Linna Cui[1]; Mansi Shrivastava[1]; Reema Banarjee[1]; Thedoe Nyunt[1]; Christopher Dunn[1]; Amit Dey[1]; Dimitrios Tsitsipatis[1]; Myriam Gorospe[1]; Nathan Basisty[1]; *[1]NIH National Institute on Aging, Baltimore, MD*

TP 368 **Atlas of N-linked protein glycosylation in the mouse**; Annie Jen[1]; Katherine A. Overmyer[1, 2, 3]; Mitchell D. Probasco[2]; Scott T. Quarmby[1, 3]; Matthew James Garland[4]; Bernd Hagedorn[4]; Johannes Petzoldt[4]; Eugen Damoc[4]; Daniel Hermanson[5]; Vlad Zabrouskov[5]; Joshua J. Coon[1, 2, 3]; *[1]Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI; [2]Morgridge Institute for Research, Madison, WI; [3]National Center for Quantitative Biology of Complex Systems, Madison, WI; [4]Thermo Fisher Scientific, Bremen, Germany; [5]Thermo Fisher Scientific, San Jose, CA*

TP 369 **Glycoprotein-Notebook: A pan-cancer glycoproteomic database and toolkit**; Hui Zhang[1]; Trung Hoang[1]; Yingwei Hu[1]; *[1]Johns Hopkins University, Department of Pathology, Baltimore, Maryland*

TP 370 **Unraveling Glycomic Shifts: A Multiplexed Study of ImmunoglobulinG, ImmunoglobulinA, and ImmunoglobulinM in Tuberculosis Infection among the Elderly**; Yun-Jung Yang[1]; Chih-Hsin Lee[2]; I-Lin Tsai[1]; *[1]Department of Biochemistry and Molecular Cell Biology, School of Medicine, College of Medicine, Taipei Medical University, Taipei, Taiwan; [2]Wan-Fang Hospital, Taipei, Taiwan*

TP 371 **N-linked and O-linked glycopeptide elucidation from ZT Scan DIA**; Stephen A Tate[1]; Claudia Alvarez[2]; *[1]SCIEX, Concord, ON; [2]SCIEX, Concord, ontario*

TP 372 **Updates to Glycoproteomics Data Analysis in FragPipe**; Daniel Polasky[1]; Jiechen Shen[1]; Fengchao Yu[1]; Alexey I. Nesvizhskii[1]; *[1]University of Michigan, Ann Arbor, MI*

TP 373 **Expanding glycopeptide identification with Match-Between-Glycans in FragPipe**; Jiechen Shen[1]; Daniel A. Polasky[1]; Shelley Jager[2, 3]; Fengchao Yu[1]; Karli R. Reiding[2, 3]; Albert J.R. Heck[2, 3]; Alexey I. Nesvizhskii[1, 4]; *[1]University of Michigan, Department of Pathology, Ann Arbor, MI; [2]Utrecht University, Biomolecular Mass Spectrometry and Proteomics, Bijvoet Center for Biomolecular Research and Utrecht Institute for Pharmaceutical Sciences, Utrecht, Netherlands; [3]Netherlands Proteomics Center, Utrecht, Netherlands; [4]University of Michigan, Department of Computational Medicine and Bioinformatics, Ann Arbor, MI*

TP 374 **Evaluating the Effects of TMT labeling on ZIC-HILIC Glycopeptide Enrichment of the Human Platelet Glycoproteome**; Nidhi Naik[1]; Adam Hawkridge[1]; *[1]Virginia Commonwealth University, Richmond, VA*

TP 375 **Real-Time Library Searching for Structural Glycoproteomics**; Kathryn Kothlow[1]; Bo Wen[1]; Chris McGann[1]; Anna G. Duboff[1]; Jacob H. Russell[1]; Emmajay Sutherland[1]; Devin Schweppe[1]; William S. Noble[1]; Nicholas M. Riley[1]; *[1]University of Washington, Seattle, WA*

TP 376 **Intact Glycoproteomics Reveals Fucosylation-Driven Glycan Heterogeneity in Clear Cell Renal Cell Carcinoma**; Fernando J Garcia-Marques[1]; Abel Bermudez[1]; Hongjuan Zhao[2]; Ru Wen[2]; James D Brooks[2]; Sharon J Pitteri[1]; *[1]Canary Center at Stanford for Cancer Early Detection, Department of Radiology, Stanford University School of Medicine, Palo Alto, CA; [2]Department of Urology, Stanford University School of Medicine, Palo Alto, CA*

TP 377 **Detection of Regulated Sites of O-GlcNAcylation and Putative PTM Cross-Talk**; Lauren E Ball[1]; Mi-Hye Lee[1]; Susana Comte-Walters[1]; Jennifer Bethard[1]; Rony Hull[1]; Mauricio Reginato[2]; *[1]Medical University of South Carolina, Pharmacology & Immunology, Charleston, SC; [2]Drexel University, Philadelphia, Pennsylvania*

TP 378 **Identifying low-abundance glycopeptides resolved by IM-MS for deep analysis of a viral spike protein**; Sabyasachi Baboo[1]; Leonard Rorrer[2]; Lauren Royer[2]; Daniel DeBord[2]; Ziqi Feng[1]; Ian A. Wilson[1]; Andrew B. Ward[1]; John R. Yates[1]; *[1]The Scripps Research Institute, La Jolla, CA; [2]MOBILion Systems, Inc., Chadds Ford, PA*

TP 379 **Automated HILIC Enrichment Coupled with Ion Mobility-Enhanced Glycopeptide Analysis for Improved and Scalable Glycoproteomic Profiling**; Hongxia Hellena Bai[1]; Klaus Lindpaintner[1]; *[1]Bruker Scientific LLC, Billerica, MA*

TP 380 **A New Polymeric ZIC-HILIC Probe for Mapping the Endogenous Serum Glycopeptidome**; Muhammad Salman Sajid[1]; Rency S Varghese[1]; Habtom W Ressom[1]; *[1]Georgetown University, Lombardi Cancer Center, Washington, DC*

TP 381 **Integrated Glycoproteomic Analysis and Glycan Spatial Biology Profiling of Prostate Cancer Using timsTOF on HILIC-enriched samples and MALDI Imaging**; Hongxia Hellena Bai[1]; Richard R Drake[2]; Klaus Lindpaintner[1]; *[1]Bruker Scientific LLC, Billerica, MA; [2]Medical University of South Carolina, Pharmacology & Immunology, Charleston, SC*

TP 382 **GlycoFASP: A Universal Method to Prepare Complex Mixtures for O-Glycoproteomic Analysis**; Shane M. Finn[1]; Keira E. Mahoney[1]; Taryn M. Lucas[1]; Valentina Rangel-Angarita[1]; Ryan J. Chen[1]; Stacy A. Malaker[1]; *[1]Yale University, New Haven, CT*

TP 383 **Leveraging workflows for comprehensive characterization of released N-glycan on monoclonal antibody and their impact on self-association**; Sanghati Bhattacharya; *University of Iowa, Iowa City, IA*

TP 384 **Proton Transfer Charge Reduction Enhances Glycoproteoform Resolution in Online and Offline Mass Spectrometry**; Tim S. Veth[1]; Kayla A. Markuson[1]; David Bergen[2]; Rafael D Melani[2]; Amanda E. Lee[2]; Chirstopher Mullen[2]; Nicholas M. Riley[1]; *[1]University of Washington, Seattle, WA; [2]Thermo Fisher Scientific, San Jose, California*

TP 385 **Deciphering O-GlcNAc Dynamics in Myocardial Ischemia: Insights from an OGT Quantitative Interactome Analysis**; Fiddia Zahra[1]; Kamau Fahie[1]; Bhargavi Narayanan[1]; Robert O'Meally[2]; Robert N Cole[2]; Mark Kohr[3]; Brian D Foster[1]; Natasha Zachara[1]; *[1]The Johns Hopkins University School of Medicine, Baltimore, MD; [2]The Mass Spectrometry and Proteomics Facility, The Johns Hopkins University School of Medicine, Baltimore, Maryland; [3]Johns Hopkins Bloomberg School of Public Health, Baltimore, MD*

TP 386 **High Field Asymmetric Waveform Ion Mobility Spectrometry (FAIMS) on the Orbitrap Astral mass spectrometer enables deep coverage of protein glycosylation**; Chia-wei Lin[1]; Sibylle Pfammatter[1]; Ralph Schlapbach[1]; Paolo Nanni[1]; *[1]Functional Genomics Center Zurich, Zurich, Switzerland*

TP 387 **Influence of N-Glycosylation on Proteolytic Processing**; Michael Girgis[1]; Diana Campos[2]; Paul Russo[1]; Mikell Paige[1]; Guanghui Zong[3]; Qiang Yang[3]; Lai-Xi Wang[3]; Miloslav Sanda[2, 4]; *[1]George Mason University, Manassas, VA/20110; [2]Max Planck Institute for Heart and Lung Research, Bad Nauheim, Germany; [3]University of Maryland, College Park, MD; [4]Georgetown University, Lombardi Cancer Center, Washington, DC*

H/D EXCHANGE: PROTEIN STRUCTURE/FUNCTION
388-413

TP 388 **Investigation of conformational dynamics of inhibitor-resistant class A β-lactamases**; Elena Bolonova[1]; Tsz-Fung Wong[1]; Pui-Kin So[1]; Zhongping Yao[1]; *[1]The Hong Kong Polytechnic University, Hong Kong, Hong Kong*

TP 389 **Probing the structural heterogeneity of Pup ligase PafA using H/D exchange mass spectrometry**; Alicia Plourde[1]; Jacquelyn C. Ogata-Bean[1]; Siavash Vahidi[1]; *[1]University of Guelph, Guelph, ON*

TP 390 **Investigating the allosteric regulation of human mitochondrial LONP1 protease using HDX-MS**; S. Quinn W. Currie[1]; Alexander F. A. Keszei[2]; Matthew Tcheng[2]; Rachel E. Wideman[1]; Mohammad T. Mazhab-Jafari[2, 3]; Aaron D. Schimmer[2]; Siavash Vahidi[1]; *[1]University of Guelph, Guelph, ON; [2]Princess Margaret Cancer Center, Toronto, ON; [3]Department of Medical Biophysics, University of Toronto, Toronto, ON*

TP 391 **Structural and functional characterization of de novo-designed inhibitors of mitochondrial human ClpP**; Jacquelyn C Ogata-Bean[1]; Monica M Goncalves[1]; Rachel E Wideman[1]; Yulia Jitkova[2]; Aaron D Schimmer[2]; Robert W Harkness[1]; Siavash Vahidi[1]; *[1]University of Guelph, Guelph, ON; [2]Princess Margaret Cancer Center, Toronto, ON*

TP 392 **Investigating conformational dynamics of the JAK2 pseudokinase-kinase domains by hydrogen/deuterium exchange mass spectrometry and molecular dynamics simulation**; Chang ZHAO[1]; Zhongping Yao[1]; *[1]The Hong Kong Polytechnic University, Hong Kong, Hong Kong*

TP 393 **Temperature-dependent hydrogen-deuterium exchange mass spectrometry identifies thermal networks in the protein scaffold of orotidine 5'-monophosphate decarboxylase**; Anthony T. Iavarone[1]; Pankaj Dubey[1]; Judith P. Klinman[1]; *[1]University of California, Berkeley, Berkeley, CA*

TP 394 **Deciphering allosteric regulation in human mitochondrial ClpP protease: insights from mass**

spectrometry; Monica M Goncalves[1]; Adwaith B. B. Uday[2]; Iain Watson[3]; S. Quinn W. Currie[1]; Taylor Forrester[1, 2]; Angelina S Kim[4]; Algirdas Velyvis[1]; Matthew S Kimber[1]; Rima Al-Awar[3]; Natalie Zeytuni[2]; Aaron D. Schimmer[5]; Siavash Vahidi[1]; *[1]University of Guelph, Guelph, ON; [2]McGill University, Ste Anne de Bellevue, QC; [3]Ontario Institute for Cancer Research, Toronto, ON; [4]University of Toronto, Toronto; [5]Princess Margaret Cancer Centre, Toronto, ON*

TP 395 **Differential conformational dynamics of the Mtb 20S core particle induced through orthosteric inhibitor binding as revealed by HDX-MS.**; Madison Turner[1]; Verena Filz[2]; Dr. Thomas Böttcher[2]; Siavash Vahidi[1]; *[1]University of Guelph, Guelph, ON; [2]University of Vienna, Vienna, Austria*

TP 396 **Integrative Characterization of Interactions between Ebola Virus Protein eVP35 and Mindbomb Protein 2 (MIB2) Using HDX-MS, XL-MS, and AlphaFold**; Xinyi Cynthia Kuang[1]; Grace Uwase[2]; Nicole D Wagner[1]; Daisy Leung[2]; Gaya Amarasinghe[2]; Michael L Gross[1]; *[1]Washington University in St. Louis, University City, MO; [2]Washington University in St. Louis School of Medicine, St. Louis, MO*

TP 397 **Mapping disordered protein-ligand interactions using in-droplet hydrogen-deuterium exchange and molecular dynamics.**; Mst Nigar Sultana[1]; Mohammad Azizur Rahman[1]; Sohag Ahmed[1]; Kevin C. Courtney[1]; Stephen J. Valentine[1]; *[1]West Virgina University, Morgantown, WV*

TP 398 **Dissecting the Role of Functionally Relevant Mutations in Adenylate Cyclase Toxin by HDX-MS**; Petr Man[1]; Zuzana Kalaninova[1, 2]; Adriana Osickova[1]; Petr Novak[1]; Jiri Masin[1]; Peter Sebo[1]; *[1]Institute of Microbiology, Prague 4, Czech Republic; [2]Faculty of Science, Prague 2, Czech Republic*

TP 399 **Protonation-induced conformational changes of CLC-ec1 studied by HDX-MS**; Jasmína M Portašiková[1, 2]; Lukáš Fojtík[1, 2]; Petr Novák[1]; Petr Man[1]; *[1]Institute of Microbiology of the Czech Academy of Sciences, Division BioCeV, Vestec, Czech Republic; [2]Department of Biochemistry, Faculty of Science, Charles University, Prague 2, Czech Republic*

TP 400 **HDX-MS reveals the conformational dynamics of the eukaryotic purine symporter UapA in lipid nanodiscs**; Charlotte Guffick[1]; Samantha A Gaytán Mondragón[2]; Euan Pyle[2, 3]; Argyris Politis[1]; Bernadette Byrne[2]; *[1]University of Manchester, Manchester, United Kingdom; [2]Imperial College London, London, United Kingdom; [3]The Francis Crick Institute, London, United Kingdom*

TP 401 **Low pH sensing triggers altered H-bonding and noncanonical conformational changes to promote bacterial virulence**; Victoria Brady[1]; Minoli Doshi[2]; Ganesh Anand[1]; *[1]Pennsylvania State University, University Park, PA; [2]Institut Pasteur, Université Paris Cité, CNRS UAR 2024, Mass Spectrometry for Biology, Paris, France*

TP 402 **Interactions of spike proteins of SARS-CoV-2 variants with neutralizing antibodies: Conformational dynamics and allostery revealed by hydrogen/deuterium exchange mass spectrometry**; Qinyu Jia[1]; Zhongping Yao[1]; Chengxi Liu[1]; *[1]the Hong Kong Polytechnic University, Kowloon, Hong Kong*

TP 403 **Hydrogen-Deuterium Exchange and Variable Temperature ESI-MS on Transthyretin Reveal Effects of ESI Buffers on Structure and Dynamics**; Emily Burningham-Lopez[1]; Carter Lantz[1]; Robert Rider[1]; Sangho Yun[1]; Arthur Laganowski[1]; David H. Russell[1]; *[1]Texas A&M University, College Station, TX*

TP 404 **Comprehensive Epitope Mapping of Borrelia burgdorferi Antigens Using Polyclonal and Standard HDX-MS**; Clint Vorauer[1]; Miklos Guttman[1]; Nick Mantis[2]; *[1]University of Washington, Seattle, WA; [2]New York State Department of Health, Albany, New York*

TP 405 **Transient structural dynamics during photo-reduction of avian cryptochrome from HDX-MS**; Suchitra Pradhan[1]; Jess Ramsay[1]; Monika Kish[1]; Daniel Kattnig[1]; Jonathan J Phillips[1]; *[1]Living Systems Institute, University of Exeter, Exeter, United Kingdom*

TP 406 **Molecular mechanism of ssDNA-mediated allosteric activation of the WYL-domain containing transcription regulator, DriD**; Emily Cannistraci[1]; Bindu Y Srinivasu[2]; Jose Chavez Orozco Jr[1]; Kevin Gozzi[3]; Thomas E Wales[2]; Maria A Schumacher[1]; *[1]Duke University Medical Center, Durham, NC; [2]Northeastern University, Boston, MA; [3]Harvard University, Cambridge, MA*

TP 407 **The Conformational effect of mutations on sliding beta clamp protein as measured by Hydrogen Deuterium Exchange Mass spectrometry**; Shreya Ghosh[1]; Melissa Liriano[1]; Penny Beuning[1]; Thomas E Wales[1]; *[1]department of chemistry and chemical biology northeastern University, Boston, MA*

TP 408 **Leveraging Hydrogen Deuterium Exchange Mass Spectrometry Data and Machine Learning to Improve Protein-Ligand Docking Pose Selection**; Vincent M Lowe[1]; Ally Smith[1]; Daniel Deredge[1]; *[1]University of Maryland School of Pharmacy, Baltimore, MD*

TP 409 **Complementary Mass Spectrometry (MS)-based Strategies to Determine Protein-Protein Interfaces in Antibody Dimerization**; Jusung Lee[1]; Michael L Gross[1]; *[1]Washington University in St. Louis, St. Louis, MO*

TP 410 **Protein folding of myoglobin studied using a PEPS-HDX-MS quench-flow apparatus**; Isini Pinipa Ranawake Arachchige[1, 2]; Rohana Liyanage[1, 2]; Jackson Lay Jr. [2, 3]; *[1]Department of Chemistry and Biochemistry, University of Arkansas, Fayetteville, AR; [2]Arkansas Statewide Mass Spectrometry Facility, FAYETTEVILLE, AR; [3]Department of Chemistry and biochemistry University of Arkansas, Fayetteville, AR*

TP 411 **Characterization of transthyretin drug binding by structural proteomics techniques combined with molecular dynamics simulations**; Evgeniy Petrotchenko[1]; Brandon Novy[2]; Konstantin I. Popov[2]; Christoph H. Borchers[3, 4]; *[1]Segal Cancer Proteomics Center, McGill University, Montreal, QC; [2]Division of Chemical Biology and Medicinal Chemistry, University of North Carolina at Chapel Hill, Chapel Hill, NC; [3]Segal Cancer Proteomics Centre, Lady Davis Institute, Jewish General Hospital, McGill University, Montreal, QC H3T 1E2; [4]Gerald Bronfman Department of Oncology, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC H3T 1E2*

TP 412 **Unifying gHDX and High-Resolution TW-SLIM to Capture the Conformational Heterogeneity of Proteins**; Nathaniel Morgan[1]; Daniel Wu[1]; Brian H. Clowers[1]; *[1]Washington State University Department of Chemistry, Pullman, WA*

TP 413 **HDgraphiX: a web-based tool for visualization of hydrogen deuterium exchange mass spectrometry data**; Kent Robert Vosper[1]; Algirdas Velyvis[1]; Siavash Vahidi[1]; *[1]University of Guelph, Guelph, ON*

IMAGING MS: METHOD DEVELOPMENT
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TP 414 **Quantification of arachidonic acid in whole-body zebrafish by IR-MALDESI qMSI**; Alena Joignant[1]; Emily Bruce[1]; Stephen Vega[1]; David Muddiman[1]; *[1]Biological Imaging Laboratory for Disease and Exposure Research, Raleigh, NC*

TP 415 **Expansion Mass Spectrometry Imaging for Subcellular Metabolomics**; Jason A Guerrero[1]; Vignesh Venkataramani[2]; Lydia Kisley[2]; Laura Sanchez[1]; *[1]University of California, Santa Cruz, Santa Cruz, CA; [2]Case Western Reserve University, Cleveland, Ohio*

TP 416 **Sample Preparation Method for MALDI Mass Spectrometry Imaging of Non-Decalcified Human Teeth**; Kayle J Bender[1]; Joanna Ellis[2]; Manish Arora[2, 3]; Elizabeth K. Neumann[1]; *[1]University of California, Davis, Davis, CA; [2]Linus Biotechnologies, Inc., North Brunswick, New Jersey; [3]Icahn School of Medicine at Mount Sinai, New York City, NY*

TP 417 **Benzoyl Chloride Derivatization for Enhanced Mass Spectrometry Imaging of Tissue and Droplets**; Ashley E Lenhart[1, 2]; Taigue W Woods[3]; Shana O Kelley[1]; Jonathan V Sweedler[1, 2, 3]; *[1]Chan Zuckerberg Biohub Chicago, Chicago, IL; [2]Beckman Institute for Advanced Science and*

Technology, University of Illinois Urbana-Champaign, Urbana, IL; [3]Department of Chemistry, University of Illinois Urbana-Champaign, Urbana, IL

TP 418 **Detection of Individual Nanoparticle Tags for Digital Mass Spectrometry Imaging**; Jan Preisler[1]; Antonin Bednarik[1]; Marek Stiborek[1]; Lenka Jindrichova[1]; Vadym Prysiazhnyi[1]; Michal Zalud[1]; Viktor Kanicky[1]; Jiri Kroupa[2]; Pavel Houska[2]; Barbora Adamova[1]; Jarmila Navratilova[1, 3]; *[1]Masaryk University, Brno, Czech Republic; [2]Brno University of Technology, Brno, Czech Republic; [3]St. Anne's University Hospital, Brno, Czech Republic*

TP 419 **Integrating Ion Mobility and Mass Spectrometry Imaging for Characterizing the Distribution of Biologically Active Disaccharide Isomers**; Ting Zeng[1]; Kevin Zematis[1]; Xueyun Zheng[1]; Brittney Gorman[1]; Dusan Velickovic[1]; Christopher R Anderton[1]; *[1]Pacific Northwest National Laboratory, Richland, Washington*

TP 420 **QMSI using targeted-DESI-MSI in MRM mode offers higher sensitivity, specificity, and rapid quantification of chloroquine drug in mice kidney**; Md. Muedur Rahman[1, 2]; Mst. Sayela Afroz[1]; Md. Al Mamun[1, 2]; Ariful Islam[3]; Takumi Sakamoto[1, 2]; Shuhei Aramaki[1]; Tomohito Sato[1]; Thanai Paxton[4]; Yutaka Takahashi[1, 2]; Tomoaki Kahyo[1, 5]; Mitsutoshi Setou[1, 6]; *[1]Department of Cellular and Molecular Anatomy, Hamamatsu University School of Medicine, Hamamatsu, Japan; [2]Preppers Co., Ltd., Hamamatsu University School of Medicine, Hamamatsu, Japan; [3]Department of Biochemistry and Microbiology, School of Health and Life Sciences, North South University, Dhaka, Bangladesh; [4]Nihon Waters K.K., Shinagawa-ku, Japan; [5]Quantum Imaging Laboratory, Division of Research and Development in Photonics Technology, International Mass Imaging and Spatial Omics Center, Institute of Photonics Medicine, Hamamatsu University School of Medicine, Hamamatsu, Japan; [6]International Mass Imaging and Spatial Omics Center, Institute of Photonics Medicine, Hamamatsu University School of Medicine, Hamamatsu, Japan*

TP 421 **Optimizing Quantitative MALDI MSI for Drug Discovery: Moving to Higher Statistical Power with Echo Acoustic Liquid Handlers**; Emily R. Sekera[1]; Nathaniel R. Twarog[1]; Rebekah DeVries[1]; P. Jake Slavish[1]; Elizabeth D. Barker[2]; Anang A. Shelat[1]; John J. Bowling[1]; *[1]St. Jude Children's Research Hospital, Memphis, TN; [2]University of Tennessee, Knoxville, TN*

TP 422 **Iterative Spatial Resolution Enhancement in Imaging Mass Spectrometry via Hydrogel Tissue Expansion and Multimodal Image Fusion**; Elijah D Mayo[1]; Jacob M Samuel[1]; Yingchan Guo[1]; Boone M Prentice[1]; *[1]University of Florida, Department of Chemistry, Gainesville, FL*

TP 423 **Spatial imaging parallel reaction monitoring with parallel accumulation serial fragmentation (iprm-PASEF) investigating 'age-protected' CD38-/- mice**; Charles A Schurman[1]; Joanna Bons[1]; Prasanna Vadhana Ashok Kumaar[1]; Jingqi Fang[1]; Rebeccah Riley[1]; Nannan Tao[2]; Eric Verdin[1]; Birgit Schilling[1]; *[1]Buck Institute for Research on Aging, Novato, CA; [2]Bruker Inc, Billerica, MA*

TP 424 **Assessing Lipid Spatial Fidelity in Expansion Imaging Mass Spectrometry**; Jacob M Samuel[1]; Sarah J. Murphy[1]; Elijah D. Mayo[1]; Tingting Yan[1]; Prentice Boone[1]; *[1]University of Florida, Gainesville, FL*

TP 425 **Novel semi-targeted mass spectrometry imaging approach using the SELECT SERIES MRT mass spectrometer with DESI XS source**; Emmanuelle Claude[1]; William Johnson[1]; Joanne Ballantyne[1]; *[1]Waters Corporation, Wilmslow, United Kingdom*

TP 426 **OzMALDI-MSI to Determine and Visualize Lipid Double-Bond Positions in Zebrafish**; Shanika Malshani Weerasinghe[1]; Josiah J Rensner[1]; Jeffrey Essner[1]; Young Jin Lee[1]; *[1]Iowa State University, Ames, IA*

TP 427 **Quantitative Mass Spectrometry Imaging of Intact Proteins**; Mushfeqa Iqfath[1]; Manxi Yang[1]; Andrew K. Swansiger[2]; Alyssa Moore[1]; Lily Miller[2]; James S. Prell[2]; Julia Laskin[1]; *[1]Purdue Univeristy, West Lafayette, IN; [2]University of Oregon, Eugene, OR*

TP 428 **Utilizing Ammonium Fluoride Doping for Quantitative Mass Spectrometry Imaging of Low Abundant Biomolecules**; Alora R Dunnavant[1]; Seth M Eisenberg[1]; Emily R Bruce[1]; David C. Muddiman[1]; *[1]Biological Imaging Laboratory for Disease and Exposure Research, Raleigh, NC*

TP 429 **Patterned Photochemical Modification for MALDI Imaging of Lipids**; Kermit K. Murray[1]; Kadeem O. Hayes[1]; *[1]Louisiana State University, Baton Rouge, LA*

TP 430 **Staining tissues with a novel dye-based matrix for MALDI MSI**; Michal Javorek[1]; Michal Hendrych[1, 2]; Katerina Ondrakova[1]; Jan Preisler[1]; Antonin Bednarik[1]; *[1]Masaryk University, Brno, Czech Republic; [2]St. Anne's University Hospital, Brno, Czech Republic*

TP 431 **Effects of Solvent Water Content on Delocalization of Analytes in MALDI Mass Spectrometry Imaging**; Won Kyu Choi[1]; Alejandro Catacora[1]; Cole C. Johnson[1]; Kristine Glunde[1]; Caitlin M. Tressler[1]; *[1]Johns Hopkins Applied Imaging Mass Spectrometry Core, Russell H. Morgan Department of Radiology and Radiological Science, Johns Hopkins School of Medicine, Baltimore, Maryland*

TP 432 **High-Resolution Imaging of plant tissue sections and 3D surfaces using AP-SMALDI Orbitrap MSI**; Carolin M Morawietz[1, 2]; Stefanie Gerbig[1]; Kerstin Strupat[3]; Bernhard Spengler[1, 2]; *[1]TransMIT GmbH, Giessen, Germany; [2]Justus Liebig University, Institute of Inorganic and Analytical Chemistry, Giessen, Germany; [3]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

TP 433 **Regression model comparison for calibration curves in MALDI and DESI MSI**; Angeliki Christakopoulou[1]; Felicia G. S. Wirtz[2]; Bin Yan[2]; Alex Dexter[2]; Josephine Bunch[2, 3]; Rory T. Steven[2]; *[1]National Physical Laboratory, London, United Kingdom; [2]National Physical Laboratory, Teddington, United Kingdom; [3]Imperial College London, London, United Kingdom*

TP 434 **Use of heavy labelled metabolites to evaluate ionisation biases in multi-organ mass spectrometry imaging**; Félicia G. S. Wirtz[1]; Alex Dexter[1]; Rory T. Steven[1]; Josephine Bunch[1, 2]; *[1]National Physical Laboratory, London, United Kingdom; [2]Imperial College London, London, United Kingdom*

TP 435 **Ion suppression and quantitation in MALDI and DESI MSI**; Félicia G. S. Wirtz[1]; Bin Yan[1]; Angeliki Christakopoulou[1]; Alex Dexter[1]; Josephine Bunch[1, 2]; Rory Thomas Steven[1]; *[1]National Physical Laboratory, London, United Kingdom; [2]Imperial College London, London, United Kingdom*

TP 436 **Sequential spotting technique for dried-drop experiments in matrix-assisted laser desorption/ionization mass spectrometry**; Joy L Maabadi[1]; Arbil Lopez[1]; Joseph H Holbrook[2]; Amanda B. Hummon[1, 2]; *[1]Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH; [2]Ohio State Biochemistry Program (OSBP), The Ohio State University, Columbus, OH*

TP 437 **FluoMALDI Imaging of the Immune Response for Label-Free In Situ Identification of Phagocytes in Francisella Novicida-Infected Mouse Tissues**; Kristine Glunde[1]; Taehun Hahm[1]; Tialfi Bergamin De Castro[2]; Alison J. Scott[2]; *[1]Johns Hopkins Applied Imaging Mass Spectrometry Core, Russell H. Morgan Department of Radiology and Radiological Science, Johns Hopkins School of Medicine, Baltimore, Maryland; [2]University of Maryland School of Dentistry, Baltimore, Maryland*

TP 438 **Tissue Expansion Mass spectrometry Imaging (TEMI) for high spatial resolution multi-omics molecular mapping**; Hua Zhang[1]; Lang Ding[2]; Amy Hu[2]; Xudong Shi[3]; Penghsuan Huang[4]; Haiyan Lu[1]; Paul W. Tillberg[2]; Meng C. Wang[2]; Lingjun Li[1, 4]; *[1]School of Pharmacy, University of Wisconsin-Madison, Madison, WI; [2]Howard Hughes Medical Institute, Janelia Research Campus, Ashburn, VA; [3]School of*

Medicine and Public Health, University of Wisconsin-Madison, Madison, WI; [4]Department of Chemistry, University of Wisconsin-Madison, Madison, WI

TP 439 **MALDI timsTOF Mass spectrometry for spatially resolved degradation profiling of tablets and blends enabling drug-excipient compatibility assessment and shelf-life prediction**; Rekha Thomas[1]; Karina Ariel Vargas[2]; Zhenqi Shi[1]; Christopher M. Crittenden[1]; Elizabeth K. Neumann[2]; *[1]Genentech, South San Francisco, CA; [2]UC Davis, Davis, CA*

TP 440 **MALDI-IHC Protein Imaging at Cellular Resolution via Ultra-dry Matrix Application**; Alyson Black[1]; Gargey Yagnik[2]; Alain Creissen[1]; Kenneth Rothschild[2]; Mark Lim[2]; *[1]HTX Technologies, Chapel Hill, NC; [2]AmberGen Inc., Billerica, MA*

TP 441 **Hybrid Imaging Analysis reveals molecular localization reflecting brain function**; Tadayuki Ogawa[1]; Eisei Tanaka[2]; Shino Takeda-Homma[3]; Takafumi Hirata[2]; Tomonari Umemura[4]; *[1]Dokkyo Medical University, Tochigi, Japan; [2]The University of Tokyo, Bunkyo-ku, Japan; [3]National Institute of Quantum Science and Technology, Inage, Japan; [4]Tokyo University of Pharmacy and Life Science, Hachioji, Japan*

TP 442 **Simultaneously imaging comprehensive metabolites on injured spinal cord by MALDI MS via employing a new cooperative matrix**; Mengjuan Li[1]; Hong Wang[2]; Jiarui Li[1]; Xinhua Guo[1]; *[1]Jilin University, Changchun, China; [2]Changchun Institute of Applied Chemistry, Changchun, China*

TP 443 **Enabling Spatial Lipidomics with MS2Imaging: A Novel Approach for Enhanced Molecular Characterization**; Varun Vashneel Sharma[1]; Gabor Toth[1]; Johan Lillja[1]; Robert Martinis[1]; Ingela Lanekoff[1]; *[1]Uppsala University, Uppsala, Sweden*

TP 444 **Advanced Molecular characterization of passivation layers in Lithium-ion batteries BY FTICR imaging Mass Spectrometry**; Théo Sombret[1, 2, 3]; Egon Kherchiche[1, 2, 3]; Julien Maillard[2, 3]; Antonin Gajan[4]; Oliver Hvidsten[5]; Mona Abdelgaid[5]; Kristin Persson[5]; Pierre Giusti[1, 2, 3]; Carlos Afonso[2, 6]; *[1]Normandie Université, CARMeN, UMR 6064 et FR 3038, Université de Rouen-Normandie, INSA de Rouen-Normandie, CNRS, IRCOF, Mont Saint Aignan Cedex., Mont Saint-Aignan, France; [2]International Joint Laboratory - iC2MC: Complex Matrices Molecular Characterization, TRTG, BP 27, 76700 Harfleur, France., Harfleur, France; [3]TotalEnergies OneTech R&D, Total Research & Technology Gonfreville, BP 27, 76700 Harfleur, France, Harfleur, France; [4]Saft, Corporate Research, 33074 Bordeaux, France, Bordeaux, France; [5]Department of Materials Sciences and Engineering, University of California, Berkeley, CA 94720, USA, Berkeley, US; [6]Normandie Univ, UNIROUEN, INSA Rouen, CNRS, CARMeN, 76000 Rouen, France., Mont Saint Aignan, France*

TP 445 **Novel method for Spatial Mapping of EGFR Protein in NSCLC via DESI-MSI**; Jingyu Jiang[1]; István Pap[2]; Horkovics-Kovats Gabriel[2]; Daniel Simon[1, 2]; Nora Alhannoush[3, 4]; Duncan Roberts[1]; Yuchen Xiang[1]; Takats Zoltan[1]; Lauren Ford[1]; Virag Sagi-kiss[1]; *[1]Division of Systems Medicine, Department of Metabolism Disgestion and Reproduction, Faculty of Medicine, Imperial College London, London, United Kingdom; [2]University of Regensburg, Department of Immune Medicine Multimodal Imaging of Intracellular Communication, Regensburg, Germany; [3]Department of Anaesthesia and Critical Care, Royal Brompton & Harefield Hospitals, Guy's and St Thomas' NHS Foundation Trust, London, United Kingdom; [4]Anesthesia Technology Department, Imam Abdulrahman bin Faisal University, Dammam, Saudi Arabia*

TP 446 **Mapping the molecular landscape of human DLBCL by GCIB-SIMS**; SImon Uzoni[1]; Daniele Zancin[1]; Vasilis Chatzikyriakos[2, 3]; Noora Neittaanmäki[2, 3]; John Fletcher[1]; *[1]Department of Chemical and Molecular Biology, University of Gothenburg, Gothenburg, Sweden; [2]Department of Laboratory Medicine, Institute of Biomedicine, Sahlgrenska Academy, University of Gothenburg, Gothenburg, Sweden; [3]Region Västra Götaland, Sahlgrenska University Hospital, Department of Clinical Pathology and Cytology, Gothenburg, Sweden*

TP 447 **Control and optimization of humidity levels for optimal in-situ tryptic digestion and MALDI MSI of peptides**; Paulina Kret[1]; Rachel S. Pryce[2]; Nidia Lauzon[3]; Anna Bodzon-Kulakowska[1]; Pierre Chaurand[2]; *[1]AGH University, Kraków, Poland; [2]Department of Chemistry, Université de Montréal, Montréal, QC; [3]McGill University, Montreal, Québec*

TP 448 **Data Fusion Strategy for MALDI-Trapped Ion Mobility Mass Spectrometry Imaging Bottom-Up Proteomics**; Varvara Nikolopoulou[1]; Reza Aalizadeh[1]; Georgia Charkoftaki[1]; Athina Lisgara[1]; Jordan Hartig[2]; Scott Pennino[2]; Vladimir V. Papov, Jr. [2]; Vasilis Vasiliou[1]; *[1]Department of Environmental Health Sciences, Yale School of Public Health, Yale University, New Haven, CT; [2]Boehringer Ingelheim Pharmaceuticals, Inc., Ridgefield, CT*

TP 449 **A High-resolution MALDI imaging mass spectrometry workflow for zebrafish whole body and organ-specific imaging**; Jacquelyn Spathies[1, 2]; Simeon Betapudi[1]; Caitlin C Murdoch[2, 3]; Lukasz G Migas[4, 5]; Katherine N Gibson-Corley[2]; Raf Van De Plas[1, 4, 5]; Eric P Skaar[2, 3]; Jeffrey M Spraggins[1, 2, 3, 6, 7]; *[1]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [2]Department of Pathology, Microbiology, and Immunology, Vanderbilt University Medical Center, Nashville, TN; [3]Vanderbilt Institute for Infection, Immunology, and Inflammation, Vanderbilt University Medical Center, Nashville, TN; [4]Department of Biochemistry, Vanderbilt University School of Medicine, Nashville, TN; [5]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [6]Department of Cell and Developmental Biology, Vanderbilt University School of Medicine, Nashville, TN; [7]Department of Biochemistry, Vanderbilt University, Nashville, TN*

TP 450 **MALDI Mass Spectrometry Imaging (MSI) of Key Metabolites of Adenosine Pathway and Methylation Pathway in Preclinical Mouse Brain Tissues**; Weiyuan Hu[1]; Weiyi Peng[2]; Xinli Liu[1]; *[1]Department of Pharmacological and Pharmaceutical Sciences, University of Houston, Houston, TX; [2]Department of Biology and Biochemistry, University of Houston, Houston, TX*

TP 451 **Novel workflow for integrating murine precision-cut lung slices with high-spatial resolution imaging mass spectrometry**; Anna J Smith[1, 2]; Katerina V Djambazova[1, 2]; Kacie A Traina[3, 4]; Jamie L Allen[1, 2]; Lukasz G Migas[5]; Madeline E Colley[1, 2]; Martin Dufresne[1, 6]; Melissa A. Farrow[1, 2]; Raf Van De Plas[1, 5, 7]; Eric P Skaar[3, 4]; Jeffrey M Spraggins[1, 2, 3, 6, 7]; *[1]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [2]Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; [3]Department of Pathology, Microbiology, and Immunology, Vanderbilt University Medical Center, Nashville, TN; [4]Vanderbilt Institute for Infection, Immunology, and Inflammation, Vanderbilt University Medical Center, Nashville, TN; [5]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [6]Department of Chemistry, Vanderbilt University, Nashville, TN; [7]Department of Biochemistry, Vanderbilt University, Nashville, TN*

TP 452 **A novel MALDI MSI approach for bottom-up proteomics: investigating peptides detection**; Athina Lisgara[1]; Georgia Charkoftaki[1]; Alvaro Santos-Neto[2]; Reza Aalizadeh[1]; Varvara Nikolopoulou[1]; Jordan Hartig[3]; Scott Pennino[3]; Vladimir V. Papov[3]; Vasilis Vasiliou[1]; *[1]Department of Environmental Health Sciences, Yale School of Public Health, Yale University, New Haven, CT; [2]São Carlos Institute of Chemistry, University of São Paulo, São Paulo, Brazil; [3]Boehringer Ingelheim Pharmaceuticals, Inc., Ridgefield, CT*

TP 453 **A pneumatically-assisted microfluidic probe for nano-DESI mass spectrometry imaging**; Lixue Jiang[1]; Julia Laskin[1]; *[1]Purdue University, West Lafayette, IN*

TP 454 **Improving MALDI-IHC Reproducibility and Sensitivity Through Gold Sputter Coating and Histologically Compatible Slides**; Andrew Bowman[1]; David S Wagner[1]; Junhai Yang[1]; *[1]AbbVie, Inc., North Chicago, IL*

TP 455 **Multimodal mass spectrometry imaging workflow to explore the role of methionine metabolism in immunotherapeutic resistance of ovarian carcinoma**; Madison Shiyuk[1, 2]; Joseph Monaghan[3]; Tian Zhao[1, 4]; Sarah MacPherson[4]; Ken Weke[1, 2]; Kyle Duncan[1, 3]; Julian J Lum[1, 4]; David R. Goodlett[1, 2]; Helena Petrosova[1, 2]; *[1]University of Victoria, Victoria, BC; [2]University of Victoria GBC Proteomics Centre, Victoria, BC, BC; [3]Vancouver Island University, Nanaimo, BC; [4]Deeley Research Centre, BC Cancer Research Institute, Victoria, BC*

INDUSTRY: TRACE ANALYSIS, QUALITY CONTROL, AND AUTOMATION

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TP 456 **Fully Automated Workflow for Volatile PFAS Analysis in Food Contact Materials Using GC-Triple Quadrupole**; Auni Wong[1]; Gwen Sin Yee Lim[2]; Aimei Zou[3]; Joel Ferrer[4]; *[1]Agilent Technologies, Singapore, Singapore; [2]CTC Analytics AG, Zwingen, Switzerland; [3]Agilent Technologies Singapore, Singapore, Singapore; [4]Agilent Technologies, Santa Clara, CA*

TP 457 **Identification of Small Molecules in Complex Cosmetic Matrices via Tandem Liquid Chromatography and High-Resolution Mass Spectrometry**; Nicole M Brundridge[1]; Heera Raghubir[1]; Elaine Rodriguez[1]; Matthew Crowe[1]; Ismael Cotte-Rodriguez[1]; *[1]L'Oreal, Clark, NJ*

TP 458 **Mass Spectrometric Detection of Polymeric and High-Mass Reaction Products from Low-Mass Siloxane Vapors under Benign Conditions: Implications for Micro-Electronic Devices**; Ryan Davis[1]; Nathan Bays[1]; David Schafer[1]; Justin Hall[1]; Tomas Babuska[1]; John Curry[1]; *[1]Sandia National Laboratories, Albuquerque, NM*

TP 459 **Determination of lithium salt in lithium battery electrolyte using ion chromatography coupled with high-resolution mass spectrometry**; Huimin Chen[1]; Zong Yang[2]; Bingjie Liu[3]; Lihai Guo[3]; *[1]SCIEX, Nanjing, China; [2]SCIEX, Shanghai, China; [3]SCIEX, Beijing, China*

TP 460 **Simplified Routine QC Monitoring of Glycans Using The ACQUITY™ QDa™ II Mass Detector**; Henry Foddy[1]; Scott Berger[2]; David Douce[1]; Cristian Cojocariu[1]; Ali Al Kaabi[3]; Andreas Fluetsch[3]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Waters Corporation, Milford, MA; [3]Johnson & Johnson Innovative Medicine, Bern, Switzerland*

TP 461 **A Novel Total Workflow for Polysorbates Analysis in Concentrated Protein Samples: from Sample Preparation to LC-ELSD Detection**; Chenchen He[1]; Limian Zhao[2]; *[1]Agilent Technologies, Wilmington, DE; [2]Agilent, WILMINGTON, DE*

TP 462 **NDSRI Risk Assessment and Trace-Level Analysis of N-Nitrosamines**; Joseph Lackey[1]; Dimple D. Shah[2]; Marian Twohigh[2]; Matthew Gregory[1]; Moritz Perscheid[1]; Amy Bartlett[2]; Peter Hancock[2]; *[1]LGC Standards, Manchester, NH; [2]Waters Corp, Milford , MA*

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TP 463 **Seeing is believing: interactive spectral annotation to aid glycoproteomics data interpretation**; Vishnu Rajan Tejus[1]; Tim S. Veth[1]; Nicholas M. Riley[1]; *[1]University of Washington, Seattle, WA*

TP 464 **Elucidating Lipid Metabolic Alterations in Early HCC Development**; Sun Jo Kim; *Chonnam National University, Gwangju, South Korea*

TP 465 **Lipid CAT: A Contaminant Annotation Tool for LC-MS Based Lipidomics**; Bowen Yang[1]; Carlos Canez[1]; Liang Li[1, 2]; *[1]University of Alberta, Edmonton, AB; [2]The Metabolomics Innovation Centre (TMIC), University of Alberta, Edmonton, AB*

TP 466 **Machine Learning-Enhanced LC-MS/MS Software Platform for High-Precision Metabolomics Quantification**; Pin-Yu Wang[1]; Rui-Yi Chen[1]; Hsiang-Yu Tang[2]; Mei-Ling Cheng[2]; Hui-Yin Chang[1, 3]; *[1]Department of Biomedical Sciences and Engineering, National Central University, Taoyuan, Taiwan; [2]Metabolomics Core Laboratory, Healthy Aging Research Center, Chang Gung University, Taoyuan, Taiwan; [3]Institute of Systems Biology and Bioinformatics, National Central University, Taoyuan, Taiwan*

TP 467 **Optimizing post-acquisition software detection of fecal amidated bile acids by LC-MS**; Stephen Barnes[1]; Landon S. Wilson[1]; Taylor F. Berryhill[1]; Youngmee Kim[2]; *[1]University of Alabama at Birmingham, Birmingham, AL; [2]University of Miami, FL, Miami, FL*

TP 468 **MassID: A Cloud-Based Untargeted Metabolomics Pipeline for Enhanced Biochemical Discovery**; Ethan Stancliffe[1]; Adam Richardson[1]; Monil Gandhi[1]; Ashima Mehta[1]; Doug Guzior[1]; Kevin Cho[2]; Tom Cohen[1]; Gary Patti[2]; *[1]Panome Bio, Saint Louis, MO; [2]Washington University in St. Louis, University City, MO*

TP 469 **An update of the asari suite of tools and an explanation of the metabolomics dark matter**; Joshua Mitchell[1]; Yuanye Chi[1]; Shuzhao Li[1]; *[1]Jackson Laboratory, Farmington, CT*

TP 470 **Rapid Human Serum Chemical Isotope Labeling LC-MS Metabolomics with Reverse Search**; Rui Qin[1]; Shuang Zhao[1]; Liang Li[1, 2]; *[1]The Metabolomics Innovation Centre, Edmonton, AB; [2]Department of Chemistry, University of Alberta, Edmonton, AB*

TP 471 **A Targeted Multi-Omic Investigation of Blood Sphingolipid Metabolism in the U-BIOPRED Cohort**; Grace Ratley[1]; Nicole Wagner[1]; Antonio Checa[1]; Ian M. Adcock[2]; Sven-Erik Dahlén[1]; Åsa M. Wheelock[1]; Craig E. Wheelock[1]; *[1]Karolinska Institutet, Solna, Sweden; [2]Imperial College London, London, United Kingdom*

TP 472 **SBML Model-Guided Metabolite Discovery: Computational Tools for Enhancing LC-MS/MS-Based Bioprocess Optimization**; Oguzcan Unver[1]; Benjamin Gerber[1]; *[1]Metastate Bio, Wilmington, DE*

TP 473 **Simulation-Based Library Optimization for Enhanced Metabolite Annotation Using KEGG and Correlation Scoring**; Nishu Nehra[1]; Jaspreet Singh[1]; Ayush Praveen[1]; Qiushi Sun[2]; Yogesh Lakhotia[1]; Rohit Swami[1]; Swetabh Pathak[1]; Richard G Kibbey[2, 3]; *[1]Elucidata, Cambridge; [2]Departments of Internal Medicine (Endocrinology), Yale University, New Haven, CT; [3]Department of Cellular & Molecular Physiology, Yale University, New Haven, CT*

TP 474 **Confident annotation of GPNAE and HexGPNAE in Caenorhabditis elegans aided by homologous series extension in LC-MS/MS data**; Nikolas Kessler[1]; Aiko Barsch[1]; Matthew R. Lewis[1]; Michael Witting[2]; *[1]Bruker Daltonics GmbH & Co.KG, Bremen, Germany; [2]Metabolomics and Proteomics Core, Helmholtz Munich, Munich, Germany*

TP 475 **Novel transformation product annotation with SIRIUS - Combining spectral libraries and structure databases**; Kai Dührkop[1]; Marcus Ludwig[1]; Martin Andre Hoffmann[1]; Markus Fleischauer[1, 2]; Martin Engler-Lukajewski[1]; Sebastian Böcker[2]; *[1]Bright Giant GmbH, Jena, Germany; [2]Friedrich Schiller University Jena, Jena, Germany*

TP 476 **MAD-Lib: A Shiny Application for Correlation-based Network Analysis of Large-Scale Metabolomics Data**; Qiushi Sun[1]; Nishu Nehra[2]; Ayush Praveen[2]; Mark P Keller[3]; Brian S Yandell[4]; Yogesh Lakhotia[2]; Alan D Attie[3, 5, 6]; Richard G Kibbey[1, 7]; *[1]Departments of Internal Medicine (Endocrinology), Yale University, New Haven, CT; [2]Elucidata Data Consulting Private Limited, San Francisco, CA; [3]Department of Biochemistry, University of Wisconsin-Madison, Madison, Wisconsin; [4]Department of Statistics, University of Wisconsin-Madison, Madison, WI; [5]Department* *of Chemistry, University of Wisconsin–Madison, Madison, WI; [6]Department of Medicine, University of Wisconsin-Madison, Madison, WI; [7]Department of Cellular & Molecular Physiology, Yale University, New Haven, CT*

TP 477 **A preliminary pan-cancer approach for ambient ionization mass spectrometry-based cancer detection**; Jacob I. Mardick[1]; Robert Tibshirani[2]; Livia S. Eberlin[1]; *[1]Department of Surgery, Baylor College of Medicine, Houston, Texas; [2]Departments of Biomedical Data Sciences and Statistics, Stanford University, Stanford, California*

TP 478 **LipidSearch 5.2: Improved Software for Parallel Processing of Large Datasets from LC-MS High Resolution Mass Spectrometry Based Lipidomics Workflows**; David A Peake[1]; Yuko Kitahashi[2]; Noritaka Masaki[2]; Yasuto Yokoi[2]; *[1]PEAKE PERFORMANCE LLC, Carmel, IN; [2]Mitsui Knowledge Industry Co., Ltd., Minato-ku, Japan*

TP 479 **Modified Cosine Similarity for Real-Time Library Search**; William Barshop[1]; Swati Anand[1]; Joshua Kelly[2]; Douglas Marchbank[2]; Jesse D. Canterbury[1]; Brandon Bills[1]; *[1]Thermo Fisher Scientific, San Jose, California; [2]Croda Canada, Concord, ON*

TP 480 **Machine learning to predict polymicrobial compositions from multi-omic HILIC-IM-MS data**; Lilith (Hongrui) Pan[1]; Kelly M Hines[1]; *[1]University of Georgia, Athens, GA*

TP 481 **Untargeted lipidomics and metabolomics studies of the navel orangeworm for monitoring in California tree nut landscape**; Anil Bhatia[1, 2]; Joshua Reger[1, 3]; Houston Wilson[1, 3]; *[1]University of California, Riverside, CA; [2]UCR Metabolomics Core, University of California, Riverside, California; [3]University of California Riverside, Kearney Agricultural Research and Extension Center, Parlier, California*

TP 482 **Integration of spatial lipidomics and transcriptomics in mouse models of Alzheimer's disease identifies culpability of the acyl chain remodeling pathway**; Laura Beth McIntire[1]; Artur Lazarian[1]; Krista Wartchow[1]; William Dartora[1]; Nicholas Bartelo[1]; Ana Costa[2]; Carmen Barrios Castellanos[1]; Jan Krumsiek[1]; Tal Nuriel[3]; Vilas Menon[3]; *[1]Weill Cornell Medicine, New York, NY; [2]University of Pittsburgh, Pittsburgh, PA; [3]Columbia University Medical Center, New York, NY*

TP 483 **Mass.Wiki as novel informatics resource for confident and transparent compound annotations in metabolomics, lipidomics and exposome research**; Oliver Fiehn[1]; Fanzhou Kong[2]; Quentin Wang[2]; Gert Wohlgemuth[2]; Yuanyue Li[2]; *[1]UC Davis, Davis, CA; [2]West Coast Metabolomics Center, University of California, DAVIS, CA*

TP 484 **The PTFI Metabolomics Data Pipeline and Library to Support the Standardized Analysis of Foods**; Steven M Watkins[1]; Chi-Ming Chien[1]; Bruce Yu[1]; Robnet Kerns[1]; Edmund Tong[1]; Selena Ahmed[2]; *[1]Verso Biosciences, Inc., Davis, CA; [2]American Heart Association, Dallas, TX*

TP 485 **CHEMPASS; A Tool for Rapid Chemical Structure Similarity Scoring and Clustering from Common Identifiers**; Kruttika Dabke[1]; Darren Kessner[1]; Jonathan E Katz[1, 2]; *[1]Ellison Medical Institute, Los Angeles, CA; [2]University of Southern California, Los Angeles, CA*

TP 486 **Multi-Fragmentation Mechanisms Enhance Small Molecule Site Localization in ModiFinder - Combining CID and EAD**; Mohammad Reza Zare Shahneh[1]; Michael Strobel[2]; Yasin El Abiead[3]; Mingxun Wang[2]; *[1]University of California, Riverside, Riverside, CA; [2]University of California, Riverside, CA; [3]Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, San Diego, CA*

TP 487 **Deep learning methods for metabolite annotation**; Hoi Yan Katharine Chau[1]; Xinran Zhang[1]; Habtom W Ressom[1]; *[1]Georgetown University, Lombardi Cancer Center, Washington, DC*

TP 488 **Reducing False Annotations in Lipidomics using Compound Discoverer 3.4 software**; Rahul Ravi Deshpande[1]; Ralf Tautenhahn[1]; Bashar Amer[1]; Giorgis Isaac[1]; Susan S Bird[1]; *[1]Thermo Fisher Scientific, San Jose, California*

TP 489 **A Multi-Agent, Domain-Specific Chatbot for Metabolomics and Lipidomics with Sub-Domain Retrieval and LLM Orchestration**; Harshani Bandara[1]; Rukshan Wijesinghe[1]; Leiver Campeon[1]; Mihira K Vithanage[1]; Lalin Theverapperuma[1]; *[1]Expert Intelligence, Santa Clara, CA*

TP 490 **Reproducibility of metabolomic profiles generated using the TruQuant platform in a multi-lab "round robin" study design**; Haley Chatelaine[1]; Chris Beecher[2]; Ewy Mathe[1]; *[1]National Center for Advancing Translational Sciences, Rockville, MD; [2]IROA Techcnologies, Chapel Hill, NC*

TP 491 **metLinkR: facilitating metaanalysis of human metabolomics data through automated linking of metabolite identifiers**; Andrew Patt[1]; Iris Pang[1]; Pin Han Lee[1]; Chiraag Gohel[2]; Eoin Fahy[3]; Vicki Stevens[1]; David Ruggieri[4]; Steven C Moore[4]; Ewy Mathé[1]; *[1]National Center for Advancing Translational Sciences (NCATS), Rockville, MD; [2]George Washington University, Washington, DC; [3]University of California San Diego, San Diego, CA; [4]National Cancer Institute, Bethesda, MD*

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TP 492 **Improved quantitative accuracy in data-independent acquisition proteomics via retention time boundary imputation**; Lincoln J Harris[1]; Michael Riffle[1]; Michael J. MacCoss[1]; William S. Noble[1]; *[1]University of Washington, Seattle, WA*

TP 493 **Ion Level Accounting Reveals Vast Untapped Potential in LC-MS Proteomics Datasets**; Mohammed Alhigaylan[1, 2]; Brendon Seale[3]; Anne-Claude Gingras[1, 3]; Hannes Röst[1, 2, 4]; *[1]Department of Molecular Genetics, University of Toronto, Toronto, ON; [2]Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, ON; [3]Lunenfeld-Tanenbaum Research Institute, Toronto, ON; [4]Department of Computer Science, University of Toronto, Toronto, ON*

TP 494 **A living proteomics benchmark for comprehensive evaluation of deep learning-based de novo peptide sequencing tools**; Marina Pominova[1]; Wout Bittremieux[1]; *[1]University of Antwerp, Antwerpen, Belgium*

TP 495 **Optimizing Peptide Selection for Quantitative Proteomics: A Mixed Method Approach to Enhance Accuracy and Precision**; Simon Perrin[1]; JEAN-CLAUDE CHARTRAND[1]; Jean-François Noel[1]; Hugo Gagnon[1]; *[1]Allumiqs, Sherbrooke, QC*

TP 496 **Effect of Imputation and Normalization Methods on Interpretation of Neuropeptide Dynamics in Label-free Peptidomics**; Elena V Romanova[1]; Yongxin Cai[2]; Jonathan V Sweedler[3]; *[1]University of Illinois at Urbana-Champaign, Urbana, IL; [2]university of Illinois-Urbana Champaign, Urbana, IL; [3]University of Illinois Urbana-Champaign, Urbana, IL*

TP 497 **Stitching together de novo peptides into full protein sequences: assembly of antibodies and beyond**; Douwe Schulte[1]; Auke Heerdink[2]; *[1]Utrecht University, Utrecht, Netherlands; [2]Utrecht University, Utrecht, Netherlands*

TP 498 **Enhancements of the Mzion Search Engine for Proteomics Data Analysis in 2025**; Qiang Zhang; *Washington University School of Medicine, St. Louis, MO*

TP 499 **Workflows for Relative Quantitation of Peptides Using Parallel-Accumulation Mobility-Aligned Fragmentation Acquisition**; Lauren C Royer[1]; Leonard Rorrer[2]; Isabel Uribe[2]; Daniel Debord[2]; *[1]MOBILion Systems, Inc, Chadds Ford, PA; [2]MOBILion Systems, Inc., Chadds Ford, PA*

TP 500 **Fast and Effective Open Modification Spectral Library Search**; Younghee Seo[1]; Seunjin Na[2]; Eunok Paek[1]; *[1]Hanyang University, Seoul, South Korea; [2]Korea Basic Science Institute (KBSI), Cheongju, South Korea*

TP 501 **Harnessing the ion mobility dimension to improve quantification in dia-PASEF**; Grzegorz Skoraczyński[1]; Sebastian Müller[1]; Oliver M. Bernhardt[1]; Monika Pepelnjak[1];

Véronique Laforte[1]; George Rosenberger[2]; Roland Bruderer[1]; Tejas Gandhi[1]; Lukas Reiter[1]; *[1]Biognosys AG, Schlieren, Switzerland; [2]Bruker Switzerland AG, Fällanden, Switzerland*

TP 502 **QuaVaProt: A Peptide Selection tool and a knowledgebase for Variant Protein Quantitation**; Constantinos Blidjios[1]; Pallab Bhowmick[1]; Vincent R. Richard[2]; Yassene Mohammed[1, 3]; Christoph H. Borchers[1, 4, 5, 6]; *[1]Gerald Bronfman Department of Oncology, Montreal, QC; [2]Segal Cancer Proteomics Centre, Jewish General Hospital, Montreal, QC; [3]LUMC, Leiden, Netherlands; [4]Segal Cancer Center, Lady David Institute, McGill University, Montreal, QC; [5]Division of Experimental Medicine, McGill University, Montreal, QC; [6]Department of Pathology, McGill University, Montreal, QC*

TP 503 **PRM-like DIA and Peptide-centric Query vs. Digital Proteomes by the first principles for Disease-specific Proteoform Discovery**; Wen Yu[1]; Jixin Wang[1]; Wenrong Chen[2]; Anqi Tu[1]; Andrew Chambers[1]; Wei Tang[1]; John Bullen[1]; Matthew Glover[1]; Bing Zhang[2]; Jonathan Mangion[3]; *[1]AstraZeneca, Gaithersburg, MD; [2]Baylor College of Medicine, Houston, TX; [3]AstraZeneca, Cambridge, United Kingdom*

TP 504 **A universal search algorithm for bottom-up proteomics**; Daniel P. Zolg[1]; Florian Seefried[1]; Michael Graber[1]; Patroklos Samaras[1]; Igor Bronshtein[2]; Lizi Mamisashvili[1]; Vishal Sukumar[1]; Samia Ben Fredj[1]; Markus Schneider[1]; Layla Eljagh[1]; Dulguun Bold[1]; Michelle T. Berger[1]; Alexander Hogrebe[2]; Siegfried Gessulat[2]; Tobias Schmidt[1]; Martin Frejno[1]; *[1]MSAID, Garching b.München, Germany; [2]MSAID, Berlin, Germany*

TP 505 **Customizable machine learning adapter improves LFQ in Mascot Distiller**; Richard J Jacob[1]; Patrick Emery[2]; Ville Koskinen[2]; *[1]Matrix Science Inc., Boston, MA; [2]Matrix Science, London, United Kingdom*

TP 506 **Examining the Capability of Ion Mobility Data to Improve Sensitivity of Open Modification Searches**; Benjamin Pullman[1]; Shreya Ahuja[1]; Shannon Marshall[1]; Matthew Glover[1]; Stewart MacArthur[2]; Sonja Hess[1]; *[1]AstraZeneca, Gaithersburg, Maryland; [2]AstraZeneca, Cambridge, United Kingdom*

TP 507 **Spectrum-centric analysis of timsTOF data with Chimerys**; Daniel P Zolg[1]; Vishal Sukumar[1]; Florian Seefried[1]; Michael Graber[1]; Patroklos Samaras[1]; Igor Bronshtein[2]; Lizi Mamisashvili[1]; Samia Ben Fredj[1]; Markus Schneider[1]; Layla Eljagh[1]; Dulguun Bold[1]; Michelle T. Berger[1]; Alexander Hogrebe[2]; Siegfried Gessulat[2]; Tobias Schmidt[1]; Martin Frejno[1]; *[1]MSAID, Garching b.München, Germany; [2]MSAID, Berlin, Germany*

TP 508 **PepCentric Enables High-Speed Repository-Scale Peptide Searching with Robust False Discovery Rate Control**; Fengchao Yu[1]; Andy T. Kong[1]; Yi Hsiao[1]; Alexey I. Nesvizhskii[1]; *[1]University of Michigan, Ann Arbor, MI*

TP 509 **Systematic assessment of deep learning-based predictors of fragmentation intensity profiles**; Mehdi Bagheri Hamaneh[1]; Aleksey Ogurtsov[1]; Oleg Obolensky[1]; Yi-Kuo Yu[1]; *[1]Division of Intramural Research, National Library of Medicine, National Institutes of Health, Bethesda*

TP 510 **O Peptide Where Art Thou: A Recommender System to Find Missing Peptides Between Runs**; Sebastian J. Paez[1]; Lillian T.A. Tatka[1]; Anastasiya Prymolenna[1]; Carolyn Allen[1]; Lindsay K Pino[1]; Alexander J. Federation[1]; William E Fondrie[1]; *[1]Talus Bioscience, Seattle, WA*

TP 511 **Improving De Novo Sequencing with Mass Errors and Retention Time Information**; Junkang Wei[1]; Fengchao Yu[1]; Alexey I. Nesvizhskii[1]; *[1]University of Michigan-Ann Arbor, Ann Arbor, MI*

TP 512 **Correction of retention time shifts between deuterated and non-deuterated fragment series for TMTpro 32plex and 35plex datasets**; David Horn[1]; Philip Loziuk[2]; Frank Berg[3]; Kai Fritzemeier[3]; Pedro Navarro[3]; Waqas Nasir[3]; Rosa Viner[4]; Dustin Frost[5]; Ryan Bomgarden[5]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Raleigh, NC; [3]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [4]Thermo Fisher Scientific, San Jose, California; [5]Thermo Fisher Scientific, Rockford, IL*

TP 513 **Integrating TagGraph into Bruker ProteoScape: Automated Open Modification Discovery with timsTOF and de novo Sequencing**; Joshua E Elias[1]; Gadi Armony[2]; Tharan Srikumar[3]; *[1]Chan Zuckerberg BioHub, Stanford, CA; [2]Bruker Nederland B.V., Leiderdorp, Netherlands; [3]Bruker Ltd., Milton, ON*

TP 514 **PG-DIA: A proteogenomic workflow for novel peptide discovery by integrating transcriptomics and data-independent acquisition proteomics**; Wenrong Chen[1]; Matthew Glover[2]; Shreya Ajuha[2]; Shannon Marshall[2]; Matthew V. Holt[3]; Wen Yu[4]; Jixin Wang[5]; Wenyan Zhong[6]; Bing Zhang[3, 7]; *[1]Baylor College of Medicine, Houston, TX; [2]Discovery Sciences, BioPharmaceuticals R&D, AstraZeneca, Gaithersburg, MD; [3]Lester and Sue Smith Breast Center, Baylor College of Medicine, Houston, TX; [4]Data Science and AI, BioPharmaceuticals R&D, AstraZeneca, Gaithersburg, MD; [5]Oncology Data Science, AstraZeneca, Gaithersburg, MD; [6]Oncology Data Science, Oncology R&D, AstraZeneca, New York, NY; [7]Department of Molecular and Human Genetics, Baylor College of Medicine, Houston, TX*

TP 515 **Introduction of AlphaPeptDeep and Carafe Automated AI Spectral Library Construction in Skyline**; David Shteynberg[1]; Brendan X. MacLean[1]; Matthew C Chambers[1]; Nicholas Shulman[1]; Brian S. Pratt[1]; Bo Wen[1]; William S. Noble[1]; Michael J MacCoss[1]; *[1]University of Washington, Seattle, WA*

TP 516 **Pioneer and Altimeter: Fast and Open-Source tools for DIA Proteomics, Optimized for Narrow Isolation Windows**; Nathan T Wamsley[1]; Ben Major[1]; Dennis Goldfarb[1]; *[1]Washington University School of Medicine, St. Louis, MO*

TP 517 **Sensitive and Interpretable Supervised Learning for Peptide Identification with Spectral Library Searching**; Hao Xu[1, 2]; Nuno Bandeira[1, 2, 3]; *[1]Center for Computational Mass Spectrometry, University of California San Diego, La Jolla, CA; [2]Department of Computer Science and Engineering, University of California San Diego, La Jolla, CA; [3]Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA*

TP 518 **Specfind: A Novel Paradigm for Peptide Identification By Searching Spectral Archives**; Ayman Hoque[1]; Henry Lam[1]; *[1]Hong Kong University of Science and Technology, HONG KONG, Hong Kong*

TP 519 **SimpliFi your Peptides: a new level of omics analysis accessible to all**; Jim Palmeri[1]; John Wilson[1]; *[1]ProtiFi LLC, Fairport, NY*

TP 520 **Enhancing quantitative proteomics with transcriptome-derived peptide databases using accurate long-read sequencing**; Regina M Edgington[1]; Jacob W Smith[1, 2]; Paul A Nicolosi[1]; Trenton J Winters[1]; Vladislav Belyy[1, 2]; Damien B Wilburn[1, 2]; *[1]The Ohio State University Department of Chemistry and Biochemistry, Columbus, OH; [2]Ohio State Biochemistry Program (OSBP), The Ohio State University, Columbus, OH*

TP 521 **Enhanced Antibody De Novo Sequencing via Transformer-Based Deep Learning**; Rukshan Wijesinghe[1]; Mihira K Vithanage[1]; Harshani Bandara[1]; Leiver Campeon[1]; Sebastian F Gómez[1]; Osanda Hemachandra[1]; Andi Krupke[1]; Lalin Theverapperuma[1]; *[1]Expert Intelligence, Santa Clara, CA*

TP 522 **Quetzal: Comprehensive Peptide Fragmentation Annotation and Visualization**; Luis Mendoza[1]; Robert L. Moritz[1]; Eric Deutsch[1]; *[1]Institute for Systems Biology, Seattle, WA*

TP 523 **Constructing a large-scale search engine training dataset of marginal peptide matches using matched-matrix calibration curves**; Brian C. Searle[1]; Teeradon Phlairaharn[1]; Ariana E. Shannon[1]; *[1]The Ohio State University, Columbus, OH*

TP 524 **Comprehensive isoform annotations and quantitation in DIA data**; Ignat Shilov[1]; Christian Heckendorf[1]; Abhishek Roushan[1]; Gary Wilson[1]; Claire Bramwell[1]; *[1]Protein Metrics, Boston, MA*

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TP 525 **Lipidomic Approach to Define Calcineurin Control over Antifungal Response in Aspergillus fumigatus**; Ahsan Hameed[1, 2]; William J Steinbach[2]; Colin D. Kay[1, 2]; Andrew J. Morris[1, 2]; Praveen R Juvvadi[2]; *[1]Arkansas Children's Nutrition Center, Little Rock, AR; [2]University of Arkansas for Medical Sciences, Little Rock, AR*

TP 526 **Changes to the Pseudo-nitzschia Lipidome After Exposure to Copepodamides Using UHPLC Coupled with High Resolution Multireflecting TOF Mass Spectrometry**; Aubrey Trapp[1]; Raphe Kudela[1]; Andrew Baker[2]; *[1]University of California Santa Cruz, Santa Cruz, CA; [2]Waters Corportaion, Pleasanton, CA*

TP 527 **MALDI MSI and Lipidomics Reveal Lipid Release in Ovarian Cancer Models**; Carlismari O. Grundmann[1]; Hannah Lusk[2]; Monica Haughan[3]; Joanna E. Burdette[3]; Laura Sanchez[2]; *[1]University of California - Santa Cruz, Santa Cruz, CA; [2]University of California, Santa Cruz, Santa Cruz, CA; [3]University of Illinois at Chicago, Chicago, IL*

TP 528 **Addressing isobaric overlaps in cholesterol ester analysis using advanced chromatography and high-resolution MS**; Goncalo Vale[1]; Daniel Smith[1]; Jeffrey G McDonald[1]; *[1]UT Southwestern, Dallas, TX*

TP 529 **Automated Deep Lipidomic Analysis of Environmental Samples using Electron Activated Dissociation and Ion-Mobility Spectrometry with Ozone Induced-Dissociation**; Patrick Mueller[1]; Dylan H. Ross[2]; Jesse B. Trejo[2]; Xueyun Zheng[2]; Aivett Bilbao[2]; Gérard Hopfgartner[1]; *[1]University of Geneva, Geneva, Switzerland; [2]PNNL, Richland, WA*

TP 530 **High-throughput plasma lipid profiling with the acoustic ejection high resolution mass spectrometry (AE HRMS)**; Eva Duchoslav[1]; Pradeep Narayanaswamy[2]; Venkatesha Gaddemane Narasimha[2]; Hyungwon Choi[3]; *[1]SCIEX, Concord, ON; [2]SCIEX, Singapore, Singapore; [3]National University of Singapore, Singapore, Singapore*

TP 531 **Lipidomics signature of obese adipocytes**; Ana Arias Marroquín[1]; Iván Torre-Villalvazo[1]; Mariana Villegas Romero[1]; Aneliz De Ita Zárate Ortiz[1]; Melanie Odenkirk[2]; Natalia Vázquez-Manjarrez[1]; *[1]Instituto Nacional de Ciencias Médicas y Nutrición, Salvador Zubirán, Mexico city, Mexico; [2]Colorado State University, Department of Horticulture and Landscape Architecture, Fort Collins, CO*

TP 532 **High-throughput nanoscale synthesis and susceptibility testing of new antibiotics using an automated desorption electrospray ionization platform**; Alexis Rae Toney[1]; Kitmin Chen[2]; Kai-Hung Huang[2]; Nicolas M Morato[2]; R. Graham Cooks[2]; *[1]Purdue University, West Lafayette, IN; [2]Purdue Univeristy, West Lafayette, IN*

TP 533 **Enhancing our understanding of viroceuticals using an optimized mass spectrometry-based lipidomics approach**; Joshua Roberts[1]; Elena Godbout[2]; Jocelyn Menard[3]; Christopher Boddy[4]; Jean-Simon Diallo[1, 2]; Jeffrey C. Smith[3]; *[1]Virica Biotech, Ottawa, ON; [2]Ottawa Hospital Research Institute, Ottawa, ON; [3]Carleton University, Ottawa, ON; [4]University of Ottawa, Ottawa, ON*

TP 534 **Breaking the ionization challenge to increase the lipidome coverage by integrating SICRIT into the inlet capillary of QTOF/LCMS**; Atsuhiko Toyama[1]; Jan-Christoph Wolf[2]; Ciara Conway[2]; Thomas Wolf[2]; Takaaki Hiraoka[3]; *[1]Shimadzu Scientific Instruments, Boston, MA; [2]Plasmion GmbH, Augsburg, Germany; [3]Shimadzu Scientific Instruments, Columbia, MD*

TP 535 **Sex Differences in the Lipidome and Their Potential Role in Predicting Metabolic Diseases**; Mariana Villegas[1]; Aneliz De Ita Zárate[1]; David Chavaro[1]; María Del Sol Pacheco[1]; Itzelly Ibarra[1]; Ana T Arias[1]; Melanie T. Odenkirk[2]; Israel García[1]; Lilia Noriega[1]; Martha Guevara[1]; Daniel Illescas[1]; Natalia Vázquez[1]; *[1]Instituto Nacional de Ciencias Médicas y Nutrición, Salvador Zubirán, Mexico city, Mexico; [2]Colorado State University, Fort Collins, CO*

TP 536 **DeepProfiling: An Untargeted Lipidomics Strategy with Optimized Data Acquisition and Processing for Enhanced Lipid Coverage**; Jian Guo[1]; Sonnet Davis[1]; Jung Suh[1]; *[1]Denali Therapeutics, South San Francisco, CA*

TP 537 **Translational lipidomics: From lipid fingerprints of CVD in experimental models to human cohorts**; Frank Kumi[1]; Beichen Sun[2]; Rajinikanth Gogiraju[2]; Katrin Schäfer[2]; Laura Bindila[2]; *[1]Mainz University Medical Center, Institute of Physiological Chemistry, Mainz, Germany; [2]University Medical Center of Mainz, Mainz, Germany*

TP 538 **Targeted metabolomics approaches the global scale: profiling lipids in brain cancer by LC-triple Quadrupole-MS (LC-QQQ-MS)**; Sierra Napoleon[1]; Jihyun Kang[1]; Michaela Schwaiger-Haber[1]; Darshak Gadara[1]; Leah P. Shriver[1]; Gary J. Patti[1]; *[1]Washington University in St Louis, St. Louis, MO*

TP 539 **Comprehensive data acquisition workflow on a Modified Orbitrap Astral MS to achieve deep lipidome coverage with high confidence annotations**; Giorgis Isaac[1]; Alan Baik[2]; Rahul Ravi Deshpande[1]; Bashar Amer[1]; Ralf Tautenhahn[1]; Isha Jain[2]; Susan Bird[1]; *[1]Thermo Fisher Scientific, San Jose, California; [2]Gladstone Institute, UCSF, San Francisco, California*

TP 540 **A chemical derivatization approach for profiling unesterified fatty acids using LC-MS with selected ion monitoring**; Joby Jose[1]; Andrea Barrera Cruz[1]; Alfred N. Fonteh[1]; *[1]Huntington Medical Research Institutes, Pasadena, CA*

TP 541 **Lipid Makeover: How Aging Transforms Adipose and Liver Tissues**; Natalia Pascuali[1]; Fernando Tobias[2]; Sofija Jovanovic Gasovic[3]; Mark Sartain[4]; Karen Yannell[4]; Almudena Veiga-Lopez[3, 5]; *[1]University of Illinois Chicago, Chicago, IL; [2]Northwestern University, Evanston, IL; [3]Department of Pathology, University of Illinois Chicago, Chicago, IL; [4]Agilent Technologies, Inc., Santa Clara, CA; [5]Chicago Center for Health and Environment, University of Illinois Chicago, Chicago, IL*

TP 542 **Identification of dysregulated lipidomic and proteomic networks in Parkinson's disease patients mutated in TMEM175 with mass spectrometry approach**; Marco Ghirimoldi[1]; Federica Carrillo[2]; Veronica De Giorgis[1]; Shahzaib Kosho[1, 3]; Elettra Barberis[4, 5]; Teresa Esposito[2, 6]; Marcello Manfredi[1, 7]; *[1]Biological Mass Spectrometry Lab, Department of Translational Medicine, University of Piemonte Orientale, Novara, Italy; [2]Institute of Genetics and Biophysics "Adriano Buzzati-Traverso", National Research Council, Naples, Italy; [3]Center for Translational Research on Autoimmune and Allergic Diseases, University of Piemonte Orientale, Novara, Italy; [4]Center for Translational Research on Autoimmune and Allergic Diseases, University of Piemonte Orientale, Novara, Piemonte, Italy, Novara, Italy; [5]Department of Sciences and Technological Innovation, University of Piemonte Orientale, Alessandria, Italy; [6]IRCCS INM Neuromed, Pozzilli, Italy; [7]IRCCS Policlinico San Donato, Institute of Molecular and Translational Cardiology, Milan, Italy*

TP 543 **Comparative assessment of liquid-liquid extraction methods for lipidomics: Insights into matrix-specific performance**; Krishnateja Konduri[1]; Jeffrey G McDonald[1]; Goncalo Vale[1]; *[1]UT Southwestern, Dallas, TX*

TP 544 **Untargeted Shotgun Lipidomics Via Sequential Precursor Ion Fragmentation on an Orbitrap Mass Spectrometer**; Jianzhong Chen[1, 2]; Thai Minh Han Nguyen[1]; Wenbo Zhi[1]; *[1]Center for Biotechnology and Genomic Medicine, Medical College of Georgia, Augusta University, Augusta, GA; [2]Department of Cellular Biology & Anatomy, Medical College of Georgia, Augusta University, Augusta, GA*

TP 545 **Cholesterol esters in focus: Lipid profile in eggs, beef, chicken and fish**; Aneliz De I Zárate Ortiz[1]; Mariana Villegas Romero[1]; Itzelly Ibarra Valdovinos[2]; Daniel Illescas[2]; Israel

García Cano[3]; Melanie T. Odenkirk[4]; Natalia Vázquez Manjarrez[1]; David Chavaro[1]; Ana T Arias[1]; María Del Sol Pacheco[1]; Lilia Noriega Lopez[1]; Martha Guevara Cruz[1]; *[1]Department of Nutrition Physiology, Metabolomics Unit, INCMNSZ, Mexico city, Mexico; [2]Department of Epidemiology, INCMNSZ, Mexico city, Mexico; [3]Department of Food Science and Technology, INCMNSZ, Mexico city, Mexico; [4]Colorado State University, Department of Horticulture and Landscape Architecture, Fort Collins, CO*

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TP 546 **Analysis of Adduct- and Collision Energy-Driven Variability in MS/MS Fragmentation Patterns**; Botao Liu[1]; Tao Huan[1]; *[1]University of British Columbia, Vancouver, BC*

TP 547 **Improving Detection of Metal-Binding Compounds in Liquid Chromatography Tandem Mass Spectrometry**; Daniel J Breiner[1]; Vanessa V Phelan[1]; *[1]CU Anschutz Skaggs School of Pharmacy and Pharmaceutical Science, Aurora, CO*

TP 548 **iModMix: Integrative Modules for Multi-omics Data Analysis**; Isis Narvaez-Bandera[1]; Ashley Lui[1]; Yonatan Ayalew Mekonnen[1]; Vanessa Rubio[1]; Noah Sulman[2]; Hayley Ackerman[1]; Oscar Ospina[1]; Guillermo Gonzalez-Calderon[1]; Elsa Flores[1]; Qian Li[3]; Ann Chen[4]; Brooke L Fridley[5]; Paul Stewart[4]; *[1]Moffitt Cancer Center, Tampa, FL; [2]University of South Florida, Tampa, FL; [3]St. Jude Children's Research Hospital, Memphis, TN; [4]Huntsman Cancer Institute, Salt Lake City, UT; [5]Children's Mercy Research Institute, Kansas City, MO*

TP 549 **Highly Sensitive Chemical Isotope Labeling LC-MS for Single Islet Metabolomics**; Xian Luo[1]; Paulo Jose Basso[2]; Sue Tsai[2]; Liang Li[3]; *[1]The Metabolomics Innovation Centre, Edmonton, AB; [2]University of Alberta, Faculty of Medicine & Dentistry - Medical Microbiology and Immunology Dept, Edmonton, Alberta; [3]University of Alberta, Faculty of Science, Chemistry Department, Edmonton, AB*

TP 550 **A workflow for Scout triggered MRM approach for targeted metabolomics at the untargeted scale for biomarkers discovery**; Rémy DE BONI[1]; Yohann CLEMENT[1]; Guillaume ROSSIGNOL[2]; Jérôme LEMOINE[1]; Sophie Ayciriex[1]; Delphine ARQUIER[1]; Jerôme RANDON[1]; Arnaud SALVADOR[1]; *[1]University Claude Bernard Lyon1, ISA, UMR5280, CNRS, Villeurbanne, France; [2]Hospices Civils de Lyon, LYON, France*

TP 551 **Metabolic Characterization of Common Bacterial Growth Media**; Megan Danielewicz[1]; Caroline Lawler[2]; Ryan D Leib[1]; Allis S Chien[1]; Emma R Guiberson[2, 3]; *[1]Stanford University Mass Spectrometry, Stanford, CA; [2]Program of Molecular Biology and Biochemistry, Middlebury College, Middlebury, VT; [3]Department of Chemistry, Middlebury College, Middlebury, VT*

TP 552 **Innovative Derivatization Strategies for LC/MS Quantitation of Phosphate-Containing Metabolites**; Alena Langova[1, 2]; Liang Li[2, 3]; Michal Holčapek[1]; *[1]University of Pardubice, Pardubice, Czech Republic; [2]University of Alberta, Edmonton, AB; [3]The Metabolomics Innovation Centre and Department of Chemistry, University of Alberta, Edmonton, AB*

TP 553 **M-TICM: A Data Alignment and Integration Approach for Multicenter Metabolomics**; Jinna Dai[1]; Xiaozhe Zhang[2]; Hong Shang[3]; *[1]National Clinical Research Center for Laboratory Medicine, Department of Laboratory Medicine, The First Hospital of China Medical University, Shenyang, China; [2]Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China; [3]National Clinical Research Center for Laboratory Medicine, Department of Laboratory Medicine, The First Hospital of China Medical University, Shenyang, China*

TP 554 **Metabolomic profiling of human monocyte differentiation into macrophages and dendritic cells**; Fernando Erra Díaz[1]; Elizabeth S Aiken[2]; Maheshwor Thapa[2]; Shuzhao Li[2, 3]; *[1]Facultad de Medicina, Instituto de Investigaciones Biomédicas en Retrovirus y SIDA Universidad de Buenos Aires, CONICET, Buenos Aires, Argentina; [2]The Jackson Laboratory for Genomic Medicine, Farmington, CT; [3]University of Connecticut School of Medicine, Farmington, CT*

TP 555 **Target metabolome profiles in human saliva distinct from those in human plasma**; Mijeong Kim[1]; HAEUN SONG[1]; Hyo Yeong Lee[1]; Su Jung Kim[1]; Hyun Ju Yoo[2]; *[1]ASAN Medical center, SEOUL, South Korea; [2]Asan Medical Center, Seoul, South Korea*

TP 556 **LCMS-MS/MS and Spatial OMIC MALDI-MSI-Based Quinomics Reveals Novel CoQ10 Metabolism in COQ4-Deficient Mice Following Treatment with BPM31510**; Juan J Aristizabal-Henao[1]; Sylwia Stopka[1]; Stephane Gesta[1]; Devon Van Cura[1]; Srada Karmacharya[1]; Megan K Cox[1]; Alba Pesini[2]; Eliana Barriocanal Casado[2]; Catarina M Quinzii[2]; Vijay Modur[1]; Niven R Narain[1, 3]; Michael A. Kiebish[1]; *[1]BPGbio, Framingham, MA; [2]Columbia University, New York, NY; [3]University of Miami, Miami, Florida*

TP 557 **Qualitative and Quantitative Analysis of Serum from Colon Cancer Patients Using Untargeted and Targeted Metabolomics**; Kevin Y Cho[1]; Ashima Mehta[2]; Monil Gandhi[2]; Adam Richardson[2]; Stephen Dearth[3]; Ethan Stancliffe[2]; Gary Patti[1]; *[1]Washington University School of Medicine, St. Louis, MO; [2]Panome Bio, Saint Louis, MO; [3]biocrates life sciences ag, Innsbruck, Austria*

TP 558 **Metabolome-Wide Association Study of Micro- and Nanoplastic Exposures in Human Placenta Cells**; Kuanliang Shao[1]; Hanna Dusza[2]; Anna Robuck[3]; Anna Young[1]; Karthikeyan Bagavathy Shanmugam[1]; Ronald D. Smith Jr. [1]; Yewei Wang[1]; Donghai Liang[1]; Juliette Legler[2]; Roel Vermeulen[2]; Douglas I. Walker[1]; *[1]Emory University, Atlanta, GA; [2]Utrecht University, Utrecht, Netherlands; [3]University of Rhode Island, Narragansett, RI*

TP 559 **Hepatocellular Metabolic Profile: Understanding Post-Thawing Metabolic Shift in Primary Hepatocytesin vitro**; Salvator Palmisano[1]; Emilio S. Rivera[1]; Tara Harvery[1]; Joshua Breidenbach[1]; Brett Blackwell[1]; Chi Yen Tseng[1]; Madison Grace Thornhill[1]; Emilia Solomon[1]; Claire Sanders[1]; Kes Luchini[1]; Erick S Lebrun[2]; Ethan M. McBride[1]; Jessica A. Salguero[1]; Francie E. Rodriguez[1]; Philip Mach[1]; Trevor G. Glaros[1]; *[1]Los Alamos National Lab, Los Alamos, NM; [2]LMI, Colorado Springs, CO*

TP 560 **Building Biologically Relevant Libraries: How Comprehensive Libraries and Deep MS/MS Coverage Enable Intelligent Library Growth**; Richard J Robinson[1]; Tess Mendoza[1]; Bashar Amer[2]; Susan S Bird[3]; Matthew W Mitchell[1]; Annie M Evans[1]; *[1]Metabolon, Durham, NC; [2]Thermo Fisher Scientific, 355 River Oaks Pkwy, San Jose, CA95134; [3]Thermo Fisher Scientific, Boston, MA*

TP 561 **Comprehensive Metabolite Profiling in Formalin-Fixed Paraffin-embedded Tissues**; Ashima Mehta[1]; Ethan Stancliffe[1]; Kevin Y Cho[2]; Monil Gandhi[1]; Douglas V Guzior[1]; Adam D Richardson[1]; Sharla Friend[1]; Tom Cohen[1]; Gary J Patti[2]; *[1]Panome Bio, St Louis, MO; [2]Washington University School of Medicine, St. Louis, MO*

TP 562 **Non-Targeted LC-HRMS and GC-MS Analysis of Illicit Flavored ENDS Products**; Diane Wallace[1]; Aliya Al-Habsha[1]; Norman Fraley[1]; Vincent Nip[1]; Manali Aggrawal[1]; Bob Moision[1]; Cameron Smith[1]; Gene Gillman[1]; *[1]Juul Labs, Washington, DC*

TP 563 **Automated and Robust CE-MS Metabolomics with Stable Isotope-Labeled Standards: From QC to Quantification**; Andrew J Percy[1]; Erin Redman[2]; J. Will Thompson[2]; *[1]Cambridge Isotope Laboratories, Inc., Tewksbury, MA; [2]908 Devices, Inc., Morrisville, NC*

TP 564 **Metabolome and Glycosphingolipidome Alterations in Pancreatic Ductal Adenocarcinoma Cells Undergoing Epithelial-Mesenchymal Transition by LC-MS/MS**; Akeem Sanni[1]; Sarah Sahioun[1]; Alfredo Reyes-Oliveras[2]; Brian Haab[2]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX; [2]Van Andel Institute, Grand Rapids, MI*

TP 565 **Simultaneous Quantitation and Discovery (SQUAD) analysis of flavonoid conjugates in blood, urine and**

food using high flow and nanoflow LC-MS/MS; Yendry Carvajal-Miranda[1]; Bashar Amer[2]; Rahul R. Deshpande[2]; Susan S. Bird[2]; Brandon Bills[2]; Debra K. M. Tacad[3]; Brian J. Bennett[3]; John W. Newman[3]; Oliver Fiehn[1]; *[1]University of California-Davis, Davis, CA; [2]Thermo Fisher Scientific, San Jose, CA; [3]USDA-ARS-WHNRC, Davis, CA*

TP 566 **SQUAD metabolomics: uniting targeted precision and untargeted discovery for in-depth fecal metabolite profiling on Orbitrap Astral MS**; Bashar Amer[1]; Steven Danielson[2]; Ayush Midha[3]; Isha Jain[3]; Rahul R. Deshpande[1]; Thomas Moehring[4]; Susan S Bird[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientfic, San Jose, CA; [3]Gladstone Institute, UCSF, San Francisco, California; [4]Thermo Fisher Scientific, Bremen, Germany*

TP 567 **Discovering Protein-Metabolite Ligand Interactions using Equilibrium Dialysis Tandem LC-MS Metabolomics**; Zihan Monshad[1]; Christina Volz[1]; Jacob West[1]; Daniel Newell[1]; Jared Rutter[1]; Kevin G. Hicks[1]; *[1]University of Utah, Salt Lake City, UT*

TP 568 **A novel QTOF with a 10x sensitivity boost enables multimodal metabolomics and lipidomics**; Vincen Wu[1]; Jason Causon[2]; Adriano Rutz[1]; Abraham Moyal[1]; Nicola Zamboni[1]; *[1]ETH Zürich, Zürich, Switzerland; [2]SCIEX, Concord, ontario*

TP 569 **Batch Correction for Metabolomics Data: Analysis of 90 Batches Acquired Over 4 Years**; Michaela Schwaiger-Haber[1]; Ethan Stancliffe[1, 2]; Gary Patti[1]; *[1]Washington University in St. Louis, St. Louis, MO; [2]Panome Bio, Saint Louis, MO*

TP 570 **High-resolution untargeted metabolomics of tea using a modified Orbitrap Astral mass spectrometer**; Bashar Amer[1]; Daniel Hermanson[2]; Eugen Damoc[3]; Anna V. Pashkova[4]; Martin Zeller[4]; Tabiwang N. Arrey[4]; Rahul R. Deshpande[2]; Thomas Moehring[4]; Susan S Bird[2]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]ThermoFisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [4]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

TP 571 **Biochemical phenotyping of null alleles in human induced pluripotent stem cell-derived cell lineages: integrating genetics with metabolomics**; Joshua M Mitchell[1]; Maheshwor Thapa[1]; Shujian Zheng[1]; Juliana Alcoforado Diniz[1]; Nelio Oliveira[1]; Yuanye Chi[1]; Amnah Siddiqa[1]; Minghao Gong[1]; Justin McDonough[1]; William Skarnes[1]; Paul Robson[1]; Shuzhao Li[1, 2]; *[1]The Jackson Laboratory for Genomic Medicine, Farmington, CT; [2]University of Connecticut School of Medicine, Farmington, CT*

TP 572 **Quantification of the Effects of Hair Treatment on Cholesterol Metabolite Concentration Via Liquid Chromatography-Mass Spectrometry**; Corinne Dilger[1]; Jenna Schuler[1]; Anjolaoluwa Favour Oyebadejo[1]; Mary Saczawa[1]; Sarah Fantin[1]; *[1]Hanover College, Hanover, IN*

TP 573 **Enhancing SQUAD Innovations: Comparative Assessment of Simultaneous Quantitation and Discovery Workflow for Organic Acids Analysis Using Multiple Chromatographic Techniques**; Justin Y Elliott[1]; Bashar Amer[2]; Priya Viathee[2]; Susan Bird[2]; Hussain A Abdulla[1]; *[1]Department of Physical and Environmental Sciences, Texas A&M University Corpus Christi, Corpus Christi, TX; [2]Thermo Fisher Scientific, San Jose, CA*

TP 574 **Expanding normalization coverage in LC-MS based untargeted metabolomics experiments**; Olivia Taverniti[1]; J. Rafael Montenegro-Burke[1]; *[1]University of Toronto, Toronto, ON*

TP 575 **Metabolite Genome-Wide Association Analysis Reveals Genetic Control of Phenolics in Breeding-Relevant Apple Germplasm**; Cristian Daniel Quiroz-Moreno; *Ohio State University, Colubus, OH*

TP 576 **Sharpen Your Peaks: Novel Column Hardware for Improved HILIC Polar Metabolite Chromatography**; Karen Yannell[1]; Cate Simmermaker[1]; Sierra D. Durham[1]; Jordy J. Hsiao[1]; *[1]Agilent Technologies, Santa Clara, CA*

TP 577 **Metabolic impact of persistent viral infections in mosquitoes**; Paul S. Soma[1]; Oshani C. Ratnayake[1]; Irma Sanchez-Vargas[1]; Samantha M. Pinto[1]; Rushika Perera[1]; *[1]Colorado State University, Fort Collins, CO*

TP 578 **Increasing confidence in non-targeted metabolite identification with library comparison and simplified unknown analysis workflow with novel software solution**; Cate Simmermaker[1]; Karen E Yannell[1]; Sierra D Durham[1]; *[1]Agilent Technologies, Santa Clara, CA*

TP 579 **Applying IROA suppression correction, normalization and batch effect algorithms to a published dataset augments previous results**; Felice A de Jong[1]; Chris Beecher[1]; *[1]IROA Technologies LLC, Nellysford, VA*

TP 580 **Metabolomic Analysis of Dried Blood Spots Collected on Multiple Collection Cards**; Monil Gandhi[1]; Ethan Stancliffe[1]; Ashima Mehta[1]; Douglas V Guzior[1]; Adam Richardson[1]; Kevin Cho[2]; Tom Cohen[1]; Gary Patti[2]; *[1]Panome Bio, Saint Louis, MO; [2]Washington University School of Medicine, St. Louis, MO*

TP 581 **Incremental Clustering for MS/MS Data in Metabolomics: A Scalable Approach for High-Throughput MS/MS Data Analysis**; Xianghu Wang[1]; Mingxun Wang[2]; *[1]University of California, Riverside, riverside, CA; [2]University of California, Riverside, CA*

TP 582 **Mechanistic insights into mitochondrial dysfunction captured by high-throughput metabolomics**; Ritchie Ly[1]; Ana S. H. Costa[2]; Jennifer M. Campbell[2]; Justin R. Cross[1]; *[1]Memorial Sloan Kettering Cancer Center, New York, NY; [2]Matterworks, Somerville, MA*

TP 583 **Evaluation of Polyunsaturated Fatty Acid Pathways in Lung Adenocarcinoma Tissue via UHPLC-HRMS/MS and MALDI-Ion Mobility-Mass Spectrometry Imaging**; Vanessa Rubio[1]; Hayley D. Ackerman[1]; Nicole Hackel[1]; Jaden Baldwin[1]; Christina Carr[1]; John H. Lockhart[1]; John M. Koomen[1]; Elsa R. Flores[1]; *[1]Moffitt Cancer Center, Tampa, FL*

TP 584 **Investigating the Role of Chain Length, Hydroxylation, and Unsaturation in Lipids Using Untargeted Lipidomics**; Minsoo Son[1]; Rencheng Wang[2]; Jaenyeon Kim[2]; Young Ah Goo[2]; *[1]Washington Univ. School of Medicine, Saint Louis, MO; [2]Washington University School of Medicine, St. Louis, MO*

TP 585 **Interpreting millions of metabolite mass spectra using DreaMS-Net – a neural network-based molecular networking**; Roman Bushuiev[1, 2]; Anton Bushuiev[2]; Josef Sivic[2]; Tomáš Pluskal[1]; *[1]IOCB Prague, Prague, Czech Republic; [2]Czech Institute of Informatics, Robotics and Cybernetics, Czech Technical University, Prague, Czech Republic*

TP 586 **Distinguishing co-eluting hexose phosphate isomers by fragmentation of alkali metal adducts**; Triston Groff[1]; Ronald Fowle-Grider[1]; Michaela Schwaiger-Haber[1]; Kevin Cho[1]; Gary J Patti[1]; *[1]Washington University in St. Louis, St. Louis, MO*

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TP 587 **Top-down characterization of intact siRNA complexes using direct infusion nanospray-MSn**; Sarah Mutchek[1]; Vladimir V. Papov, Jr. [2]; Scott Pennino[2]; Daniele Fabris[1, 3]; *[1]University of Connecticut, Storrs, CT; [2]Boehringer Ingelheim Pharmaceuticals, Inc., Ridgefield, CT; [3]RiboDynamics, Manchester, CT*

TP 588 **LC-HRMS and Hydrogen-Deuterium MS study for characterization of oxidative impurities of phosphorothioate oligonucleotide for CNS acting oligonucleotide therapeutics nusinersen**; Vijay S Bhalekar[1]; Ravi P Shah[1]; *[1]National Institute of Pharmaceutical Education and Research, Ahmedabad (NIPER-A),, Gandhinagar, India*

TP 589 **Discovery of Novel DNA-Histone Cross-links by Mass Spectrometry**; Kun Yang[1]; Ying Peng[1]; *[1]University of Texas at Austin, Austin, TX*

TP 590 **Characterization of mRNA Modifications by Ion-pairing LC-MS Techniques**; Xiaomei He; *ProtaGene, Burlington, MA*

TP 591 **Characterization of tRNA methylationusing the ZenoTOF® 7600 system**; Longlong Hu[1]; Ji Luo[1]; Hongxu Chen[2]; Bingjie Liu[2]; *[1]SCIEX, Shanghai, China; [2]SCIEX, Beijing, China*

TP 592 **Application of a Sequence-Specific Thermophilic Ribonuclease to Bottom-up RNA Analysis by LC-MS/MS**; Benjamin F Jepson[1]; Eric J Wolf[2]; Nan Dai[2]; Ivan R Correa Jr.[2]; Erbay Yigit[1]; *[1]New England Biolabs, Ipswich, MA; [2]New England Biolabs, Beverly, MA*

TP 593 **Examining a multi-enzyme strategy for mapping tRNA Modifications using LC-MS/MS**; Bibek Hamal[1]; Asif Rayhan[1]; Patrick A Limbach[1]; *[1]University of Cincinnati, Cincinnati, OH*

TP 594 **mRNA Sequence Mapping via Endonuclease Digestion and LC-MS Analysis with Novel Informatics Workflows**; Catalin E Doneanu[1]; Chris Preston[2]; Matt Gorton[2]; Tatiana Johnson[1]; Bala Addepalli[1]; Nick Pittman[2]; Ying Qing Yu[1]; *[1]Waters Corporation, Milford, MA; [2]Waters Corporation, Wilmslow, United Kingdom*

TP 595 **Multiple endonucleases for digestion of tRNA anticodon regions to conduct modification mapping by LC-MS/MS**; Hina Zain[1]; Yu Sun[2]; Bibek Hamal[1]; Asif Rayhan[1]; Ann Ehrenhofer-Murray[2]; Patrick Limbach[1]; *[1]University of Cincinnati, Cincinnati, OH; [2]Humboldt-Universität zu Berlin, Berlin, Germany*

TP 596 **Enhancing RNA modification mapping by LC-MS/MS through off-line fractionation of complex samples**; Aastha Gyawali[1]; Scott Abernathy[1]; Patrick Limbach[1]; *[1]University of Cincinnati, Cincinnati, OH*

TP 597 **Simplifying Total tRNA Modification Mapping: Advantages of the Universal Mass Exclusion List**; Asif Rayhan[1]; Bala Addepalli[2]; Patrick Limbach[1]; *[1]University of Cincinnati, Cincinnati, OH; [2]Waters Corporation, Milford, MA*

TP 598 **LC-MS/MS/MS for Assessing the Incorporation and Repair of O2-Alkylthymidine lesions in Genomic DNA**; Chen Wang[1]; Pengcheng Wang[1]; Lin Li[1]; Yinsheng Wang[1]; *[1]University of California, Riverside, Riverside, CA*

TP 599 **Improving LC-MS Analysis of mRNA: Enzymatic Digestion and LC-MS Analysis for Characterization of mRNA Modifications and Sequence Integrity**; Pierre Alexander Mücke[1]; Anke Schnabel[1]; Daniel Waldera-Lupa[1]; Sascha Rexroth[2]; *[1]ProtaGene GmbH, Dortmund, Germany; [2]Shimadzu Europa GmbH, Duisburg, Germany*

TP 600 **HPLC Fractionation for the LC-MS/MS Characterization of Eukaryotic tRNA mixtures**; Jennifer Kist[1]; Cassandra Herbert[1]; Patrick Limbach[1]; *[1]University of Cincinnati, Cincinnati, OH*

TP 601 **Toward standardized epitranscriptome analytics: An inter-laboratory comparison of mass spectrometric detection and quantification of modified ribonucleosides in human RNA**; Tulsi Bhandari[1]; Martin Hengesbach[2]; Alan Bruzel[3]; Chi-Kong Chan[4]; Michael S. DeMott[4]; Ganna Podoprygorina[2]; Guangxin Sun[4]; Vivian Cheung[3]; Peter Dedon[4]; Mark Helm[2]; Patrick A. Limbach[1]; *[1]University of Cincinnati, Cincinnati, OH; [2]Institute for Pharmaceutical and Biomedical Sciences, Johannes Gutenberg University,, Staudingerweg 5, Germany; [3]Department of Molecular Biology, Cell Biology & Biochemistry, Brown University, Providence, RI; [4]Department of Biological Engineering, Massachusetts Institute of Technology, Cambridge, MA, USA, Cambridge, MA*

TP 602 **Creating a mass spectrometry for the absolute quantification of RNA nanoparticles in eye tissue**; Mohammed Hassan[1]; Kevin S Li[1]; Patrick A. Limbach[1]; *[1]University of Cincinnati, Cincinnati, OH*

TP 603 **Comprehensive analysis of Oligonucleotide gas-phase stability and fragmentation: Impact of 2'-modifications, base composition, and charge states**; Christopher Gawlig[1]; Mattis Kaumann[1]; Güngör Hanci[1]; Barbara Pfaff[1]; Michael Rühl[1]; *[1]BioSpring Gesellschaft für Biotechnologie mbH, Frankfurt am Main, Germany*

TP 604 **Confirming Stereochemical Identity of Stereopure Oligonucleotides Through Enzymatic Digestion and Analysis with Liquid Chromatography – Mass Spectrometry**; Brooke Koshel[1]; Amber Lindsey[1]; Gina Lein[1]; Keith Bowman[1]; Chandra Vargeese[1]; *[1]Wave Life Sciences, Lexington, MA*

TP 605 **Single Quadrupole Mass Spectrometry Quick Workflows Specified to Oligonucleotides Screening**; Kosuke Uchiyama[1]; Noriko Kato[1]; Simon Ashton[2]; Neil Loftus[2]; Risa Suzuki[3]; Yuka Fujito[1]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]Shimadzu Corporation, Manchester, United Kingdom; [3]Shimadzu Scientific Instruments, Columbia, MD*

TP 606 **Top-down fragmentation of native and denatured G-quadruplex oligonucleotides using the timsOmni platform**; Rim Chiba[1]; Arjun Mani Mallika[1]; Jean-François Greisch[2]; Athanasios Smyrnakis[3]; Dimitris Papanastasiou[3]; Frederic Rosu[1]; Valerie Gabelica[1]; *[1]University of Geneva, Geneva, Switzerland; [2]Bruker Switzerland AG, Fällanden, Switzerland; [3]Fasmatech Science & Technology, Athens, 15233, Greece*

TP 607 **Novel fragmentation strategies on the timsOmni platform for the characterization of oligonucleotide therapeutics**; Arjun Mani Mallika[1]; Rim Chiba[1]; Jean-François Greisch[2]; Athanasios Smyrnakis[3]; Dimitris Papanastasiou[3]; Frederic Rosu[1]; Valerie Gabelica[1]; *[1]University of Geneva, Geneva, Switzerland; [2]Bruker Switzerland AG, Fällanden, Switzerland; [3]Fasmatech Science & Technology, Athens, 15233, Greece*

TP 608 **Mass spectrometry-based structural analysis of oligonucleotide DNA duplexes**; Alexandre Ferreira Gomes[1]; Martin Gilar[1]; *[1]Waters Corporation, Milford, MA*

TP 609 **Detailed study into ASO impurity analysis, lessons learned, and myths dispelled while creating compliant platform methods**; Ulrik Mistarz[1]; Alexander Schwahn[2]; Simon Szwandt[3, 4]; Ken Cook[3]; *[1]Thermo Fisher Scientific, Copenhagen, Denmark; [2]Thermo Fisher Scientific, Reinach, Switzerland; [3]Thermo Fisher Scientific, Morpeth, United Kingdom; [4]Thermo Fisher Scientific, Hemel Hempstead, United Kingdom*

TP 610 **Quantitative Proteomics Identifies Multiple Pseudouridine-binding Proteins**; Songbo Wei[1]; Yinsheng Wang[1]; *[1]UCR, RIVERSIDE, CA*

TP 611 **Optimization of Sample Pretreatment Methods for LC-MS/MS Determination of Oligonucleotide Drugs in Tissues and Excreta**; Jin Xie[1]; Yan Song[1]; Ting Wang[1]; Peiyun An[1]; Jinlian Lu[1]; Zhiyu Li[1]; Lili Xing[1]; Yi Tao[1]; Liang Shen[1]; *[1]WuXi AppTec, Shanghai, China*

TP 612 **An Efficient and Environmentally Friendly Method for Determination of Nucleoside Phosphate Compounds by LC-MS/MS**; Shuo Zhang[1]; Xiongfei Wu[1]; Wuyun Gong[1]; Xianchun Zhang[1]; Zhiyu Li[1]; Lili Xing[1]; Yi Tao[1]; Liang Shen[1]; *[1]WuXi AppTec, Shanghai, China*

TP 613 **Predicting long-term stability of oligonucleotides by using Accelerated Stability Assessment Program modelling and High-Resolution Mass Spectrometry**; Geert Van Raemdonck[1]; Kevin Roeleveld[1]; Birger Zutterman[1]; Koen Iterbeke[1]; *[1]AnaBioTec, Evergem, Belgium*

TP 614 **An automated quality control system for ribonucleoside analysis**; Guadalupe Espadas[1, 2]; Roger Olivella[1, 2]; Olga Pastor[1, 2]; Eduard Sabidó[1, 2]; *[1]Centre for Genomic Regulation (CRG), Barcelona, Spain; [2]Universitat Pompeu Fabra (UPF), Barcelona, Spain*

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TP 615 **Fragmentation chemistry through the eyes of a deep neural network**; Joel Lapin[1]; Maksim Iuzhaniov[1]; Adrian Hölzlwimmer[1]; Nikita Levin[2, 3]; Shabaz Mohammed[3]; Mathias Wilhelm[1]; *[1]Technical University of Munich, Freising, Germany; [2]Rosalind Franklin Institute, Didcot, United Kingdom; [3]University of Oxford, Oxford, United Kingdom*

TP 616 **ExD vs EThcD: What`s better for Top-Down sequencing of natural amphibian disulfide peptides**; Albert T Lebedev[1, 2]; Dmitrii M Mazur[1]; Tatiana Y. Samgina[1, 2]; Yury V Vasil'ev[3]; Michael C Hare[3]; Yinan Li[4]; *[1]Shenzhen MSU-BIT University, Shenzhen, China; [2]Moscow State University, Moscow, Russian Federation; [3]Agilent Technologies, Inc., Corvallis, OR; [4]University of Hong Kong, Hong Kong, China, HONG KONG, China*

TP 617 **In-depth peptide mapping of biopharmaceuticals using an electron-transfer/higher-energy collision dissociation (EThcD) implemented on a modified Orbitrap Hybrid MS**; Reiko Kiyonami[1]; Cong Wang[2]; Peter Krueger[2]; Roberto Gamez[3]; Heiner Koch[2]; Min Du[1]; *[1]Thermo Fisher Scientific, Lexington, MA; [2]Thermo Fisher Scientific, Bremen, Germany; [3]ThermoFisher Scientific, Lexington, MA*

TP 618 **Tandem mass spectrometry of linear depsipeptides with alpha-hydroxy acid residues**; Brison A Shira[1, 2]; Elin C Herndon[1]; Michael W. Giuliano[1]; Jay G Forsythe[1]; *[1]College of Charleston, Charleston, SC; [2]Purdue University, West Lafayette, IN*

TP 619 **Evaluation of Peptide Identification Performance by Microflow Liquid Chromatography Coupled to Trapped Ion Mobility Time of Flight Mass Spectrometry**; Anh Tran[1]; Meghan C. Burke[1]; Tytus D Mak[1]; Katharina S Yandrofski[1, 2]; Ioannis L Karageorgos[1, 2]; William E Wallace[1]; *[1]NIST, Gaithersburg, MD; [2]IBBR, Rockville, MD*

TP 620 **Overcoming Singly Charged Peptide Exclusion in Mass Spectrometry for Improved Nt-Acetylation Analysis**; Marco Hadisurya[1]; Zhuojun Luo[1]; Amirhesam Mashaollahi[1]; Yanyan Du[1]; W. Andy Tao[1, 2, 3]; *[1]Department of Biochemistry, Purdue University, West Lafayette, IN; [2]Department of Chemistry, Purdue University, West Lafayette, IN; [3]Tymora Analytical Operations, West Lafayette, IN*

TP 621 **Bioprospecting the Host Defense Peptidome of the Largest Salamander in North America, Cryptobranchus alleganiensis (Hellbender)**; Syeda Raika Shahid[1]; Barney Bishop[1]; Edward Bentil[1]; *[1]George Mason University, fairfax, VA*

TP 622 **Streamlined analysis of synthetic peptides with non-standard amino acid chemistry**; Rachel Franklin[1]; Adrian Guthals[1]; Joseph C. Meeuwsen[1]; *[1]Agilent Technologies, Inc., Corvallis, OR*

TP 623 **Advanced Data Analysis of Peptide LC-MS Spectra through In Silico Fragmentation**; Alexander Bourque[1]; Anne Marie Smith[1]; Artyom Petrovskiy[1]; Vitaly Lashin[1]; *[1]ACD/Labs, Toronto, ON*

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TP 624 **Integrated Single-Tip Enrichment Enables Simultaneous and Efficient Analysis of Plant Phosphoproteomics and N-glycoproteomics**; Chin-Wen Chen[1]; Ting-An Chen[1]; Pei-Yi Lin[1]; Shu-Yu Lin[2]; Chuan-Chih Hsu[1]; *[1]Institute of Plant and Microbial Biology, Academia Sinica, Taipei city, Taiwan; [2]Academia Sinica Common Mass Spectrometry Facilities for Proteomics and Protein Modification Analysis, Academia Sinica, Taipei city, Taiwan*

TP 625 **Characterization and Quantification of Glucagon-Like Peptide-1 Agonists and their Impurities Using Liquid Chromatography/Mass Spectrometry (LC/MS)**; David L Wong[1]; Suresh Babu Cugati Vishweshwaraiah[2]; *[1]Agilent Technologies, Inc., Santa Clara, CA; [2]Agilent Technologies Singapore (sales) Pte Ltd, Singapore, Singapore*

TP 626 **Site localization of Protein-Primed Non-templated DNA synthesis using HCD-triggered-EThcD**; Nolan Neville[1]; Edwin Escobar[1]; Andrew Hanneman[1]; Robert Trachman[1]; *[1]New England Biolabs, Beverly, MA*

TP 627 **Untargeted Identification and Localization of Isomerized Residues in Neuroendocrine Peptides**; Samuel Okyem[1, 2]; Jonathan V. Sweedler[2, 3]; *[1]University of Illinois Urbana-Champaign, Urbana, IL; [2]Beckman Institute for Advanced Science and Technology, University of Illinois Urbana-Champaign, Urbana, IL; [3]university of Illinois-Urbana Champaign, Urbana, IL*

TP 628 **Peptide Mapping of Therapeutic Proteins Using Electron-Activated Dissociation: A Comparative Analysis with Electron Transfer Dissociation**; Yasmine Bouchibti[1]; Shuai Wu[1]; Iain Campuzano[1]; *[1]Amgen, Inc., Thousand Oaks, CA*

TP 629 **Characterization of Synthetic peptide drug and impurities using High-performance liquid chromatography (HPLC) and Liquid chromatography/mass spectrometry (LC/MS)**; Chae Young Ryu; *Agilent Technologies Inc., Seoul, South Korea*

TP 630 **Enrichment of Sialylated and Phosphorylated Glycopeptides via a Very Weak Anion Exchange Chromatography Method**; Peng-Kai Liu[1]; Danqing Wang[2]; Ting-Jia Gu[3]; Bin Wang[3]; Hung-Yu Chiang[1]; Lingjun Li[1, 2, 3]; *[1]Biophysics Graduate Program, University of Wisconsin-Madison, Madison, WI; [2]Department of Chemistry, University of Wisconsin Madison, Madison, WI; [3]School of Pharmacy, University of Wisconsin-Madison, Madison, WI*

TP 631 **Electron-transfer/higher-energy collision dissociation (EThcD) coupled to FAIMS improves ADP-ribose peptides fragmentation**; Taku Kasai[1]; Masanori Aikawa[1, 2, 3]; Sasha A. Singh[1]; *[1]Center for Interdisciplinary Cardiovascular Sciences, Division of Cardiovascular Medicine, Department of Medicine, Brigham Women's Hospital, Harvard Medical School, Boston, MA; [2]Center for Excellence in Vascular Biology, Cardiovascular Division, Brigham and Women’s Hospital, Harvard Medical School, Boston, MA; [3]Channing Division of Network Medicine, Department of Medicine, Brigham Women's Hospital, Harvard Medical School, Boston, MA*

TP 632 **Top-Down and Bottom-Up timsMS Histone PTM Screening of Non-annotated Insect Model Organisms**; Andrea Ramirez Torres[1]; Cassandra N. Fuller[1]; Lilian Valadares Tose[1]; Kevin Jeanne Dit Fouque[1]; Francisco Fernandez-Lima[1]; *[1]Florida International University, Miami, FL*

TP 633 **Histidine-Rich Glycoprotein Sialylation Affects its Inhibition of FXII Autoactivation**; Yang Zou[1, 2, 3]; Rensong Ji[2, 3]; Arnoud Marquart[4]; Joost Meijers[4]; Marta Šiborová[2, 3]; Karli R. Reiding[2, 3]; Albert J.R. Heck[2, 3]; *[1]Radboud University Medical Center, Nijmegen, Netherlands; [2]Utrecht University, Utrecht, Netherlands; [3]Netherlands Proteomics Center, Utrecht, Netherlands; [4]Sanquin Research and Landsteiner Laboratory, Amsterdam, Netherlands*

TP 634 **Developing a platform for the Quantitative profiling of Lipidated proteins**; Kavita R Matange[1]; Maria Antonelli[1]; Paolo Cifani[1]; *[1]Cold Spring Harbor Laboratory, Cold Spring Harbor, NY*

TP 635 **Confident and sensitive identification of semaglutide degradation products using liquid chromatography-high resolution accurate mass (HRAM) mass spectrometry**; Xiaoxi Zhang[1]; Xuepu Li[2]; Roberto Gamez[3]; Frank Steiner[4]; Min Du[5]; *[1]ThermoFisher Scientific, Shanghai, China; [2]Thermo Fisher Scientific, Shanghai, China; [3]Thermo Fisher Scientific, Austin, TX; [4]Thermo Fisher Scientific, Germering, Germany; [5]Thermo Fisher Scientific, Lexington, MA*

TP 636 **A comprehensive solution for PTM analysis: integrating input normalization and stoichiometry calculations**; Veronique Laforte[1]; Damiano Robbiani[1]; Monika Puchalska[1]; Anamarija Pfeiffer[1]; Tejas Gandhi[1]; Lukas Reiter[1]; *[1]Biognosys AG, Schlieren, Switzerland*

TP 637 **Unbiased Proteomic Profiling and Computational Software for Post-translational Arginylation**; Zongtao Lin[1]; Joanna Gongora[2]; Xingyu Liu[2]; Emily Zahn[2]; Bibhuti Bhusana Palai[2]; Daniel Ramirez[2]; Richard M. Searfoss[2]; Francisca NDL Vitorino[2]; Rashmi Karki[2]; Benjamin A Garcia[2]; *[1]Washington University in St. Louis, St. Louis, MO; [2]Washington University in St. Louis, St. Louis, Missouri*

TP 638 **Advanced Characterization of Semaglutide and Its Impurities Using a Heart-Cutting 2D-LC/MS Workflow for Biopharmaceutical Analysis**; Paramjeet Khandpur[1]; Ashish Pargaonkar[1]; Preeti Bharatiya[1]; *[1]Agilent technologies, Bangalore, India*

TP 639 **Deep N-terminome profiling via graphene oxide-based depletion of internal peptides derivatized with 2,3-naphthalene-dicarboxaldehyde**; William LeFever[1]; Zhuojun Luo[2]; R. Graham Cooks[3]; W. Andy Tao[2, 3]; *[1]Purdue University, West Lafayette, IN; [2]Department of Biochemistry, Purdue University, West Lafayette, IN; [3]Department of Chemistry, Purdue University, West Lafayette, IN*

TP 640 **Prosit-PTM: Deep Learning Enhances Detection and Localization of Unseen PTMs**; Wassim Gabriel[1]; Daniel P Zolg[2]; Polina Prokofeva[2]; Ludwig Lautenbacher[1]; Chien-Yun Lee[3]; Rebecca Meelker González[3]; Guillaume Médard[2, 4]; Bernhard Kuster[2]; Mathias Wilhelm[1]; *[1]Computational Mass Spectrometry, School of Life Sciences, Technical University of Munich, Freising, Germany; [2]Chair of Proteomics and Bioanalytics, School of Life Sciences, Technical University of Munich, Freising, Germany; [3]Young Investigator Group: Mass Spectrometry in Systems Neurosciences, School of Life Sciences, Technical University of Munich (TUM), Freising, Germany; [4]Proteomics Core Facility, National & Kapodistrian University of Athens, Athens, Greece*

TP 641 **Enhancing Phosphoproteomic Insights through Protein Abundance Normalization in TMT-plex Analysis**; Sogol Sedighi[1]; Ting Liu[1]; Robert O'Meally[2]; Robert N Cole[2]; Brian O' Rourke[1]; D. Brian Foster[1]; *[1]Division of Cardiology, Johns Hopkins University School of Medicine, Baltimore, MD; [2]Department of Biological Chemistry, The Johns Hopkins University School of Medicine, Baltimore, MD*

TP 642 **Improving Sulfoproteome Coverage by Reducing Competition from Highly Abundant Isobaric Protein Phosphorylation in Mouse Macrophages**; Hye Kyong Kweon; *The University of Michigan, Ann Arbor, MI*

TP 643 **Mass Spectrometric Characterization of UV-C and Methylene Blue Treated Mouse Plasma and Related Changes in Sample Processing Modifications**; Edward Bentil[1]; Barney N Bishop[1]; Shannon Carney[2]; Caitlin Woodson[2]; Michelle Theus[2]; Kylene Kehn-Hall[2]; Dionisio Davis Garcia[3]; *[1]George Mason University, Manassas, VA; [2]Virgina Institue of Technology, Blacksburg, VA/20110; [3]George Mason University, Manassas, VA/20110*

TP 644 **Monitoring Stability and Impurity Products of GLP-1 Agonists Using a Novel Single Quadrupole LC/MS**; Mahsan Miladi; *Agilent Technologies, Santa Clara, CA*

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645-656

TP 645 **DOE-Based Comparative Analysis of MAM on Thermo Fisher Q Exactive™ HF and Exploris™ 240 for Therapeutic Antibodies**; Jianji Chen[1]; Erin Weisenhorn[1]; Rosalynn Molden[2]; *[1]Just_Evotec Biologics, Seattle, WA; [2]Just Evotec Biologics, Redmond, WA*

TP 646 **Comparison of High-Resolution Tofs for Cell Culture Media Nutrient and Metabolite Analysis**; Courtney Walton[1]; Yun Alelyunas[2]; *[1]Waters Corp., Milford, MA; [2]Waters Corporation, Milford, MA*

TP 647 **Enhancing Bioprocess Development through Automated Spent Media and Titer Analysis by LC-MS with Data Connectivity via Statistical Software**; Elizabeth Embrey[1]; Yun Alelyunas[2]; Mark Wrona[2]; Guillaume Béchade[3]; Patrick Boyce[1]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Waters Corporation, Milford, MA; [3]Waters Corporation, Saint Quentin en Yvelines, France*

TP 648 **Online LC/MS method for measurement of monoclonal antibody glycosylation from a bioreactor**; Michael D Knierman[1]; Bruce Dolby[2]; Christian Lambrecht[2]; Haiko Herschbach[2]; Sebastian Weinig-Berger[3]; Thomas Walker[4]; Patrick Cronan[4]; Matthew Wong[5]; James Angelo[5]; Jean-Luc Gerling[5]; *[1]Agilent Technologies, Santa Clara, CA; [2]Agilent Technologies, Inc., Waldbronn, Germany; [3]Agilent Technologies, Inc., Santa Clara, CA; [4]Agilent Technologies, Lexington, MA; [5]Millipore Sigma, Bedford, MA*

TP 649 **Enhancing Process Development for Synthetic GLP-1 Agonists Leveraging Negative Polarity LC-MS**; Brock R Juliano[1]; Hsi-Chun Chao[1]; Gordon R Lambertus[1]; *[1]Eli Lilly and Company, Indianapolis, IN*

TP 650 **Evaluating the Impact of Glucose Feed and Temperature Modulation of Bioreactors Using Microfluidic CE-MS for Metabolic Profiling and Product Characterization**; Erin Redman[1]; Hampus Engstroem[2]; Katherine Raiche[2]; Stephanie Klaubert[2]; Awab Nehela[2]; Scott Miller[2]; Graziella Piras[2]; J. Will Thompson[1]; *[1]908 Devices, Inc., Morrisville, NC; [2]908 Devices Inc., Boston, MA*

TP 651 **High-throughput Characterization of Therapeutic Proteins by Peptide Mapping Using Dual Binary Pumps and Dual Columns In-Tandem**; Andrew Dykstra[1]; Prashant Jethva[1]; Daniel Woodall[1]; Pavel Bondarenko[1]; *[1]Amgen, Thousand Oaks, CA*

TP 652 **An Automated, Sterile Bioreactor Sampling Workflow for Rapid, In-Process Media and Product Quality Attribute (PQA) Monitoring via Microfluidic CE-MS**; Katherine Raiche[1]; Stephanie Klaubert[1]; Jeremy Bechen[1]; J. Will Thompson[2]; Erin Redman[2]; J. Scott Mellors[2]; *[1]908 Devices Inc., Boston, MA; [2]908 Devices Inc, Morrisville, NC*

TP 653 **High-Throughput Peptide Mapping with Excellent Sequence Coverage Using Parallel Accumulation–Mobility Aligned Fragmentation**; Catherine Riley[1]; Jack Eifert[1]; Lake Paul[1]; Lauren Royer[2]; Leonard Rorrer[3]; Daniel DeBord[2]; *[1]BioAnalysis LLC, Philadelphia, PA; [2]Mobilion Systems Inc., Chadds Ford, PA; [3]MOBILion Systems, Inc, Chadds Ford, PA*

TP 654 **Gas-phase Deuterodeboronation for GC-MS/GC-IR Structure Elucidation of Aryl Boronic Acids**; Brett M. Marsh[1]; Hannah Zimmerman-Federle[1]; *[1]Corteva Agriscience, Indianapolis, IN*

TP 655 **Standardized tools for biologics analyses and QC: glyPAQ™ and the Turbo MAM Kit**; Sandra L. Wilson[1]; Melinda Wojtkiewicz[2]; Rebekah Gundry[2]; John P. Wilson[1]; *[1]ProtiFi LLC, Fairport, NY; [2]University of Nebraska Medical Center, Omaha, NE*

TP 656 **Walkup In-Line Batch Reaction Monitoring with LCMS**; Muhammad Asif Alimuddin; *Pfizer Inc, San Diego, CA*

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TP 657 **Target Identification Using Affinity Selection Mass Spectrometry and a Protein Library of 17,000 Proteins, Including Membrane Proteins**; Xianshu Yang[1]; Naoki Tarui[1]; Masaharu Nakayama[1]; *[1]SEEDSUPPLY INC., 26-1, Muraoka-Higashi 2-Chome Fujisawa, Kanagawa 251-0012, Japan*

TP 658 **Ion-Mobility Mass Spectrometry Provides Insight into How Ligands Stabilize Transthyretin**; Robert Rider[1]; Carter Lantz[1]; Sangho Yun[1]; Emily Birmingham-Lopez[1]; Arthur Laganowsky[1]; David H Russell[1]; *[1]Texas A&M University, College Station, TX*

TP 659 **Mapping the Interactome of FtsH and YidC inE. coliUsing XL-MS**; Mehmet Çalıseki[1, 2]; Burak V Kabasakal[1]; *[1]Turkish Accelerator and Radiation Laboratory, Ankara, Turkey; [2]Sabancı University, Istanbul, Turkey*

TP 660 **Direct protein-protein interaction using crosslinking and high-mass MALDI-MS for drug discovery**; Congrui Tan[1]; Yuye Zhou[1]; Renato Zenobi[1]; *[1]ETH Zurich, Zurich, Switzerland*

TP 661 **Characterization of complexes formed by polyphosphate and platelet factor 4**; Yi Du[1]; Igor A Kaltashov[2]; *[1]University of Massachusetts-Amherst, Amherst, MA; [2]University of Massachusetts Amherst, Amherst, MA*

TP 662 **Characterization of Nanobody and Affibody Complexes via Native Mass Spectrometry and Ultraviolet Photodissociation**; Jessica G Pauling[1]; Mady S Telford[1]; Bryan W Davies[1]; Jennifer S Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX*

TP 663 **Characterization of the USP18-ISG15-STAT2 complex using mass spectrometry and biophysical analysis**; Graham West[1]; Xidong Feng[2]; Ian McCombes Tolis[2]; Masaya Yamaguchi[2]; Kris Borzilleri[2]; Erik Ralph[2]; Agustin Casimiro-Garcia[3]; *[1]Pfizer, Groton, CT; [2]Pfizer Inc., Groton, CT; [3]Pfizer Inc., Cambridge, MA*

TP 664 **Multi-dimensional High-Throughput Molecular Glue Screening via Gas Phase Affinity Selection Native Mass Spectrometry and Cryo-EM Analysis**; Weijing Liu[1]; Kheewoong Baek[2]; Eric Fischer[3]; Albert Konijnenberg[4]; Wenfei Song[4]; Christopher Mullen[1]; Yuan Xiong[3]; Ken Durbin[5]; Shane Bechler[6]; Rosa Viner[7]; Thomas Moehring[8]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Dana-Farber Cancer Institute, Boston, MA; [3]Dana-Farber Cancer Institute, Boston, Massachusetts; [4]Thermo Fisher Scientific, Eindhoven, Netherlands; [5]Proteinaceous, Evanston, IL; [6]Thermo Fisher Scientific, Sunnyvale, CA; [7]ThermoFisher Scientific, San Jose, CA; [8]Thermo Fisher Scientific, Bremen, Germany*

TP 665 **Complexin-1 mediates interactions of Synaptotagmin-1 with the SNARE complex**; Julia Bieber[1]; Carla Schmidt[1]; *[1]Johannes Gutenberg University, Mainz, Germany*

TP 666 **Scalable Mapping of Ligand-Receptor Interactions and Cell Surface Protein Neighborhoods via Proximity Labeling with Radius Modulation**; Jonathan J Swietlik[1, 2]; Benedikt O Gansen[3]; Alexander Henrici[4]; Felix Kühner[2]; Jonathan J Scheler[3]; Felix Meissner[2, 3]; *[1]Odyssey Therapeutics, Boston, MA; [2]Max Planck Institute of Biochemistry, Munich, Germany; [3]Institute of Innate Immunity, University of Bonn, Bonn, Germany; [4]Institute of Virology, Technical University of Munich, Munich, Germany*

TP 667 **Metabolic Control of Glycosylation Forms for Establishing Glycan-Dependent Protein Interaction Networks**; Xingyu Liu[1]; Yi Li[2]; Zongtao Lin[1]; Siyu Chen[3]; Ying Sheng[3]; Shunyang Wang[3]; Carlito B. Lebrilla[3]; Benjamin A Garcia[1]; Yixuan Xie[2]; *[1]Washington University in St. Louis School of Medicine, St. Louis, MO; [2]Fudan University, Shanghai, China; [3]UC Davis, Davis, CA*

TP 668 **Exploring the transient interactome of a mitochondrial membrane complex via crosslinking mass spectrometry**; Vanessa Linke[1, 2]; Tereza Kadavá[3]; Agnieszka Chacińska[1]; Albert J.R. Heck[3]; *[1]IMol Polish Academy of Sciences, Warsaw, Poland; [2]IIMCB (International Institute of Molecular and Cell Biology), Warsaw, Poland; [3]Utrecht University, Utrecht, Netherlands*

TP 669 **Noncovalent interactions and ionization polarity impact the formation of nonspecific adducts during native-ESI MS**; Madeline G Bannon[1]; Alexandra M Cupples[1]; Elyssia S Gallagher[1]; *[1]Baylor University, Waco, TX*

TP 670 **Native MS Reveals the Different DNA Binding States of a DNA Annealing Protein Complex**; Zihao Qi[1, 2]; Carter T. Wheat[3, 4]; Charles E. Bell[1, 3, 4]; Vicki H. Wysocki[1, 2, 4]; *[1]Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH; [2]Native Mass Spectrometry Guided Structural Biology Center, The Ohio State University, Columbus, OH; [3]Department of Biological Chemistry and Pharmacology, The Ohio State University, Columbus, OH; [4]Ohio State Biochemistry Program (OSBP), The Ohio State University, Columbus, OH*

TP 671 **Native and top-down mass spectrometry of membrane and glycoproteins on the timsOmni platform**; Abraham O Oluwole[1, 2]; Mariangela Kosmopoulou[3]; Athanasios Smyrnakis[3]; Dimitris Papanastasiou[3]; Carol V Robinson[1, 2]; Weston Struwe[2, 4]; *[1]Department of Chemistry, University of Oxford, Oxford, United Kingdom; [2]Kavli Institute for Nanoscience Discovery, University of Oxford, Oxford, United Kingdom; [3]Fasmatech Science & Technology, Chalandri, Greece; [4]Department of Biochemistry, University of Oxford, Oxford, United Kingdom*

TP 672 **Identifying and probing the endogenous RORβ interactome in astrocytes using rapid immunoprecipitation mass spectrometry**; Nadeska I Montalvan[1, 2]; Timothy R O'Leary[2]; Mi Ra Chang[2]; Kuang-Ting Kuo[1, 2]; Patrick R Griffin[1, 2]; *[1]Skaggs Graduate School of Chemical and Biological Sciences, The Scripps Research Institute, Jupiter, FL; [2]Department of Molecular Medicine, The Herbert Wertheim UF Scripps Institute for Biomedical Innovation & Technology, Jupiter, FL*

TP 673 **Unveiling BCL-2/xL-Specific PROTAC Efficiencies and Dissociation Pathways Using Native Mass Spectrometry**; Mohamed Ibrahim Gadallah[1]; Digant Nayak[2]; Jinhui Zhang[3]; Guangrong Zheng[3]; Shaun K. Olsen[2]; Daohong Zhou[4]; Jennifer S Brodbelt[1]; *[1]Department of Chemistry, University of Texas at Austin, Austin, Texas, United States., Austin, TX; [2]Department of Biochemistry & Structural Biology, University of Texas Health Science Center at San Antonio, San Antonio, TX; [3]Department of Medicinal Chemistry, College of Pharmacy, University of Florida, Gainesville, Florida; [4]Department of Biochemistry and Structural Biology and Center for Innovative Drug Discovery, School of Medicine, University of Texas Health Science Center at San Antonio, San Antonio, TEXAS*

TP 674 **Low-Resolution Structural Characterization of RNA-Binding Proteins during Cellular Stress on a Proteome-Wide Scale**; Benjamin Steinmetz[1, 2]; Luca Riermeier[1, 2]; Alexander Leitner[1]; *[1]ETH Zurich, Zurich, Switzerland; [2]Life Science Zurich Graduate School, Zurich, Switzerland*

TP 675 **Integrated interactome profiling of transglutaminase 2 via proximity labeling and affinity purification mass spectrometry**; Hong-Beom Park[1, 2, 3]; Gyuri Park[2, 3, 4]; Sinae Lee[2, 3, 5]; Eunseo Kim[1, 2, 3]; Hyeon Chang Lee[2, 3, 4]; Minhyeok Kang[2, 3, 4]; Soeun Yun[1, 2, 3]; Jin Lee[1, 2, 3]; Dohyun Han[2, 3, 6]; *[1]Department of Biomedical Science, College of Medicine, Seoul National University, Seoul, South Korea; [2]Department of transdisciplinary medicine, Seoul National University Hospital, Seoul, South Korea; [3]Proteomics Core Facility, Biomedical Research Institute, Seoul National University Hospital, Seoul, South Korea; [4]Molecular Medicine and Biopharmaceutical Sciences, WCU Graduate School of Convergence Science and Technology Seoul National University, Seoul, South Korea; [5]Cancer Research Institute, Seoul National University college of medicine, Seoul, South Korea; [6]Department of Medicine, Seoul National University College of Medicine, Seoul, South Korea*

TP 676 **Characterizing Lactoferrin-DNA Interaction Using Native Mass Spectrometry: Insights into Modulating NET Formation**; Ruolan Cheng[1]; Igor A. Kaltashov[1]; *[1]University of Massachusetts Amherst, Amherst, MA*

TP 677 **Monomer exchange experiment using nMS to evaluate druggability for TNF**; Xidong Feng[1]; Wenyi Hua[1]; Ian Tolis[1]; Jing Yan[2]; Jie Quan[2]; Fabien Vincent[1]; Michael Primiano[2]; *[1]Pfizer Inc., Groton, CT; [2]Pfizer Inc., Cambridge, MA*

TP 678 **AP-DIA-MS Interrogation of Protein Quality Control to Target Deficiency of Adenosine Deaminase 2 (DADA2)**; Lea A Barny[1, 2]; Minsoo Kim[1, 2]; Yijin Shen[1]; Lars Plate[1, 2]; *[1]Vanderbilt University, Nashville, TN; [2]Vanderbilt Medical Center, Nashville, TN*

TP 679 **Serially Integrated and Mutually Validated De Novo Protein Networks (SIMUV) by Crosslinking Mass Spectrometry and Complexome Profiling in Cardiac Tissues**; Hugo A Amedei[1]; Olexandr Dybkov[2]; Olivia Langer[2]; Brian Foo[3, 4]; D. Brian Foster[1]; Stephan E Lehnart[3, 4]; Henning Urlaub[2, 4]; Christof Lenz[2, 4, 5]; *[1]Division of Cardiology, Johns Hopkins University School of Medicine, Baltimore city, MD; [2]Bioanalytical Mass Spectrometry Group, Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany; [3]Cellular Biophysics and Translational Cardiology Section, Department of Cardiology and Pneumology, Heart Research Center Göttingen, University Medical Center Göttingen, Göttingen, Germany; [4]Cluster of Excellence "Multiscale Bioimaging: from Molecular Machines to Networks of Excitable Cells" (MBExC), Georg August University, Göttingen, Germany; [5]Bioanalytics Group, Department of Clinical Chemistry, University Medical Center Götttingen, Göttingen, Germany*

TP 680 **Ligand Binding to Replicative Hexameric Helicase Characterized by Native Mass Spectrometry**; William Moeller[1, 2]; Mark P Foster[3]; Vicki H Wysocki[1, 2]; *[1]Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH; [2]Native Mass Spectrometry Guided Structural Biology Center, The Ohio State University,* *Columbus, OH; [3]Department of Chemistry and Biochemistry, The Ohio State University, Columbus, Ohio*

TP 681 **A cross-linking mass spectrometry method (LLPS-CLIR-MS) for characterizing protein-RNA interactions in phase-separated systems**; Tebbe De Vries[1]; Mihajlo Novakovic[1]; Yinan Ni[1]; Izabela Smok[1]; Clara Inghelram[1]; Maria Bikaki[1]; Chris Sarnowski[1]; Yaning Han[1]; Leonidas Emmanouilidis[1]; Giacomo Padroni[1]; Alexander Leitner[1]; Frederic Allain[1]; *[1]ETH Zurich, Zurich, Switzerland*

TP 682 **Molecular Mechanism of B Cell Kinase Activation on the Membrane through Lipid Bilayer Native Mass Spectrometry**; Rachel A McAllister[1]; Moitrayee Bhattacharyya[2]; Kallol Gupta[3, 4]; *[1]Yale University, West Haven, CT; [2]Department of Pharmacology, Yale University, New Haven, CT; [3]Department of Cell Biology, Yale School of Medicine, New Haven, CT; [4]nanobiology Institute, Yale University, New Haven, CT*

TP 683 **Simultaneous Native/Intact Analysis of Protein Complexes for Drug Screening Using DynaChip Online Buffer Exchange and Taylor-Aris Dispersion**; Casey Vantucci[1]; Carter Asef[1]; Austin Culberson[1]; Mason Chilmonczyk[1]; *[1]Andson Biotech, Atlanta, GA*

TP 684 **Native mass spectrometry characterization of the interactions between viral RNA silencing suppressor protein p19 and duplex RNA**; Micah T Donor[1]; Nicholas P Sysum[1]; *[1]George Fox University, Newberg, OR*

TP 685 **Capturing heterogenous assemblies of membrane proteins directly from the membrane through CDMS: Chasing after ultrafast synaptic vesicle fusion**; Samantha O Shepherd[1]; Aniruddha Panda[1]; Kallol Gupta[1]; *[1]Yale University - West Campus, West Haven, CT*

TP 686 **The impact of protein charge on nonspecific binding in positive- and negative-mode ESI-MS**; Alexandra M. Cupples[1]; Madeline G. Bannon[1]; Elyssia S. Gallagher[1]; *[1]Baylor University, Waco, TX*

TP 687 **Deciphering the interaction between LRH-1 and PPIB as its novel co-repressor**; Nereida Abad-Yang[1, 2]; Valentine Courouble[1, 2]; Jielei Wang[1, 2]; Patrick R Griffin[1, 2]; *[1]The Scripps Research Institute, La Jolla, CA; [2]Herbert Wertheim UF Scripps Institute for Biomedical Innovation and Technology, Jupiter, FL*

TP 688 **Amyloid-beta 1-16 Homodimer—Regorafenib Complex Revealed by Novel Top-Down Carbene Footprinting done within the Ion Source**; Paul Martino; *Houghton University, Houghton, NY*

TP 689 **Identifying and Characterizing Protein-Protein Interactions of Nuclear Receptor RORB by a Combination of Immunoprecipitation Mass Spectrometry and Crosslinking Mass Spectrometry**; Denis Shutin[1]; Timothy R O'Leary[1]; Mi Ra Chang[1]; Patrick R. Griffin[1]; *[1]UF Scripps, Florida, Jupiter, FL*

TP 690 **MutSβ nucleotide binding and hydrolysis probed by nMS**; Xidong Feng[1]; Amir Arellano-Saab[2]; Erik Ralph[2]; Zane Wenzel[2]; Paula Loria[2]; Ellene Mashalidis[2]; Ian Tolis[1]; *[1]Pfizer Inc., Groton, CT; [2]Pfizer Worldwide Research, Groton, CT*

TP 691 **Large-scale tumor antigen proximity labeling identifies novel pairings for bispecific antibody targeting**; Noah Dephoure[1]; Kendall Johnson[1]; Tali Vittum[1]; Chris May[1]; Rebecca Howell[1]; Cody Scandore[1]; Jeffrey Guernsey[1]; Pam Holland[2]; Scott Lesley[1]; Niyi Fadeyi[1]; Rob Oslund[1]; *[1]InduPro, Cambridge, MA; [2]InduPro labs, Cambridge, MA*

PROTEOMICS: INTACT PROTEINS AND TOP DOWN ANALYSIS II

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TP 692 **Autocalibration of Top-Down Mass Spectra Data to Improve Processing Results**; Joseph B. Greer[1, 2]; Michael D. Kim[2]; Michael A. R. Hollas[1, 2]; Ryan T. Fellers[1, 2]; Bryan P. Early[1, 2]; Matthew T. Robey[1]; Neil L. Kelleher[2]; Kenneth R. Durbin[1]; *[1]Proteinaceous, Evanston, IL; [2]Northwestern University, Evanston, IL*

TP 693 **Precision Serology with Single-clone Resolution using Automated Top-Down Sequencing of Light and Heavy Chains from Human Blood**; Neil L. Kelleher[1]; Benjamin J. Des Soye[1]; Taojunfeng Su[2]; Ryan T. Fellers[1]; Michael A. R. Hollas[1]; Philip Compton[3]; Ken Durbin[4]; Troy David Fisher[1]; Jared O. Kafader[1]; *[1]Proteomics Center of Excellence, Northwestern University, Evanston, IL; [2]Northwestern University, Evanston, IL; [3]Integrated Protein Technologies, Evanston, IL; [4]Proteinaceous, Evanston, IL*

TP 694 **Leveraging Machine Learning to Enhance Intact Protein Acquisition and Analysis**; Abdul Rehman Basharat[1]; Ryan Tal Fellers[1, 2]; Troy David Fisher[1, 2]; Bryan Patrick Early[1, 2]; Matthew T. Robey[1]; Michael A. R. Hollas[1, 2]; Kenneth Robert Durbin[1]; *[1]Proteinaceous, Evanston, IL; [2]Northwestern University, Evanston, IL*

TP 695 **Quantitative Profiling of Arginylated Proteoforms Through Discovery Top-Down Proteomics**; Richard M Searfoss[1]; Xingyu Liu[1]; Zongtao Lin[1]; Benjamin A. Garcia[1]; *[1]Washington University School of Medicine, St. Louis, MO*

TP 696 **Putting Capillary Electrophoresis – Mass Spectrometry (CE-MS) to the Test: Multi-Lab Benchmarking for Top-Down Proteomics**; Kevin Jooß[1]; Noah Gould[2]; Qianjie Wang[3]; Alexander R. Ivanov[2]; Liangliang Sun[3]; *[1]Vrije Universiteit Amsterdam, Amsterdam, Netherlands; [2]Northeastern University, Boston, MA; [3]Michigan State University, Department of Chemistry, East Lansing, MI*

TP 697 **Optimization of HeLa Cell Lysis Buffer and Conditions for Top-down Proteomics Analysis**; Ashlyn Solenberger[1]; Trishika Chowdhury[2]; Anju Teresa Sunny[2]; Kellye A Sutton[2]; Si Wu[2]; *[1]The University of Alabama, Tuscaloosa, AL; [2]University of Alabama, Tuscaloosa, AL*

TP 698 **Methionine Oxidation Footprinting in Intact Proteins (MOFIP) to Examine the Effect of Kinase Inhibitor-Induced Structural Changes on Human Cancer Cells**; Patrycja Szamweber[1]; Anju Teresa Sunny[1]; Kellye Cupp Sutton[1]; Si Wu[1]; *[1]University of Alabama, Tuscaloosa, AL*

TP 699 **Building a Data-Driven Top-down Fragmentation Strategy for Characterizing Monoclonal Antibodies**; Troy D Fisher[1, 2]; Taojunfeng Su[1]; Ryan T. Fellers[1, 2]; Michael A. R. Hollas[1, 2]; Abdul Rehman Basharat[2]; Matthew T. Robey[1, 2]; Ken Durbin[2]; Neil L. Kelleher[1, 3]; *[1]Northwestern University, Evanston, IL; [2]Proteinaceous, Evanston, IL; [3]Northwestern University, Feinberg School of Medicine, Chicago, IL*

TP 700 **A Novel Approach to De Novo Sequencing for Top-Down Proteomics**; Lissa C. Anderson[1, 2]; Krishna Saketh Kamadana[3]; Xian Mallory[3]; Nathan K. Kaiser[1]; *[1]National High Magnetic Field Laboratory, Tallahassee, FL; [2]Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL; [3]Department of Computer Science, Florida State University, Tallahassee, FL*

TP 701 **Probing the Stability of Protein Complexes utilizing Native Top-down Mass Spectrometry and Ion Mobility Mass Spectrometry**; Luchen Wuyang[1]; Joseph A. Loo[1]; Rachel R. Loo[1]; *[1]UCLA, Los Angeles, CA*

TP 702 **Top-Down Proteomics Reveals Histone Proteoform Dynamics during Neonatal Swine Heart Development**; Zhan Gao[1]; Tang Ling[2]; Scott J Price[3]; Matthew S Fisher[4]; Wuqiang Zhu[2]; Ying Ge[5]; *[1]UW-MADISON, Madison, WI; [2]Department of Cardiovascular Diseases, Physiology and Biomedical Engineering, Center for Regenerative Medicine, Mayo Clinic Arizona, Scottsdale, 85259, USA, Scottsdale, Arizona; [3]Department of Medicine, University of Wisconsin-Madison, Madison, Wisconsin 53705, USA, Madison, Wisconsin; [4]Department of Chemistry, University of Wisconsin–Madison, Madison, WI; [5]Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI*

TP 703 **In-Source Charge Reduction Enhances Top-Down Characterization of Denatured Proteins**; Rachel Franklin[1]; Yury V. Vasilev[1]; John Mehl[2]; *[1]Agilent Technologies, Inc., Corvallis, OR; [2]Agilent Technologies, Inc., Wilmington, Delaware*

TP 704 **Applying tandem mass spectrometry to identify antimicrobial host defense peptides from caecilian skin secretions**; Joan Rozario[1]; Barney Bishop[1]; Edward Bentil[1]; Carly Muletz Wolz[2]; Brian Gratwicke[2]; Luke Linhoff[2]; Mike Kirby[2]; Matt Evans[2]; Sara Hasentab[2]; *[1]George Mason*

University, Manassas, VA; [2]Smithsonian's National Zoo and Conservational Biology Institute, Washington, DC

TP 705 **Direct Histone Proteoform profiling based on TIMS-q -ExD/UVPD -MS/MS**; Md Shofiul Alam[1]; Cassandra N. Fuller[1]; Kevin Jeanne Dit Fouque[1]; Lilian Valadares Tose[1]; Richard M Searfoss[2]; Benjamin A Garcia[2]; Francisco Fernandez-Lima[1, 3]; *[1]Florida International University, Miami, FL; [2]Washington University School of Medicine Dept. of Biochemistry and Molecular Biophysics, St. Louis, MO; [3]Biomolecular Sciences Institute, Florida International University, Miami, FL*

TP 706 **Direct detection and characterization of S-nitrosohemoglobin using intact, native and top-down mass spectrometry.**; Saylor Stottlemeyer[1]; Tiffany Cho[1]; P. Matthew Joyner[1]; Ireland Plunkett[1]; Andrew K Goring[2]; Fabien Scalzo[1]; Joseph A. Loo[2]; *[1]Pepperdine University, Malibu, CA; [2]UCLA, Los Angeles, CA*

TP 707 **Comprehensive proteoform analysis of E. coli using sequential extraction, size-exclusion chromatography fractionation, and capillary zone electrophoresis-tandem mass spectrometry**; Jorge Colon-Rosado[1]; Liangliang Sun[2]; *[1]Michigan State University, East Lansing, MI; [2]Michigan State University, Department of Chemistry, East Lansing, MI*

TP 708 **Characterization of Proteoforms by Top-Down and Bottom-Up Mass Spectrometry with Database Search and De Novo Sequencing**; Shuyang Zhang[1]; Wenting Li[2]; Lei Xin[1]; Weiwu Chen[1]; Yandong Zhu[1]; Zheng Chen[1]; Baozhen Shan[3]; *[1]Bioinformatics Solutions Inc., Waterloo, N2J; [2]Bioinformatics Solution Inc., Waterloo, CA; [3]Bioinformatics Solutions Inc., Waterloo, ON*

TP 709 **An Optimized Bead-Mediated Protein Aggregation Method for Proteoform Identification Via Top-Down Mass Spectrometry**; Isabella G Feltenstein[1]; Maria Margineantu[1]; Bryon S. Drown[1]; *[1]Purdue University, West Lafayette, IN*

TP 710 **Decoy spectrum for accurate proteoform-level FDR estimation in top-down proteomics**; Ayesha Feroz[1]; Oliver Kohlbacher[1, 2, 3]; Kyowon Jeong[1, 2]; *[1]Applied Bioinformatics, Department for Computer Science, University of Tübingen, Tübingen, Germany; [2]Institute for Bioinformatics and Medical Informatics, University of Tubingen, Tubingen, Germany; [3]Translational Bioinformatics, University Hospital Tübingen, Tübingen, Germany*

TP 711 **Is CZE-MS ready for multi-omics analysis of complex biological samples with high long-term reproducibility?**; Guijie Zhu[1]; Liangliang Sun[2]; *[1]Michigan State University, East Lansing, MI; [2]Michigan State University, Department of Chemistry, East Lansing, MI*

TP 712 **Guided Amino Acid Sequence Determination of Antibody Light and Heavy Chains using Direct Mass Technology Fragmentation Spectra**; Ryan T Fellers[1, 2]; Michael A. R. Hollas[1, 2]; Bryan P. Early[1, 2]; Joseph B. Greer[1, 2]; Matthew T. Robey[2]; Abdul R. Basharat[2]; Taojunfeng Su[1]; Neil L. Kelleher[1]; Kenneth R. Durbin[2]; *[1]Northwestern University, Evanston, IL; [2]Proteinaceous, Evanston, IL*

TP 713 **Evaluation of top-down mass spectrometry analysis of exosome proteoforms enriched from plasma utilizing four different enrichment approaches**; Amal Mohamed Kamal Eltobshi[1]; Amy Carfagno[1]; Luca Fornelli[1]; *[1]University of Oklahoma, Norman, OK*

TP 714 **Increasing knowledge from Top Down Protein Analysis**; Stephen A Tate[1]; Lyle Burton[2]; *[1]SCIEX, Concord, ON; [2]SCIEX, Concord, ontario*

TP 715 **Top-Down Analysis of Malignant Cell Lines Reveals an Expanded RAS Proteoform Landscape**; Grace M Scheidemantle[1]; Robert A. D'Ippolito[1]; Kanika Sharma[1]; Nicole Fer[1]; Brian Smith[1]; Mackenzie Meyer[1]; Scott Eury[1]; Abigail Neish[1]; Alexandria L Sohn[1]; Min Hong[1]; Matthew R Drew[1]; Jennifer Mehalko[1]; Katie Powell[1]; Vanessa Wall[1]; William Burgan[1]; Dominic Esposito[1]; Anna E. Maciag[1]; Frank McCormick[1, 2]; Dwight V Nissley[1]; Caroline DeHart[1]; *[1]Frederick National Laboratory for Cancer Research, Frederick, MD; [2]Helen Diller Family Comprehensive Cancer Center, University of California, San Francisco, California*

TP 716 **Parameter Optimization for Proteoform-Specific Top-Down LC-MS/MS Leveraging Model Populations of RAS**; Alexandria L Sohn[1]; Grace M Scheidemantle[1]; Min Hong[1]; Matthew R Drew[1]; Jennifer Mehalko[1]; Katie Powell[1]; Vanessa Wall[1]; William Burgan[1]; Dominic Esposito[1]; Frank McCormick[1, 2]; Dwight V Nissley[1]; Caroline DeHart[1]; *[1]Frederick National Laboratory for Cancer Research, Frederick, MD; [2]Helen Diller Family Comprehensive Cancer Center, University of California, San Francisco, California*

TP 717 **Characterizing Recombinant RAS Proteoforms Using An Optimized High-Throughput Top-Down Proteomic Method and OptiMSe Software**; Grace M Scheidemantle[1]; Robert A. D'Ippolito[1]; Alexandria L Sohn[1]; Matthew R Drew[1]; Peter Frank[1]; Min Hong[1]; Jennifer Mehalko[1]; Simon Messing[1]; Shelley Perkins[1]; Kelly Snead[1]; Vanessa Wall[1]; Carissa Grose[1]; William Burgan[1]; William Gillette[1]; Dominic Esposito[1]; Frank McCormick[1, 2]; Dwight V Nissley[1]; Caroline DeHart[1]; *[1]Frederick National Laboratory for Cancer Research, Frederick, MD; [2]Helen Diller Family Comprehensive Cancer Center, University of California, San Francisco, California*

TP 718 **High efficiency electron capture dissociation enables top-down and bottom-up discovery proteomics at chromatographic and ion mobility timescales with a LC-Q-TOF**; Lester S. Manly[1]; Anne M. Roberts[1]; Joseph S. Beckman[2]; Blaine R. Roberts[1]; *[1]Emory Univ. School of Medicine, Atlanta, GA; [2]Oregon State University, Corvallis, OR*

TP 719 **Top-Down Proteomic MS Workflow to Screen for Specific, Reversible, and Covalent Natural Product-Derived Inhibitors**; Samantha J Knott[1]; Pelle Simpson[1]; Kurt Morgenstern[1]; William Old[1]; Marvin Yu[1]; *[1]Enveda Biosciences, Boulder, CO*

PROTEOMICS: QUANTITATIVE II
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TP 720 **Evaluation of a Modified Orbitrap Astral Mass Spectrometer for Label-Free Quantitation of Proteomic Samples**; Anna V. Pashkova[1]; Tabiwang N. Arrey[1]; Eduard Denisov[1]; Pedro Navarro[1]; Frank Berg[1]; Christoph Henrich[1]; Johannes Petzoldt[1]; Eugen Damoc[1]; *[1]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

TP 721 **Data driven optimization of the chromatographic peak sampling in dia-PASEF for optimal biomarker discovery workflows**; Bettina Streckenbach[1]; Christopher Below[1]; Ino Karemaker[1, 2]; Roland Bruderer[1]; Oliver M. Bernhardt[1]; Lukas Reiter[1]; *[1]Biognosys AG, Schlieren, Switzerland; [2]ETH Zürich, Zürich, Switzerland*

TP 722 **Global Mapping of Baseline Protein Turnover in 22 Murine Tissues and Fluids Using Pulse SILAM Proteomics**; Götz-Norman Hagemann[1]; Leonie Reichart[1]; Alexander Betz[1]; Catalina Cepeleaga[1]; Andreas Köpke[2]; Barbara Schnitzer[1]; Christin Zasada[1]; Hannes Hahne[1]; Kathrin Grundner-Culemann[1]; *[1]OmicScouts GmbH, Freising, Germany; [2]bioExpert, Nieder-Olm, Germany*

TP 723 **A targeted multiomics approach to differentiate clinically similar kidney diseases from liquid biopsy samples**; Jake T Kline[1]; Amy Carfagno[1]; Qingling Li[2]; Amal M Kamal[1]; Philip Remes[2]; Cristina Jacob[2]; Brittany Lee[2]; Lilian Heil[2]; Charles E. Maxey[2]; Amirmansoor Hakimi[2]; Stephanie N. Samra[2]; Romain Huguet[2]; Lorenzo Gallon[3]; Luca Fornelli[1]; *[1]University of Oklahoma, Norman, OK; [2]ThermoFisher Scientific, San Jose, CA; [3]University of Illinois Chicago, Chicago, IL*

TP 724 **Comprehensive Apolipoprotein Profiling Using Targeted Proteomics and Incident Cardiovascular Disease Events in the General Population**; Andrea Villanueva Raisman[1]; Tamas Szili-Torok[2, 3]; Daniel Eklund[3, 4]; My Nguyen[3]; Stephan JL Bakker[2]; Uwe JF Tietge[3, 4]; Fredrik Edfors[1]; *[1]SciLifeLab, KTH Royal Institute of Technology, Solna, Sweden; [2]Department of Internal Medicine, University Medical Center Groningen, University of Groningen,*

Groningen, Netherlands; [3]Division of Clinical Chemistry, Department of Laboratory Medicine, Karolinska Institutet, Stockholm, Sweden; [4]Medical Unit of Clinical Chemistry, Karolinska University Laboratory, Karolinska University Hospital, Stockholm, Sweden

TP 725 **Development of a CellenONE-automated top-down TMT-labeling platform for human cells**; Trishika Chowdhury[1]; Samin Anjum[1]; Anju Teresa Sunny[1]; Kellye A Sutton[1]; Si Wu[1]; *[1]University of Alabama, Tuscaloosa, AL*

TP 726 **Chemometric optimization of bottom-up proteomics sample preparation for absolute quantification of proteins in human plasma**; Margret Thorsteinsdottir[1, 2, 3]; Kari Arnarson[1, 3, 4]; Kristrun Yr Holm[1, 2]; Valdis Gunnarsdottir Thormar[2, 4]; Sigridur Klara Bodvardsdottir[2, 4]; Yassene Mohammed[5, 6, 7]; Christoph H. Borchers[6, 7, 8, 9]; Finnur Freyr Eiriksson[1, 3]; *[1]Faculty of Pharmaceutical Sciences, University of Iceland, Reykjavik, Iceland; [2]BioMedical Center, University of Iceland, Reykjavik, Iceland; [3]ArcticMass, Reykjavik, Iceland; [4]Faculty of Medicine, University of Iceland, Reykjavik, Iceland; [5]Leiden University Medical Center, Leiden, Netherlands; [6]Segal Cancer Center, Lady David Institute, McGill University, Montreal, QC; [7]Gerald Bronfman Department of Oncology, Montreal, QC; [8]Division of Experimental Medicine, McGill University, Montreal, QC H4A 3J1; [9]Department of Pathology, McGill University, Montreal, QC*

TP 727 **Decoding Aging and Health in Mice: High-Throughput Proteomics from Low Serum Samples**; Amit K Dey[1]; Bradley Olinger[1]; Maria Emilia Fernandez[1]; Nathan L Price[1]; Rafael De Cabo[1]; Nathan Basisty[1]; *[1]National Institute on Aging-NIH, Baltimore, Maryland*

TP 728 **High-throughput Proteomics Using Narrow Window DIA on a Modified Orbitrap Astral Mass Spectrometer**; Till Reinhardt[1]; Tabiwang N. Arrey[1]; Anna Pashkova[1]; Eduard Denisov[1]; Johannes Petzoldt[1]; Bernd Hagedorn[1]; Yannick Mueller[1]; Immo Colonius[1]; Arne Kreutzmann[1]; Hamish Stewart[1]; Christian Hock[1]; Eugen Damoc[1]; *[1]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

TP 729 **Single-cell Proteome Profiling of the Early Developing Xenopus laevis Embryo**; Ailing Li[1]; Isabelle Luz[1]; Peter Nemes[1]; *[1]University of Maryland, College Park, MD*

TP 730 **Expanding targeted instrumentation to discovery proteomics: Complement reporter ion quantification with an ion trap**; Qi Zhang[1, 2]; Edward Cruz[2, 3]; Alex Johnson[1, 2]; Philip Remes[4]; Vyas Pujari[2, 3]; Thao Nguyen[2, 3]; Michael Stadlmeier[2, 3]; Jessica Wang[2, 3]; Cristina Jacob[4]; Graeme McAlister[4]; Martin Wühr[2, 3]; *[1]Department of Chemical and Biological Engineering, Princeton University, Princeton, NJ; [2]Lewis-Sigler Institute of Integrative Genomics, Princeton University, Princeton, NJ; [3]Department of Molecular Biology, Princeton University, Princeton, NJ, United States, Princeton, NJ; [4]Thermo Fisher Scientific, San Jose, CA*

TP 731 **Quantitative Proteomics and Phosphoproteomics of Extracellular Vesicle by Multiplexed Data-Independent Acquisition**; Yi-Kai Liu[1]; Nathaniel Miller[1]; Marco Hadisurya[1]; Zheng Zhang[1]; W. Andy Tao[1, 2, 3, 4]; *[1]Department of Biochemistry, Purdue University, West Lafayette, IN; [2]Department of Chemistry, Purdue University, West Lafayette, IN; [3]Purdue Institute for Cancer Research, Purdue University, West Lafayette, IN; [4]Tymora Analytical Operations, West Lafayette, IN*

TP 732 **Proteoform-resolved kinetic measurement of deubiquitinase mediated polyubiquitin hydrolysis by top-down mass spectrometry**; Debapriya Bhattacharya[1]; Rishi Patel[2]; Chittaranjan Das[2]; Bryon S. Drown[2]; *[1]Purdue University, West Lafayette, IN; [2]Purdue Univeristy, West Lafayette, IN*

TP 733 **Selection of candidate factors that contribute to liver fibrosis using Olink Explore and LC-MS/MS analyses**; Ian TA Green[1]; James Rooney[1]; Chunna Guo[1]; Whitney Smith-Kinnaman[1]; Jessica Maiers[1]; Amber Mosley[1]; *[1]Indiana University School of Medicine, Indianapolis, IN*

TP 734 **Proteomic and phenotypic insights into a peripheral tissue model of Huntington's Disease**; Ephraim Chidi Ezeigbo[1]; Herbi Yuliantoro[1]; Anthony Debastiani[1]; Peng LI[1]; Justin Legleiter[2]; Stephen J Valentine[1]; *[1]West Virginia University, Morgantown, WV; [2]University of Nevada Reno, Reno, NV*

TP 735 **Insights into Biguanide-Protein Binding Mechanisms via Thermal Proteome Profiling**; Suman Choudhary[1]; Utham Valekunja[1]; Pawan K. Jha[1]; Yamazaki Shintaro[1]; Jing Chen-Roetling[1]; Akhilesh B. Reddy[1]; *[1]University of Pennsylvania, Perelman School of Medicine, Philadelphia, PA*

TP 736 **Impact of Isolation Window Width and Dynamic Range of Differential Expression on Quantitative FDR in DIA Experiments**; Anton Poliakov[1]; Nicolas Hartel[1]; Kent W Seeley[1]; *[1]Thermo Fisher Scientific, San Jose, California*

TP 737 **Detailed Investigation into Proteoform Inference from Mass Spectrometry based Plasma Proteomics and Affinity-based Platform Data**; Aron Phong[1]; Douglas Kirsher[2]; Shreya Chand[2]; Bich Nguyen[2]; Balazs Szoke[2]; Sara Ahadi[2]; *[1]Alkahest Inc., San Carlos, CA; [2]Alkahest, Inc., San Carlos, CA*

TP 738 **Identification and Functional Characterizations of U2AF1 protein interactome in MDS/AML Diseases**; Caroline Marie Johnston[1]; Yinsheng Wang[2]; Xiaomei He[1]; *[1]East Carolina University, Greenville, NC; [2]University of California, Riverside, CA*

TP 739 **Evaluation of a Novel Ion Source Using a Large-Scale Targeted Liquid Chromatography Mass Spectrometry (LC-MS) Assay for Translational Proteomics Research**; Jimmy Yi Zeng[1]; Ranjan Bhadra[1]; Hao Qian[1]; Sangeet Adhikari[1]; Katherine Walker[2]; Joshua A Silveira[2]; Cornelia L Boeser[2]; Eloy R. Wouters[2]; Jessica Chan[1]; Adam Poltorak[1]; Robert Zawada[1]; Philip Ma[1]; Bruce Wilcox[1]; *[1]Prognomiq, Inc., San Mateo, CA; [2]Thermo Fisher Scientific, San Jose, California*

TP 740 **A Proteomics Approach to Study the Concentration-Dependent Efficiency and Specificity of PD-L1 PROTACs with Low Cell Count Samples**; David Foreman[1]; Pooja Saklani[2]; Guang Yang[2]; Ahad Hossain[2]; Gaurav Chopra[2]; *[1]Purdue University, West Lafayette, IN; [2]Purdue Univeristy, West Lafayette, IN*

TP 741 **Profiling of Aryl Hydrocarbon Receptor Activation in Cell Lines Using Label-free Quantitative Proteomics**; Mayumi Pasqual[1]; Robert Jervine V Ortega[1]; Xudong Yao[1]; *[1]University of Connecticut, Storrs, CT*

TP 742 **Analysis and visualization of quantitative PTM proteomics data using FragPipe-Analyst and FragPipeAnalystR**; Yi Hsiao[1]; Haijian Zhang[2]; Yamei Deng[3]; Fengchao Yu[3]; Ralf B Schittenhelm[2]; Alexey I. Nesvizhskii[1, 3]; *[1]Department of Computational Medicine and Bioinformatics, University of Michigan, Ann Arbor, MI; [2]Monash University, Clayton, Australia; [3]Department of Pathology, University of Michigan, Ann Arbor, MI*

VIRUSES AND VIRUS-LIKE PARTICLES

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TP 743 **Characterizing the content and structure of AAV capsids by Size Exclusion Chromatography and Charge Detection Mass-Spectrometry**; Kanchan Pathak[1]; Gustavo Perrotti[1]; Steve J. Rosa[2]; Graham Robinett[2]; Lance Kasper[2]; James Q. Xia[3]; Carlos R. Escalante[1]; Fabio P. Gomes[1]; *[1]Virginia Commonwealth University, Richmond, VA; [2]Agilent Technologies, Santa Clara, CA; [3]CMP Scientific Corp, Brooklyn, NY*

TP 744 **Photodissociation charge detection mass spectrometry**; Lilou Duplantier[1]; Tessa Reinert[1]; Sylvain Maclot[1]; Lars Thiede[2, 3]; Ronja Pongan[2, 3]; Jürgen Müller-Guhl[2, 3, 4]; Sanne Ugelstad[2, 3]; Charlotte Uetrecht[2, 3]; Rodolphe Antoine[1]; *[1]Université Claude Bernard Lyon 1, Lyon, France; [2]CSSB Centre for Structural Systems Biology, Deutsches Elektronen-Synchrotron DESY & Leibniz Institute of Virology (LIV) & University of Lübeck, Notkestraße, Hamburg, Germany; [3]Institute of Chemistry and Metabolomics,* *University of Lübeck, Hamburg, Germany; [4]Bernhard Nocht Institute for Tropical Medicine (BNITM), Hamburg, Germany*

TP 745 **Determination of Empty/Full Capsid Ratio for Adeno-associated viruses: A comparison between Q Exactive UHMR Mass Spectrometer and Analytical Ultracentrifugation**; Yilong Zheng[1]; Jason Dugger[1]; Jie Ding[1]; *[1]PPD Clinical Research Services, Thermo Fisher Scientific, Middleton, WI*

TP 746 **The Size the Limit: STORI-method Orbitrap Charge Detection Mass Spectrometry of Species Greater Than 10 MDa**; Kyle Patrick Bowen[1]; Weijing Liu[1]; Zoltan Szabo[1]; Mike Senko[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

TP 747 **Use of Mass Spectrometry to Analyze USP AAV Reference Standard, Including Analysis of Full, Partial, and Empty Capsid Particles**; Anthony J Blaszczyk[1]; Ben Clarke[1]; Jerome Jacques[1]; *[1]United States Pharmacopeia, Rockville, MD*

TP 748 **Analysis of genome encapsidated in Adeno-associated virus vector by orbitrap-based charge detection mass spectrometry**; Ryoji Nakatsuka[1, 2, 3]; Yuki Yamaguchi[1]; Aoba Matsushita[4]; Yasuo Tsunaka[1]; Mitsuko Fukuhara[1, 4]; Tetsuo Torisu[1]; Susumu Uchiyama[1]; *[1]Department of Biotechnology, Graduate School of Engineering, Osaka University, Suita, Japan; [2]Technology Research Laboratory, Shimadzu Corporation, Kyoto, Japan; [3]Osaka University Shimadzu Analytical Innovation Research Laboratories, Osaka University, Suita, Japan; [4]U-Medico Inc, Suita, Japan*

TP 749 **Characterization of Qβ virus-like particles using Orbitrap-based charge detection mass spectrometry (CDMS)**; Ying-Ting Chiou[1]; Hung-Wei Yang[2]; Weijing Liu[3]; Szu-Hsueh Lai[1]; *[1]Department of Chemistry, National Cheng Kung University, Tainan, Taiwan; [2]Department of Biomedical Engineering, National Cheng Kung University, Tainan, Taiwan; [3]Thermo Fisher Scientific, 355 River Oaks Pkwy, San Jose, CA95134*

TP 750 **The application of mass photometry on the characterizations of recombinant adeno-associated virus**; Yuki Yamaguchi[1]; Saki Shimojo[1]; Tomohiko Ikeda[1]; Risa Shibuya[1]; Mitsuko Fukuhara[1, 2]; Yasuo Tsunaka[1]; Tetsuo Torisu[1]; Susumu Uchiyama[1]; *[1]Osaka University, Suita-shi, Japan; [2]U-Medico Inc, Suita, Japan*

TP 751 **Robust, scalable virus-host proteomics with AI-generative library of life kingdoms and iterative search of zoological space**; Quanqing Zhang; *UC Riverside, Riversdie, CA*

TP 752 **Structural Insights into Virus-Like Particles using Charge Detection Mass Spectrometry**; Anisha Haris[1]; Kevin Giles[1]; David Bruton[1]; Keith Richardson[1]; Jakub Ujma[1]; David Ballantyne[1]; Lars Thiede[2, 3]; Ronja Pogan[2, 3]; Jocky Chun Kui Kung[2, 3]; Charlotte Uetrecht[2, 3]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]CSSB Centre for Structural Systems Biology, Deutsches Elektronen-Synchrotron DESY & Leibniz Institute of Virology (LIV) & University of Lübeck, Notkestraße, Hamburg, Germany; [3]Institute of Chemistry and Metabolomics, University of Lübeck, Hamburg, Germany*

TP 753 **Epitope Mapping and Characterization of Anti-SARS-CoV-2 Nucleocapsid Nanobodies**; Rachelle A. Louis-Jacques[1]; Ann Maria P. John[1]; Peter C. Fridy[2]; Junjie Wang[2]; Michael P. Rout[2]; Brian T. Chait[2]; Erica Jacobs[1, 2]; *[1]St. John's University, Jamaica, NY; [2]Rockefeller University, New York, NY*

TP 754 **Recombinant Adeno Associated Virus (rAAV) Characterization and Comparison using Sedimentation Velocity-Analytical Ultra Centrifugation (SV-AUC) and Charge Detection Mass Spectrometry (CDMS)**; Anisha Haris[1]; Kevin Giles[1]; David Bruton[1]; Keith Richardson[1]; Yousef Abugalyon[2]; Cameron Raphael[2]; Suparna Taneja-Bageshwar[2]; Ashoka Maddur Appajaiah[2]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]FUJIFILM Diosynth Biotechnologies, College Station, TX*

TP 755 **A Novel Pipeline for Saliva Metaproteomics Using MetaNovo and MetaMorpheus Capable of Detecting Viral Mutations**; Yanjia Zhang[1]; Aaron Timperman[1]; *[1]University of Pennsylvania, Philadelphia, PA*

TP 756 **Detection and Characterization of Dynamic Protein Methylation Signatures in Cellulophaga balticaVirocells During Bacteriophage Infection**; Andrew J. Stai[1, 2]; Cristina Howard-Varona[3]; Marion Urvoy[3]; Natalie E. Solonenko[3]; Matthew B. Sullivan[3]; Robert L. Hettich[1]; *[1]Biosciences Division, Oak Ridge National Laboratory, Oak Ridge, TN; [2]University of Tennessee Knoxville, Knoxville, TN; [3]Department of Microbiology, Ohio State University, Columbus, OH*

TP 757 **Simplified nanoESI-MS analysis of AAV capsid proteins following MauriceFlex icIEF fractionation and DynaChip online buffer exchange**; Mason Chilmonczyk[1]; Carter Asef[1]; Austin Culberson[1]; Srinivasa Rao[2]; Will McElroy[2]; Jiaqi Wu[2]; Casey Vantucci[1]; Chris Heger[2]; *[1]Andson Biotech, Atlanta, GA; [2]ProteinSimple, a Bio-Techne Brand, San Jose, CA*

TP 758 **Mass Measurement of Extracted AAV Genomes Coupled with Intact Capsid Analysis to Assess Sequence Integrity and Protein**; Benjamin E Draper[1]; Lohra M Miller[1]; Gwendolyn J Jarrold[1]; Junping Zhang[2]; Weidong Xiao[2]; Martin Jarrold[1]; *[1]Megadalton Solutions, Bloomington, IN; [2]Indiana University School of Medicine, Department of Pediatrics, Indianapolis, IN*

TP 759 **Evaluation of mass spectrometry for characterization of adeno-associated virus serotype 9 (AAV9) identity, structure and distribution**; Allison N Schorzman[1]; Hunter Walker[1]; *[1]BridgeBio Gene Therapy, Raleigh, NC*

TP 760 **Probing the thermal behaviors of co-formulated dual vector AAVs by desalting size-exclusion chromatography coupled to charge detection mass spectrometry**; Chen Du[1]; Victoria C Cotham[1]; Shunhai Wang[1]; Ning Li[1]; *[1]Regeneron, Tarrytown, NY*

TP 761 **Empty and Full Capsid Ratio Analysis of SF9-Baculovirus Produced AAV After Each Step of the Downstream Purification Process**; Noah Miller-Medzon[1]; Timothy Fenn[1]; Rebecca D'Esposito[2]; Ying Qing Yu[2]; *[1]LEXEO Therapeutics, New York, NY; [2]Waters Corp., Milford, MA*

TP 762 **Mass Spectral Evidence from a Chaotic Assembly Process is Key to Reliable Copy Number Estimation of Tailed Phage Virion Components**; Trang Phan[1]; Grace Sullinger[1]; Fletcher Austin[1]; Natalie D'Alimonte[1]; Skye Bixler[1]; Caleb Emmons[2]; Sammy Pardo[3]; Dana Molleur[3]; Susan T. Weintraub[3]; Julie Thomas[1]; *[1]Rochester Institute of Technology, Rochester, NY; [2]Proteome Software, Portland, OR; [3]Univ. of Texas Health Science Center at San Antonio, San Antonio, TX*

TP 763 **Perturbations and Proteoforms: Deep proteomic investigation of HIV-1 Maturation Inhibitors Bevirimat and Lenacapavir on HIV-1 Virions**; Claire E Boos[1]; Mark Scalf[1]; James W Bruce[1]; Nathan M Sherer[1]; Lloyd M. Smith[1]; *[1]University of Wisconsin-Madison, Madison, WI*

TP 764 **Protein MS analysis of viral factories**; Joshua Sargeant[1]; Paul Gershon[1]; *[1]UC-Irvine, Irvine, CA*

TP 765 **Defining the Impacts of Intercellular Communication on the Three-Dimensional Virus Microenvironment**; Colter S Brainard[1]; Krystal K Lum[1]; James C Kostas[1]; Ileana M Cristea[1]; *[1]Princeton University, Princeton, NJ*

TP 766 **Robust Adeno-Associated Virus Aggregate Analysis with Reduced Sample Consumption on Biozen™ dSEC-7 Size Exclusion Column**; Crystal Holt; *Phenomenex, STOCKTON, CA*

TP 767 **Test**; Jennifer Anne Watson; *ASMS Office, Santa Fe, NM*

WEDNESDAY POSTERS

WEDNESDAY POSTERS

Set-up for all Monday posters
6:30 - 9:00 am

ALL POSTERS PRESENT

10:30 - 12:00 pm AND 1:00 - 2:30 pm

Remove all Monday posters
5:00 - 8:00 pm

Ambient Ionization: Applications ... 001-032
Biomarkers: Quantitative Analysis I ... 033-059
Carbohydrates ... 060-075
Drug and Metabolite Analysis ... 076-103
Environmental: General II ... 104-139
Food Safety & Chemistry: Foodomics, Allergens, Bacteria, Foods, and Supplements ... 140-176
Fundamentals: Formation and Structures of Big Ions ... 177-181
Fundamentals: Ion Structure/Energetics/Reactions ... 182-202
Glycomics ... 203-223
High Throughput MS I ... 224-246
Imaging MS: Instrumentation ... 247-258
Imaging MS: Pharmaceuticals, Metabolites, Lipids, and Glycans I ... 259-286
Imaging: Spatially-Resolved Omics I ... 287-306
Informatics: Algorithms and Statistical Advances ... 307-335
Instrumentation: General ... 336-353
Ion Mobility: Applications ... 354-373
Isotope Labeling and Fluxomics Applications ... 374-376
LC/MS: Sample Preparation I ... 377-399
Lipids: ID and Structural Analysis ... 400-420
Metabolomics: Clinical Applications ... 421-438
Metabolomics: Identification of Unknown Metabolites ... 439-459
Metabolomics: Sample Preparation ... 460-464
Neuroscience and Neurodegenerative Disease Research I ... 465-488
Nucleic Acids and Oligonucleotides II ... 489-515
Peptidomics and Immunopeptidomics ... 516-544
Phosphopeptides and Phosphoproteins ... 545-556
Plant Biology and Biotechnology ... 557-568
Protein Therapeutics: Structural Characterization ... 569-605
Proteins: Conformation Analysis and Structural Biology ... 606-628
Proteomics: Chemoproteomics ... 629-650
Proteomics: Clinical Applications ... 651-678
Proteomics: Infectious Diseases ... 679-693
Proteomics: New Approaches I ... 694-719
Single Cell MS I ... 720-747
Stable Isotope Labeling ... 748-762

AMBIENT IONIZATION: APPLICATIONS
001-032

WP 001 **Rapid Identification of Prohibited Substances in Sports Black Market Products using ASAP-MS**; Alisha Henderson[1]; Oliver Krug[2]; David Douce[3]; Ashley Sage[3]; Mario Thevis[2]; Liam M Heaney[1]; *[1]Loughborough University, Loughborough, United Kingdom; [2]German Sport University Cologne, Cologne, Germany; [3]Waters Corporation, Wilmslow, United Kingdom*

WP 002 **Rapid Multiplex Antimicrobial Resistance Profiling and Bacterial Identification by LAP-MALDI MS Biotyping**; Lily R Adair[1]; Ian Jones[2]; Rainer Cramer[1]; *[1]Department of Chemistry, University of Reading, Reading, United Kingdom; [2]School of Biological Sciences, University of Reading, Reading, United Kingdom*

WP 003 **Streamlining Fungal Natural Product Discovery using the Liquid Microjunction Surface Sampling Probe**; Jess Deng[1]; Jennifer L. Kolwich[1]; Georgia Reed[2]; Avena C Ross[1]; Randy E. Ellis[2, 3, 4, 5]; Richard D. Oleschuk[1]; *[1]Department of Chemistry, Queen's University, Kingston, ON; [2]School of Computing, Queen's University, Kingston, ON; [3]Department of Mechanical and Materials Engineering, Queen's University, Kingston, ON; [4]Department of Surgery, Queen's University, Kingston, ON; [5]Department of Biomedical and Molecular Sciences, Queen's University, Kingston, ON*

WP 004 **Quick and easy on-target sample cleanup method for Liquid AP-MALDI**; Agata Kowalczyk[1]; Jeffery Brown[2]; Rainer Cramer[1]; *[1]University of Reading, Reading, United Kingdom; [2]Waters Corporation, Wilmslow, United Kingdom*

WP 005 **Intermittent Headspace Sampling and Profiling of Volatile Organic Compounds via Dielectric Barrier Discharge Ionization: Application to Aroma Differentiation in Wine**; Daniel A Heffernan[1]; Nicole Strittmatter[2]; Frederik Oleinek[2]; Paak Wai Lau[2]; Ayla Schueler[2]; Alina Meindl[3]; Mathias Senge[4]; Aleksei Karpenko[2]; *[1]Technical University of Munich, Garching, Germany; [2]Technical University of Munich, Garching bei Muenchen, Germany; [3]Department Design & Green Engineering Fachhochschule, Salzburg, Austria; [4]Trinity college, Dublin, Ireland*

WP 006 **Utilizing Direct Analysis in Real Time Mass Spectrometry for Sample Normalization in Quantitative Metabolomics**; Yousef Haidar[1]; Liang Li[1, 2]; *[1]University of Alberta, Faculty of Science, Chemistry Department, Edmonton, AB; [2]The Metabolomics Innovation Centre (TMIC), University of Alberta, Edmonton, AB*

WP 007 **Semi quantitative nicotine analysis and screening of electronic cigarette oils using Waters™ RADIAN™ ASAP mass spectrometer**; Thomas G Milnes[1]; Nick Birse[1]; Simon JS Cameron[1]; *[1]Queens University Belfast, belfast, United Kingdom*

WP 008 **Rapid Discrimination and Quality Assessment of Chinese Baijiu Flavor Profiles using SICRIT-MS Analysis**; Fuyuan Tan[1]; Charles C. Liu[2]; Xiaokun Duan[2]; *[1]Tinghua Liquor Industry Co., Ltd, Yibin, China; [2]ASPEC Technologies, Beijing, China*

WP 009 **Identification of Cigarette Ashes by Direct Analysis in Real Time Mass Spectrometry (DART-MS)**; Shujun Liu[1]; Xiaokun Duan[2]; Charles C. Liu[2]; *[1]Shenyang Fire Science and Technology Research Institute of MEM, Shenyang, China; [2]ASPEC Technologies, Beijing, China*

WP 010 **Simultaneous CID and EI-Like Fragmentation of Odd-Electron Ions using DBDI with Atomospheric Pressure-Inlet Mass Spectrometer**; Ciara Conway[1, 2]; Markus Weber[1, 2]; Jan-Christoph Wolf[2]; Christoph Haisch[1]; *[1]Technical University of Munich, Garching, Germany; [2]Plasmion, Augsburg, Germany*

WP 011 **Using the Waters RADIAN™ ASAP mass spectrometer to develop rapid and cost-effective tests for food safety**; Annette O Farrell[1]; Nick Birse[2]; Panagiotis Manesiotis[1]; Simon JC Cameron[1]; *[1]Queens University Belfast, Belfast, United Kingdom; [2]Queens University Belfast, belfast, United Kingdom*

WP 012 **Heat pulse desorption mass spectrometry of low-volatility compounds using an AC corona discharge ion source enclosed in a PFA tube**; Stephanie Rankin-Turner[1]; Satoshi Ninomiya[2]; Kenzo Hiraoka[2]; *[1]University of Pittsburgh, Pittsburgh, PA; [2]University of Yamanashi, Kofu, Japan*

WP 013 **Identification of the Polymer Composition of Food Contact Articles using DART-HRMS**; Victoria M Anderson[1]; Jānis Ruško[2]; Ingus Pērkons[2]; Kristen Reese[1]; Luke K. Ackerman[1]; *[1]FDA, College Park, MD; [2]BIOR Institute of Food Safety, Animal Health and Environment "BIOR", Laboratory of Chemistry, Riga, Latvia*

WP 014 **Use of Ambient Ionization Mass Spectrometry for a Semiquantitative Screening of Muscle Enhancers in Illegal Products**; Alzbeta Nemeskalova[1, 2]; Jana Knytlova[1]; Iveta Silhankova[1]; Petra Dinisova[3]; Martin Kuchar[1]; Michael Volny[1, 2]; *[1]University of Chemistry and Technology in Prague, Prague 6 - Dejvice, Czech Republic; [2]Institute of Microbiology, Prague 4, Czech Republic; [3]Pragolab s.r.o., Nad Krocinkou 285/55, Prague 9, Czech Republic*

WP 015 **Approach to analysis of autopsy material with possible implementation in medical diagnostics**; Ekaterina Parochkina[1]; Andrey Temnov[2]; Anatoly Sorokin[1]; Mikhail Oliferenko[1]; Anna Rumyantseva[1]; Denis Bormotov[1]; Stanislav Pekov[1, 3]; Igor Popov[1]; *[1]MIPT, Dolgoprudny, Russia; [2]Institute of Cell Biophysics, Puschino, Russia; [3]Skoltech, Skolkovo, Russia*

WP 016 **Classification of edible oils analyzed with ambient ionization mass spectrometry**; Rachel L Theriault[1]; Malek Hassan[2]; Richard David Oleschuk[2]; Randy E Ellis[1]; *[1]Queen's University, School of Computing, Kingston, Ontario; [2]Queen's University, Department of Chemistry, Kingston, Ontario*

WP 017 **Rapid, multi-class volatile analyses using Solid Phase Microextraction Sheets and Direct Analysis in Real Time Mass Spectrometry (SPMESH-DART-MS)**; Zoë C Scott[1]; Andre P Kalenak[1]; Gavin L Sacks[1]; *[1]Cornell University, Ithaca, NY*

WP 018 **Development and Validation of Method for Quantification of Antimycotics utilizing DART-MS**; Zahuindanda Aventura[1]; Lukas Brunner[2]; Anna Bui[2]; Saulė Nickutė[2]; Gernot Wolfram[2]; *[1]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [2]RECIPE Chemicals + Instruments GmbH, Munich, Germany*

WP 019 **Direct, Targeted Ambient Ionization Mass Spectrometry Analysis of Enzyme-Facilitated Degradation of Nylon Polymers**; Miranda E. Lockley[1]; Malek Hassan[1]; Mikaela K. Coleman[1]; Maria E. Cleveland[1]; Graeme W. Howe[1]; Richard D. Oleschuk[1]; *[1]Department of Chemistry, Queen's University, Kingston, Ontario*

WP 020 **Colorectal Cancer phenotyping pathways using ambient ionisation mass spectrometry from early diagnosis to precision treatment**; Lauren Ford[1]; Elmeri J Latvanen[2]; Duncan Roberts[2]; Petra Paizs[1]; Eftychios Manoli[1]; Maria Sani[1]; James Mckenzie[2]; James Kinross[1]; Zoltan Takats[2, 3]; *[1]Imperial college london, London, United Kingdom; [2]Imperial College London, Division of Systems Medicine, London, United Kingdom; [3]University of Regensburg, Department of Immune Medicine Multimodal Imaging of Intracellular Communication, Regensburg, Germany*

WP 021 **Rapid Screening Using Ambient Ionisation Mass Spectrometry Uncovers Chemotherapy-Induced Phospholipidosis and Lipid Metabolic Reprogramming in Ovarian Cancer Cells**; Wangxing Guo[1]; Amar Rai[1, 2]; Klaudia Mitiajew[1]; Yu Wang[3]; Apostolia Galani[4]; Maria Paraskevaidi[4]; Yuchen Xiang[1]; Robert Murray[3]; Maria Kyrgiou[4]; Zoltan Takats[1, 5]; Stefania Maneta-Stavrakaki[1]; *[1]Imperial College London, Division of Systems Medicine, London, United Kingdom; [2]Rosalind Franklin Institute, Didcot, United Kingdom; [3]Imperial College London, Department of Physics, London, United Kingdom; [4]Imperial College London, Institute of Reproductive Developmental Biology, London, United Kingdom; [5]University of Regensburg, Department of Immune Medicine Multimodal Imaging of Intracellular Communication, Regensburg, Germany*

WP 022 **Small Solutions to Big Problems: Using Submicron Diameter Emitters to Electrospray Directly from Standard Biophysical Conditions**; Jacob S Jordan[1]; Nicklas Österlund[1]; Michael Götze[1]; Kevin Pagel[1]; *[1]Freie Universität Berlin, Berlin, Germany*

WP 023 **Rapid Quantification of PFAS compounds in water utilizing a weak anion exchange coated blade spray mass spectrometry**; Thomas Kane[1]; Ryan Micklitsch[1]; Shane Stevens[1]; Diego Lopez[1]; Mathew Lininger[1]; Gary Stidsen[1]; Tracey Peters[1]; *[1]Restek Corporation, Bellefonte, PA*

WP 024 **Forensic Application of Sandpaper Spray Ionization Mass Spectrometry (SPS-MS): Chemotaxonomic Classification of Brazilian and Canadian Woods**; Karl Angelo M Rodrillo[1]; Thays V.C. Monteiro[2]; Rodinei Augusti[3]; Maíra Fasciotti[2]; Demian Rocha Ifa[1]; *[1]Department of Chemistry, York University, Toronto, ON; [2]National Institute of Metrology, Quality and Technology, Vitória, Brazil; [3]Universidade Federal de Minas Gerais, Belo Horizonte, Brazil*

WP 025 **Sorbent Mesh Design Improves Detection Limits for Rapid Trace Volatile Analyses by SPMESH-DART-MS**; Andre P Kalenak[1]; Gavin L Sacks[1]; *[1]Cornell University Dept. of Food Science, Ithaca, NY*

WP 026 **Abiotic Disaccharide Formation in Aqueous Microdroplets Investigated via Mass Spectrometry**; Myles Edwards[1]; Dylan T Holden[2]; R. Graham Cooks[2]; *[1]Purdue University, West lafayette, Indiana; [2]Purdue Univeristy, West Lafayette, IN*

WP 027 **Monitoring spatiotemporal dynamics of soil microbe co-culture metabolites using ambient mass spectrometry**; Jess Deng[1]; Jennifer L. Kolwich[1]; Kyla Toshack[1]; Avena C Ross[1]; Richard Oleschuk[2]; *[1]Queen's University, Department of Chemistry, Kingston, Ontario; [2]Queen's University, Kingston, ON*

WP 028 **Detection of Glioma Biomarkers using Touch Spray Tandem Mass Spectrometry**; Mahdiyeh Shahi[1]; Kenneth Lane Virgin[2, 3]; Diogo Moniz Garcia[4]; Alfredo Quiñones-Hinojosa[4]; Robert Graham Cooks[5]; *[1]Purdue University, west lafayette, IN; [2]Purdue University, West Lafayette, IL; [3]Indiana University School of Medicine, Indianapolis, IN; [4]Mayo Clinic, Jacksonville, FL; [5]Purdue Univeristy, West Lafayette, IN*

WP 029 **Analytical Characterization of Polyfluorinated Coatings on Paper Food Packaging**; Luke K Ackerman[1]; Clark Ridge[1]; Jennifer Janovick[2]; Iris Yourick[3, 4]; Victoria Anderson[1]; Jordan Escavage[1]; Elsie Peprah[1]; Sarah Prebihalo[1]; Katherine Carlos[1]; Peter F Scholl[5]; *[1]FDA Human Foods Program, College Park, MD; [2]Joint Institute for Food Safety and Applied Nutrition (JIFSAN), University of Maryland, College Park, MD; [3]Oak Ridge Institute for Science and Education, Oak Ridge, TN; [4]UCSD, San Diego, CA; [5]Retired - FDA Human Foods Program, College Park, MD*

WP 030 **New Ionization Mechanism in LC-ESI-MS for Highly Polar Pesticides: A Strategy to Improve Sensitivity**; Diego A Grassi[1]; Facundo Larregui[1]; Pablo Blasco[1]; Daniela Morello[2]; Ricardo Petersen[2]; *[1]Analytical Technologies, Buenos Aires, Argentina; [2]Proanalisis S.A., Buenos Aires, Argentina*

WP 031 **Metabolic Profiling in Long COVID Using an Embossed Paper Platform for Paper Spray Mass Spectrometry Analysis**; Monica Duarte Silva[1]; Abraham K. Badu-Tawiah[2]; *[1]The Ohio State University, Columbus, OH; [2]The Ohio State University Department of Chemistry and Biochemistry, Columbus, OH*

WP 032 **Qualitative and quantitative MS, different parts of similar equations for EI,CI, MALDI, ESI MS, a Beer's Law Analogy?**; Drew Sauter; *Nanoliter, LLC, Henderson, NV*

BIOMARKERS: QUANTITATIVE ANALYSIS I
033-059

WP 033 **Characterization and Quantification of Human IgG Light Chain in Biological Samples by High-Resolution Mass Spectrometer**; Chunhai Ruan[1]; Gus Hui[1]; Gang Xu[1]; Shane Woolf[1]; Kumar Shah[1]; Moucun Yuan[1]; William Mylott Jr. [1]; *[1]PPD, part of Thermo Fisher Scientific, Richmond, VA*

WP 034 **Towards the Development of a Liquid Chromatography Free Workflow for Measurement of Clinically Important Proteins**; Ruben Shrestha[1]; Matthew Willets[2]; Daniel Hornburg[1]; Gary Kruppa[3]; Christopher Clark[2]; Ganesh Balasubramanian[1]; Richard Yip[4]; Andrew Hettle[4]; Morteza Razavi[5]; Leigh Anderson[4]; *[1]Bruker Daltonics GmbH & Co. KG, San Jose, CA; [2]Bruker Daltonics GmbH & Co. KG, Billerica, MA; [3]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [4]SISCAPA Assay Technologies Inc., Washington D.C., DC; [5]SISCAPA Assay Technologies Inc., Victoria, BC*

WP 035 **Developing a Targeted UPLC-MS/MS Method from Untargeted Work to Measure Diverse Urinary Phase II Metabolites**; Jin Y Chen[1]; Zhengzhi Xie[1]; Pawel Lorkiewicz[1]; Sanjay Srivastava[1]; *[1]University of Louisville, Louisville, KY*

WP 036 **Metabolomic biomarkers of acute radiation syndrome and delayed effects of acute radiation exposure : correlation with histological and clinical endpoints**; Swarnima Pandey[1]; Nageswara Pilli[2]; Praveen Kumar[2]; Jace W. Jones[2]; George Parker[3]; Catherine Booth[4]; Gregory Tudor[4]; Ann M. Farese[5]; Thomas J. MacVittie[5]; Polly Chang[6]; Maureen A. Kane[2]; *[1]University of Maryland, Baltimore, MD; [2]University of Maryland, School of Pharmacy, Department of Pharmaceutical Sciences, Baltimore, MD; [3]Charles River Laboratories, Edinburgh, United Kingdom; [4]Epistem Ltd., Manchester, United Kingdom; [5]University of Maryland, School of Medicine, Department of Radiation Oncology, Baltimore, MD; [6]SRI International, 333 Ravenswood Ave Menlo Park, CA*

WP 037 **Transforming Plasma Proteomics: Leveraging the Performance of SysQuan for Absolute Quantitation**; Yassene Mohammed[1, 2]; Vincent R. Richard[1, 3]; M. Immanuel Reyes Madlangsakay[4]; Ying Lao[4]; Victor Spicer[4]; Claudia Gaither[5, 6]; Pradyumn Maheshwari[5]; Eileen Tudorica[5]; Stoyan Stoychev[7]; Timon Geib[8]; Robert Popp[5]; René P. Zahedi[4, 9, 10, 11]; Dorte B. Bekker-Jensen[7]; Nicolai Bache[7]; Christoph H. Borchers[1, 3, 12, 13, 14]; *[1]Segal Cancer Proteomics Centre, Jewish General Hospital, Montreal, QC; [2]Leiden University Medical Center, Leiden, Netherlands; [3]McGill University - Lady Davis Institute, Montréal, QC; [4]Manitoba Centre for Proteomics and Systems Biology, Winnipeg, MB; [5]MRM Proteomics Inc, Montreal, Quebec; [6]Faculty of Veterinary Medicine, Department of Clinical Sciences, University of Montreal, Montreal, QC; [7]Evosep Biosystems, Odense, Denmark; [8]McGill University - Lady Davis Institute, Montreal, QC; [9]Department of Internal Medicine, University of Manitoba, Winnipeg, MB; [10]Department of Biochemistry and Medical Genetics, University of Manitoba, Winnipeg, MB; [11]Paul Albrechtsen Research Institute, CancerCare Manitoba, Winnipeg, MB; [12]Gerald Bronfman Department of Oncology, Montreal, QC; [13]Division of Experimental Medicine, McGill University, Montreal, QC; [14]Department of Pathology, McGill University, Montreal, QC*

WP 038 **Develop and Validate an Accurate LC-MS/MS Method to Quantify 5-Methylthioadenosine in Human Plasma**; Chenggang Li[1]; Changjian Zhao; Jinzhi Liu; Laixin Wang[1]; Yuhuan Ji; *[1]Resolian, Chongqing, China*

WP 039 **Develop and Validate an Ultra-sensitive LC-MS/MS Method to Simultaneously Quantify Angiotensin II and Aldosterone in Human Plasma**; Chenggang Li[1]; Changjian Zhao[1]; Jinzhi Liu[1]; Laixin Wang[2]; Yuhuan Ji[1]; *[1]Resolian, Chongqing, China; [2]Chongqing Denali Medpharma Co.,Ltd, Chongqing, China*

WP 040 **Proteomic Analysis of Host Response to CD437 Treatment in MRSA-Infected C57BL/6 Mouse Lung**; Mehari M. Weldemariam[1]; Samuel Krug[1]; Ravineel Singh[2]; Keven M. Robinson[2]; Maureen A. Kane[1]; *[1]University of Maryland Baltimore, Baltimore, MD; [2]University of Pittsburgh, School of Medicine, Department of Medicine, Pittsburgh, PA*

WP 041 **Protein breakdown: How sample preparation affects peptide-based protein quantification**; Ceren Kul[1]; Pelin Yildiz[1]; Sureyya Ozcan[1]; *[1]Department of Chemistry, METU, Ankara, Turkey*

WP 042 **Automated Clinical Sample Preparation and Triple Quadrupole LC-MS/MS Analysis via Reverse Trap-and-Elute Chromatography of Serum Vitamin D Metabolites**; Stanislaw Krzyzanowski[1]; Praveen K Alla[2]; Mathew S Hautman[1]; Milaan Thirukumaran[1]; Alyssa S Aebersold[2]; Nazim Boutaghou[1]; *[1]Shimadzu Scientific Instruments, Columbia, Maryland; [2]CompuNet, Moraine, Ohio*

WP 043 **Streamlined automated sample preparation and protein quantification of tissue lysates for improved throughput and normalization of LCMS measurements**; Andrea Casasola-LaMacchia[1]; Nick Psychogios[1]; Evan Mettenbrink[1]; Alyssa Myers[1]; Krista Carpenter[1]; Hannah Pepper[1]; Jay Johnson[1]; Katherine Wright[1]; Hendrik Neubert[1]; *[1]Pfizer Inc., Andover, MA*

WP 044 **Point-of-Care Alcohol Consumption Monitoring by Aziridination of Phosphatidylethanol (PEth)**; Joseph Caruso[1]; Muhammad Ali[2]; Kai-Hung Huang[2]; Veronica Feng[2]; Nicolas M Morato[2]; Peter Anderson[3]; Kristina Brooks[3]; R. Graham Cooks[2]; *[1]Purdue University, West Lafayette, IN; [2]Purdue Univeristy, West Lafayette, IN; [3]University of Colorado Anschutz, Aurora, CO*

WP 045 **Quantitation of galactosemia biomarkers by chemical derivatization LC-MRM/MS**; Jun Han[1, 2]; Madeleine Chan[1]; Juncong Yang[1]; Jasmine Benoit[1]; Jason Bi[1]; Dave Schibli[1, 2]; David R. Goodlett[1, 3]; *[1]Genome BC Proteomics Centre, University of Victoria, Victoria, BC; [2]Division of Medical Sciences, University of Victoria, Victoria, BC; [3]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC*

WP 046 **Oxylipin Quantification in Plasma of People with Heart Failure: A Mass Spectrometry-Based Investigation of Inflammation-Driven Disease Progression**; Dominique A Baldwin[1]; Jericha Mill[2]; Farhan Raza[2]; Judith Simcox[2, 3]; *[1]University of Madison-Wisconsin, Madison, WI; [2]University of Wisconsin-Madison, Madison, WI; [3]Howard Hughes Medical Institute, Chevy Chase, Maryland*

WP 047 **An ultra-sensitive LC-MS strategy for absolute, accurate quantification of membrane proteins revealed substantial presence of FcRn on cell surface**; Qingqing Shen[1]; Chao Xue[1]; Xiaoyu Zhu[1]; Huiting Tang[1]; Jun Qu[1]; *[1]State University of New York at Buffalo, Buffalo, NY*

WP 048 **Method Transfer of Testosterone, 4-Androstene 3, 17-dione, and Pregnenolone in Human Serum Using Liquid Chromatography and Tandem Mass Spectrometric Detection**; Matthew W Probst; *Labcorp, Indianapolis, IN*

WP 049 **Revolutionizing translational research: large-scale targeted PRM proteomics assays enabled by Stellar mass spectrometer (MS)**; Qingling Li[1]; Cristina C. Jacob[1]; Philip M. Remes[2]; Jared Deyarmin[1]; Amirmansoor Hakimi[3]; Stephanie N. Samra[3]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientfic, San Jose, CA; [3]Thermo Fisher Scientific, San Jose, California*

WP 050 **Highly Multiplex Targeted Proteomics Assays in Plasma using Stellar Mass Spectrometer with Adaptive RT**; Qingling Li[1]; Jared Deyarmin[2]; Stephanie N. Samra[1]; Cristina C. Jacob[1]; Kerry Hassell[3]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific, San Jose, California*

WP 051 **Large-scale targeted biomarker analysis of volatile organic compounds in breath by TD-GS-Orbitrap**; Darren Barrington-Light[1]; Mircea Martiniuc[2]; Tilly Woodland[2]; Kayleigh Arthur[2]; Annamaria Szabo[2]; Lourenco Saco[2]; Laercio Fernandes[1]; *[1]Thermo Fisher Scientific, Altrincham, United Kingdom; [2]Owlstone Medical Ltd., Cambridge, United Kingdom*

WP 052 **Sensitive and selective quantitation of bile acids in children with autism spectrum disorder using targeted**

MS2/MS3 on the Stellar MS; Jingshu Guo[1]; Lauren Bishop[2]; Bashar Amer[2]; Alexey V Melnik[3]; James B. Adams[4]; Rosa Krajmalnik-Brown[4]; Khemlal Nirmalkar[4]; Charles E. Maxey[2]; Cristina Jacob[2]; Kerry Hassell[2]; Scott M. Peterman[2]; Susan S Bird[2]; *[1]Thermo Fisher Scientific, Roseville, MN; [2]Thermo Fisher Scientific, San Jose, CA; [3]BileOmix Inc., Farmington, Connecticut; [4]Arizona State University, Tempe, AR*

WP 053 **Metabolomic Response to Non-Steroidal Anti-Inflammatory Drugs**; Soumita Ghosh[1]; Nick Lahens[2]; Kayla Barekat[1]; Soon Yew Tang[2]; Katherine Theken[1]; Emanuela Ricciotti[2]; Arjun Sengupta[2]; Robin Joshi[2]; Federic D Bushman[2]; Aalim Weljie[2]; Tilo Grosser[3]; Garret A FitzGerald[1]; *[1]University of Pennsylvania, Philadelphia, PA; [2]University of Pennsylvania, Perelman School of Medicine, Philadelphia, PA; [3]Bielefeld University, Bielefeld, Germany*

WP 054 **Rapid, Derivatization-Free Separation and Quantification of D- and L-2-Hydroxyglutaric Acid via Chiral LC-MS/MS**; Taylor A. Harmon[1]; Mioara Larion[1]; *[1]National Cancer Institute, Bethesda, MD*

WP 055 **Optimization of extraction parameters to maximize recovery of diverse analyte classes from dried blood spots**; Omar Aboul-Houda[1]; Austin Pickens[1]; Samantha L. Isenberg[1]; Rachel Lee[1]; Carla Cuthbert[1]; *[1]CDC, Atlanta, GA*

WP 056 **Deep Spatial Proteomics of Primary Cilia: Unlocking Subcellular Proteome Composition with Nanoscale Precision**; Yi-De Chen[1]; Chantal Hoi Yin Cheung[1]; Hsiao-Jen Chang[1]; Chia-Wen Chung[1]; Chun-Kai Huang[1]; Weng Man Chong[1]; Jung-Chi Liao[1]; Christoph Krisp[2, 3]; Taiga Arai[4]; Daniel Hornburg[4]; *[1]Syncell Inc, Taipei, Taiwan; [2]Bruker Daltonics GmbH & Co.KG, Bremen, Germany; [3]MDC-Bruker Center of Excellence for Single Cell Omics, Max Delbrück Center – Berlin Institute for Medical Systems Biology, Berlin, Germany; [4]Bruker, Billerica, MA*

WP 057 **Development and Evaluation of a Multiplexed Health Surveillance Panel using ultra-high throughput PRM-MS in an Inflammatory bowel disease cohort**; Qin Fu[1, 2]; Philip Remes[2]; Jihyeon Lee[1]; Cristina Jacob[2]; Dalin Li[1]; Manasa Vegesnas[1]; Koen Raedschelders[1]; Ali Haghani[1]; Sandy Joung[1]; Susan Cheng[1]; Scott M. Peterman[2]; Justyna Fert-Bober[1]; Dermot P. B. McGovern[1]; Christopher I. Murray[1]; Jennifer E. Van Eyk[1]; *[1]Cedars Sinai Medical Center, Los Angeles, CA; [2]Thermo Fisher Scientific, 355 River Oaks Pkwy, San Jose, California*

WP 058 **Accurate LC-MS-based protein quantification in deep plasma profiling enabled by end-to-end enrichment workflow with the Evotip Pure**; Joel Vej-Nielsen[1]; Frederik Tolberg[1]; Stoyan Stoychev[1]; Dante' Johnson[1]; Nicolai Bache[1]; Dorte Bekker-Jensen[1]; *[1]Evosep, Odense, Denmark*

WP 059 **Bridging Computational Complexity and Biological Discovery: Interactive Differential Abundance Analysis in MD 3.0**; Mansi Aggarwal[1]; Sara Ceccacci[2, 3]; Kevin Roger[2]; Ida Chiara Guerrera[2]; Anna Quaglieri[1]; *[1]Mass Dynamics, Melbourne, Australia; [2]Necker Proteomics, Université Paris Cité - Structure Fédérative de Recherche Necker, INSERM US24/CNRS UAR3633, Paris, France; [3]Université Paris Cité, INSERM, UMR 1163, Institut Imagine, Laboratory of Genetic Skin Diseases, Paris, France*

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WP 060 **Trifluoromethyl Carbohydrate Footprinting for Probing Protein Binding Components of Oligosaccharides Mixture**; Quadrat Yusuph[1]; Sandeep K Misra[1]; Joshua S Sharp[1]; *[1]University of Mississippi, Oxford, MS*

WP 061 **B3GALT5-mediated SIAE and glycoRNA let-7a regulates colon mucosal barrier function in ulcerative colitis**; Xiaotong Wang[1]; Guoqiang Ma[2]; Duanmin Hu[3]; Shuang Yang[2]; *[1]Department of Hepatology and Gastroenterology, The Affiliated Infectious Hospital of Soochow University, Suzhou, China; [2]Soochow University, Suzhou, China; [3]Department of Gastroenterology, The Second Affiliated Hospital of Soochow University, Suzhou, China*

WP 062 **Rapid Profiling of Human Milk Oligosaccharides at Enhanced Coverage of Isobaric and Isomeric Heterogeneity Using TIMS-Enabled MALDI Mass Spectrometry**; Marko Mank[1]; Aliye Ozalp[1]; Arndt Asperger[2]; Bernd Stahl[1, 3]; Klaus Lindpaintner[4]; *[1]Danone Research & Innovation, Utrecht, Netherlands; [2]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [3]Department of Chemical Biology & Drug Discovery, Utrecht Institute for Pharmaceutical Sciences, Utrecht University, Utrecht, Netherlands; [4]Bruker Scientific LLC, Billerica, MA*

WP 063 **Characterization of Saccharide Isomers via MS/MS spectra of Negative Chloride Adducts Using an Advanced Scoring Algorithm with Diagnostic Ion**; Shixiang Xu[1]; Santosh Raman Acharya[1]; Ruth M Speidel[1]; Badu-Tawiah Abraham[1]; *[1]Ohio State University, Columbus, OH*

WP 064 **Bespoke SEC calibration for carbohydrates using direct infusion high-resolution mass spectrometry**; Yu-Ping Huang[1]; Michael Bukowski[1]; *[1]Methods and Application of Food Composition Laboratory, Beltsville Human Nutrition Research Center, USDA-ARS, Beltsville, MD*

WP 065 **Characterization ofLipopolysaccharidesin Outer Membrane Vesicles and Vaccine Conjugates via FAIMS and Kendrick Mass Defect Plots**; Abanoub Mikhael[1, 2]; Darryl Hardie[2]; Helena Petrosova[1, 2]; Alan Cross[3]; Robert K Ernst[3]; David R. Goodlett[1, 2]; *[1]University of Victoria, Victoria, BC; [2]University of Victoria GBC Proteomics Centre, Victoria, BC, BC; [3]University of Maryland, Baltimore, MD*

WP 066 **Label-Free Glycomic Strategy for Differentiating Acidic Monosaccharide Isomers from Marine Polysaccharides**; Nari Seo[1, 2]; Hyun Joo An[1, 2]; *[1]Chungnam National University, Daejeon, South Korea; [2]Asia Glycomics Reference Site, Daejeon, South Korea*

WP 067 **Towards Spatially Resolved 'Saccharide' Analyses: TIMS Analysis of Chondroitin Sulphate in situ.**; Anthony J Devlin[1]; Alice Bertocchi[2]; Ffion R. Hammond[2]; Daniel Simon[3]; Zoltan Takats[3]; Felicia Green[1]; *[1]Rosalind Franklin Institute, Didcot, United Kingdom; [2]Kennedy Institute of Rheumatology, Oxford, United Kingdom; [3]Imperial College London, London, United Kingdom*

WP 068 **Development of an (IM-MS)2 Method with Multi-Pass Cyclic Ion Mobility Spectrometry for Enhanced Glycan Structural Elucidation**; Chaoshuang Xia[1]; Elias Mernie[1]; Joseph Zaia[1]; Catherine E Costello[1]; Cheng Lin[1]; *[1]Boston University Chobanian & Avedisian School of Medicine, Boston, MA*

WP 069 **Acidic Sheath Liquid Capillary Electrophoresis to Increase Charge States of GAGs for More Efficient Electron-Based Fragmentation**; Jonathan Choi[1]; I Jonathan Amster[1]; *[1]University of Georgia, Athens, GA*

WP 070 **Compositional Analysis and Investigation of Prebiotic Potential of Oligosaccharides in Plant-Based Dairy Alternatives:Insights from Oat, Soy, Coconut, and Almond Beverages**; Han Peng[1]; Jerina Rugji[2]; Yuchen Gu[1]; Romina Diaz[1]; David Andrew Mills[1]; Gulustan Ozturk[2]; Daniela Barile[1]; *[1]University of California, Davis, Davis, CA; [2]University of Wisconsin-Madison, Madison, WI*

WP 071 **Comparing ionization efficiencies and fragmentation patterns of carbohydrates in various solvent systems using positive- and negative-ion mode mass spectrometry**; Lyssa A Garber[1]; Alexes N Thurman[1]; Elyssia Gallagher[1]; *[1]Baylor University, Waco, TX*

WP 072 **Determination of lactose content using HILIC amide column on a single quad LCMS system**; Aubrey Jean Stout[1]; Md Asaduzzaman[1]; Samantha Olendorff[2]; Prateek Sharma[3]; *[1]Department of Nutrition, Dietetics and Food Science, Utah State University,, Logan, Utah, USA; [2]Shimadzu Scientific Instruments,, Kansas, USA, Kansas; [3]NDFS Department, Utah State University, Logan, UT, United States, Logan, UT*

WP 073 **Novel Approach Combining the Benefits of IM-MS and EED for Separation and Definition of Unique Glycan Structures**; Chaoshuang Xia[1]; Hayley L. Knox[2]; Christine A. Arbour[3]; Cheng Lin[1]; Barbara Imperiali[3]; Karen N. Allen[2]; Catherine E Costello[1]; *[1]Center for Biomedical Mass*

Spectrometry, Boston University Chobanian & Avedisian School of Medicine, Boston, MA; [2]Department of Chemistry, Boston University, Boston, MA; [3]Department of Biology and Department of Chemistry, Massachusetts Institute of Technology, Boston, MA

WP 074 **Exploring the Carbohydrate Composition of Chardonnay Pomace Through Multi-Omics Approaches**; Han Peng[1]; Bruna Paviani[1]; Ece Surek[2]; Elisa García[3]; Daniela Barile[1]; *[1]University of California, Davis, Davis, CA; [2]Istinye University, Istanbul, Turkey; [3]Consejo Superior de Investigaciones Científicas (CSIC), Madrid, Spain*

WP 075 **Structural Identification of Unusual Complex N-Glycans Using Mass Spectrometry**; Chi-Kung Ni[1]; Yen-Ting Lin[2, 3]; *[1]Academia Sinica, Taipei, Taiwan; [2]Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei City, Taiwan; [3]Department of Chemistry, National Tsing Hua University, Hsinchu, Taiwan*

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WP 076 **Automated Soft-Spot Identification in Hydrolyzed Cyclic Peptides Using MASSPEC Structural Elucidation Software with HPLC/ESI Exact-Mass MS and MSMS Data**; Marshall M. Siegel[1]; Gary Walker[2]; Serhiy Hnatyshyn[3]; Rostyslav Hnatyshyn[4]; Joe R. Cannon[3]; Haiying Zhang[3]; *[1]MS Mass Spec Consultants, Fair Lawn, NJ; [2]MS Mass Spec Consultants, Fair Lawn, New Jersey; [3]Bristol-Myers Squibb.Co, Lawrence, NJ; [4]Arizona State University, School of Computing and Augmented Intelligence, Tempe, AZ*

WP 077 **Metabolites Identification of Oligonucleotide Drug Trecovirsen Using a QTOF mass spectrometer**; Pengyi Hou[1]; Dandan Si[1]; Zhimin Long[1]; Bingjie Liu[1]; *[1]SCIEX, Beijing, China*

WP 078 **Structure Analysis of Reactive Metabolites of Hepatotoxic Drugs by Electron Activated Dissociation to Identify the Site of Metabolic Activation**; Kazuko Inoue; *Eisai Co.,Ltd., Tsukuba, Japan*

WP 079 **Identification of AC-262536 human urinary metabolites after single oral administration of the drug by UHPLC-HRMS**; Ekaterina Dmitrieva[1, 2]; Azamat Temerdashev[3]; Elina Gashimova[3]; *[1]Shenzhen MSU-BIT University, Shenzhen, China; [2]Moscow State University, Moscow, Russia; [3]Kuban State University, Krasnodar, Russia*

WP 080 **Exploring the Translation of Organ-on-a-Chip Technology for Human Relevant Diagnostic Biomarkers**; Elizabeth Dhummakupt[1]; Gabrielle Rizzo[1]; Conor Jenkins[1]; Tyler Goralski[1]; Priscilla Lee[1]; Dylan Fudge[1]; Allison Clay[2]; *[1]U.S. Army Combat Capabilities Development Command (DEVCOM) Chemical Biological Center (CBC), Aberdeen Proving Ground, MD; [2]Precise Systems, Lexington Park, MD*

WP 081 **Leveraging feature-based molecular networking for advancing in vitro metabolic profiling of fenbendazole across species**; Young-Heun Jung[1]; Dong-Cheol Lee[1]; Junyoung O. Park[2]; Ju-Hyun Kim[1]; *[1]Yeungnam University, Gyeongsan-si, South Korea; [2]University of California, Los Angeles, Los Angeles, CA*

WP 082 **A Simple Cost-Effective Determination of Histamines in Gentamicin by HPLC/MS**; John Wright[1]; Donna Payne[2]; Sue D'Antonio[1]; *[1]Agilent Technologies, Santa Clara, CA; [2]AnalytEval, Missouri City, TX*

WP 083 **Evaluation of matrix effects in post-ICP chemical ionization MS for standard-free quantitation of halogenated metabolites in biological matrices**; Zahra Afsharsaveh[1]; Samuel White[1]; Grace Hahm[1]; Matthew A. Cerny[2]; Kaveh Jorabchi[1]; *[1]Georgetown Univ., Washington, DC; [2]Pfizer, Groton, CT*

WP 084 **Automation in Metabolite Identification Workflows with Software-Assisted Processing of Mass Spectrometry Data**; Savannah M Mason[1]; Ismael Zamora[1]; Luca Morettoni[1]; Paula Cifuentes[1]; Ramon Adalia[1]; *[1]Mass Analytica, S.L., Sant Cugat del Vallés, Spain*

WP 085 **Profiling and Characterization of ZD10Q and Metabolites in Rat, Dog, Monkey, and Human Hepatocytes**; Alex (Hong) Zhang[1]; Bruce Sachais[2]; Connor McCloskey[2]; Sarah McMahon[2]; Toufiq Ul Amin[1]; Luis Ramos[1]; Xiaokun Cai[1]; Wenbin Liu[1]; Lata Venkatarangan[1]; Ragu Ramanathan[1]; *[1]QPS, LLC, Newark, DE; [2]New York Blood Center, New Tork, NY*

WP 086 **Empowering peptide catabolite discovery: software-aided electron activated dissociation (EAD) based orthogonal fragmentation analysis**; Robert Clapper[1]; Rahul Baghla[2]; Eshani Galermo[2]; Zoe Zhang[2]; *[1]Sciex, Framingham, MA; [2]Sciex, Redwood City, CA*

WP 087 **Implementation of 18O-labelled water to aid identifying degradation products of pharmaceutical and agricultural molecules by high-resolution mass spectrometry**; Rong Chen[1]; Chengli Zu[1]; *[1]Corteva Agriscience, Indianapolis, IN*

WP 088 **The micro-QuEChERS meets LC-MS/MS for the first time in antifungal drugs monitoring in capillary blood microsamples: ANTISEPSIS study**; Arkadiusz Kocur[1, 2]; Mateusz Moczulski[1, 2]; Agnieszka Czajkowska[1]; Anna Częczek[1]; Małgorzata Mikaszewska-Sokolewicz[3]; *[1]Therapeutic Drug Monitoring, Clinical Pharmacokinetics and Toxicology Unit, Department of Clinical Biochemistry, The Children's Memorial Health Institute in Warsaw, Warsaw, Poland; [2]Department of Drug Chemistry, Pharmaceutical and Biomedical Analysis, Faculty of Pharmacy, Medical University of Warsaw, Warsaw, Poland; [3]Anesthesiology and Intensive Care Clinical Department, The Children's Memorial Health Institute in Warsaw, Warsaw, Poland*

WP 089 **Development and clinical application of HILIC-LC-MS/MS method for simultaneous determination of ganciclovir and creatinine in capillary blood microsamples: NEOGANC study**; Arkadiusz Kocur[1, 2]; Mateusz Moczulski[1, 2]; Justyna Czech-Kowalska[3]; *[1]Therapeutic Drug Monitoring, Clinical Pharmacokinetics and Toxicology Unit, Department of Clinical Biochemistry, The Children's Memorial Health Institute in Warsaw, Warsaw, Poland; [2]Department of Drug Chemistry, Pharmaceutical and Biomedical Analysis, Faculty of Pharmacy, Medical University of Warsaw, Warsaw, Poland; [3]Department of Neonatology and Neonatal Intensive Care, The Children's Memorial Health Institute in Warsaw, Warsaw, Poland*

WP 090 **Using mass spectrometry-based approaches to interrogate complex metallodrug components**; Ludovic Muller[1]; James Polli[2]; Bruce Yu[2]; Sarah Michel[2]; Maureen Kane[3]; *[1]University of Maryland Baltimore, Baltimore, MD; [2]University of Maryland, Baltimore, Baltimore, MD; [3]Universityof Maryland Baltimore, Baltimore, MD*

WP 091 **New Method Analysis of Illicit, Prescription, Over the Counter, and Addiction Treatment Drugs in Wastewater to Support Public Health Surveillance**; Thomas D Sinkway[1]; Sarah Robinson[1]; Francisco Paneque[1]; Camden Camacho[1]; Nicole Winn[1]; Tara Sabo-Attwood[1]; John Bowden[1]; Joseph H Bisesi[1]; *[1]University of Florida, Gainesville, Florida*

WP 092 **High Resolution MS Metabolic Profiling of Astragali Radix in rats based on Multi Reflecting Time-of-Flight MS combined with Mass-Metasite software**; Sijian Chen[1]; Yisheng Xu[2]; Yingyuan Lu[1]; Pengfei Tu[1]; *[1]Peking University, beijing, China; [2]Waters Technology (Beijing) Co., Ltd., Beijing, China*

WP 093 **Fast and Sensitive Metabolite Profiling of the Antisense Oligonucleotide Tofersen in liver homogenates Using UHPLC-HRAM mass spectrometry**; Robert L Ross[1]; Min Du[1]; Hao Yang[1]; Roberto Gamez[2]; *[1]Thermo Fisher Scientific, Lexington, MA; [2]Thermo Fisher Scientific, Austin, TX*

WP 094 **Innovative drug metabolite identification and characterization using electron activated dissociation**; Rahul Baghla[1]; Ben Jiang[2]; Min Wang[2]; Eshani Galermo[1]; *[1]Sciex, Redwood City, CA; [2]Amgen, South San Francisco, CA*

WP 095 **Rapid UHPLC Energy-Resolved Mass Spectrometry Technique to Identify Co-eluting Isobaric Products**; Kevin Colizza[1]; Timothy A Brown[1]; *[1]GSK, Collegeville, PA*

WP 096 **An Analysis of the Effects of Variable Concentration Salt on Faradaic Ion Concentration Polarization Coupled to a Mass Spectrometric Device**; Jamison R Polley[1]; Varadaraju Vadakekatte Dyavegowda[1]; Lahiru Wedasingha[1]; Magnus P Rydberg[1]; Nicholas E Manicke[1]; [1]*Indiana University Indianapolis, Indianapolis, IN*

WP 097 **prio-PASEF: Precision and Discovery in MetID Workflows**; Beixi Wang[1]; Xuejun Peng[1]; Jonathan R. Plante[2]; Reena G. Patel[2]; Kyle P. Mummau[2]; Elke S. Perloff[2]; Melvin Blaze[2]; Heiko Neuweger[3]; Erica Marie Forsberg[4]; [1]*Bruker Scientific LLC, San Jose, California;* [2]*Discovery Life Sciences, Woburn, MA;* [3]*Bruker Daltonics GmbH & Co.KG, Bremen, Germany;* [4]*Bruker Daltonics, San Jose, CA*

WP 098 **Simulation of Sildenafil Metabolism using an Electrochemical Oxidation System**; Unyong Kim[1]; Sumin Seo[1]; Jiyu Kim[1]; Chohee Jeong[1]; Woojin Jeong[1]; Sang Beom Han[1]; [1]*College of Pharmacy, Chung-Ang University, Seoul, South Korea*

WP 099 **A universal LC-HRMS method for rapid and comprehensive metabolite profiling and identification of oligonucleotide therapeutics**; Yuqing Zhao[1]; Chongzhuang Tang[1]; Yue Yang[1]; Allan Xu[2]; Mingshe Zhu[3]; [1]*XenoFinder, Suzhou, China;* [2]*Keystone Bioanalytical, North Wales, PA;* [3]*MassDefect Technologies, Princeton, NJ*

WP 100 **Identification of Montelukast Metabolites in Rat Plasma Using LC/MS-Based Metabolomics Analysis**; Jinchun Sun[1]; Ashley Kaswer[1]; Richard Beger[1]; Jessica Oliphant[1]; [1]*NCTR / USFDA, Jefferson, AR*

WP 101 **LC-QTOF- and LC-TIMS-qQTOF-MS Analysis of Fecal Inoculum Biotransformation Products and LC-MRM-MS Analysis of Human Withanolide Pharmacokinetics of an Ashwagandha Supplement**; Jessica L Etter[1, 2]; Luke Marney[1, 2]; Jaewoo Choi[1, 2]; Liping Yang[1, 2]; Eli Smart[3]; Alex Speers[4]; Axel Lozano-Ortiz[2, 4, 5]; Ella Limoico[2, 4, 6]; Amala Soumyanath[2, 4]; Jan F. Stevens[2, 7, 8]; Claudia S. Maier[1, 2, 8]; [1]*Department of Chemistry, Oregon State University, Corvallis, OR;* [2]*BENFRA Botanical Dietary Supplements Research Center, Oregon Health and Science University, Portland, OR;* [3]*Department of Biochemistry and Biophysics, Oregon State University, Corvallis, OR;* [4]*Department of Neurology, Oregon Health and Science University, Portland, OR;* [5]*Department of Biology, Portland State University, Portland, OR;* [6]*Department of Chemistry, Portland State University, Portland, OR;* [7]*Department of Pharmaceutical Sciences, Oregon State University, Corvallis, OR;* [8]*Linus Pauling Institute, Oregon State University, Corvallis, OR*

WP 102 **Stability of N- and O-glucuronides in aqueous solutions at various pH and in human feces**; Zhoupeng Zhang[1]; April Chen[1]; Niresh Hariparsad[1]; [1]*AstraZeneca, Waltham, MA*

WP 103 **Minimizing in source fragmentation without compromising sensitivity: A nitrosamine drug substance-related impurity (NDSRI) method supporting regulatory research at the FDA**; Jinhui Zhang[1]; Jingyue Yang[2]; Xiaoming Xu[3]; Patrick J. Faustino[3]; [1]*FDA, Silver Spring, MD;* [2]*Food and Drug Administration, St. Louis, MO;* [3]*Food and Drug Administration, Silver Spring, MD*

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WP 104 **Detection of Microcystin-RR and Microguanidine Complex During UHPLC-ESI-MS**; Sanduni H Premathilaka[1]; Dragan Isailovic[1]; [1]*University of Toledo, Toledo, OH*

WP 105 **Analysis of Per- and Polyfluoroalkyl Substances (PFAS) in Leachate by EPA Method 1633A Using LC-MS/MS**; Tiffany Liden[1]; Ruth Marfil-Vega[1]; Om Shrestha[1]; Robert English[1]; Toshiya Matsubara[1]; Kevin A Schug[2]; Evelyn Wang[1]; [1]*Shimadzu Scientific Instruments, Columbia, Maryland;* [2]*University of Texas at Arlington, Arlington*

WP 106 **Comprehensive Non-Targeted PFAS Analysis Using Quadrupole Time-of-Flight (QToF) Mass Spectrometry with a Multi-Approach Data Processing Workflow**; Om Shrestha[1]; Toshiya Matsubara[1]; Ruth Marfi-Vega[1]; Jeff Dahl[1]; [1]*Shimadzu Scientific Instruments, Columbia, Maryland*

WP 107 **Simplifying EPA 1633 analyses with an improved dual bed solid-phase extraction method**; Jason Hoisington[1]; Alexis Shelow[1]; Jason Thomas[1]; Colton Myers[1]; Diego A. Lopez[1]; [1]*Restek Corporation, Bellefonte, PA*

WP 108 **A study of bioaccumulation of drugs of abuse in darters (Etheostomaspp.) in southern Ontario, Canada**; Diana M Cardenas-Soraca[1]; Milica Kecman[1]; Sandra Salic[1]; Rashne Vakharia[1]; Paola A. Ortiz-Suarez[1]; Leslie M. Bragg[1]; Mark R. Servos[1]; [1]*Deparment of Biology, University of Waterloo, Waterloo, ON*

WP 109 **Dioxins analysis by GC-HRTOFMS and GC-MS/MS as alternative to GC-SectorMS**; Masahiro Hashimoto[1]; Jun Onodera[1]; Masaaki Ubukata[1]; Norihisa Hatakeyama[1]; [1]*JEOL Ltd., Akishima, Japan*

WP 110 **Analysis of Per-and-polyfluoroalkyl substances in soil and wastewater/groundwater using a benchtop multi-reflecting Time-of-flight XevoTM MRT mass spectrometer**; Hania Khoury-Hollins[1]; Henry Foddy[1]; Sara Stead[1]; Stuart J Adams[1]; Jayne Kirk[1]; Richard Lock[1]; [1]*Waters Corporation, Wilmslow, United Kingdom*

WP 111 **Interrogation of a fluoropolymer dispersion prepared with a non-fluorinated polymerization aid by liquid chromatography high resolution mass spectrometry**; Jill Boyle[1]; John C. Sworen[1]; Peter A. Morken[1]; Adam P. Smith[2]; Maria D. Cervantes Garcia[1]; Jordyn Kramer[1]; Michael P. Wadsley[1]; Michael C. Davis[1]; [1]*Chemours Company, Newark, DE;* [2]*Chemours Company, Washington, WV*

WP 112 **Ultra-sensitive PFAS analysis according to EU and EPA regulations in drinking water**; Arnd Ingendoh[1]; Miguel Angel Perez[2]; Zahuindanda Aventura[3]; Carsten Baessmann[4]; Radhika Madana Mohan[5]; [1]*Bruker Daltonics, Bremen, Germany;* [2]*Bruker Espanola, Madrid, Spain;* [3]*Bruker Inc, Billerica, MA;* [4]*Bruker Daltonics GmbH & Co. KG, Bremen, Germany;* [5]*Bruker Scientific, Billerica, MA*

WP 113 **De Novo PFAS Annotation and Classification Using Highly Accurate Formula Prediction and Kaufmann Algorithms Embedded in FluoroMatch Suite**; Jeremy Koelmel[1]; Michael Kummer[2]; David Schiessel[2]; Olivier Chevallier[3]; David Godri[4]; Christian Klein[3]; Emma E Rennie[3]; Krystal J Godri Pollitt[1]; [1]*Yale University, New Haven, CT;* [2]*Innovative Omics, Sarasota, FL;* [3]*Agilent Technologies, Santa Clara, CA;* [4]*3rd Floor Solutions, Caledon, ON*

WP 114 **Rapid screening of environmental PAFS contaminated samples by targeted DESI MRM triple quadrupole system**; Emmanuelle Claude[1]; Alex Birsan[2]; Emrys Jones[1]; Joanne Ballantyne[1]; [1]*Waters Corporation, Wilmslow, United Kingdom;* [2]*Waters Limited, Quebec, Quebec*

WP 115 **Routine EPA 1633 PFAS analysis with a novel slotted bandpass ion guide to improve signal response robustness**; Stuart J Adams[1]; Kari Organtini[2]; David Gould[1]; Peter Hancock[1]; Narendra Meruva[2]; [1]*Waters Corporation, Wilmslow, United Kingdom;* [2]*Waters Corporation, Milford, MA*

WP 116 **Improvements in Detection and Characterization of PFAS Molecules Using Enhanced Inclusion and Exclusion Features in Data Dependent Acquisition (DDA)**; Chris Hughes[1]; Stephen Griffin[2]; Michael McCullagh[1]; Stuart J Adams[1]; [1]*Waters, Wilmslow, United Kingdom;* [2]*Waters Corporation, Milford, MA*

WP 117 **Investigating Fire Fighter and E-waste Handlers Exposure to PFAS Using Liquid Chromatography and Cyclic Ion Mobility Mass Spectrometry**; Michael McCullagh[1]; Iggy Kass[2]; Stuart Adams[1]; Sarah Dowd[2]; David Megson[3]; Pennante Bruce-Vanderpuije[4]; [1]*Waters Corporation, Wilmslow, United Kingdom;* [2]*Waters Corp., Milford, MA;* [3]*Manchester Metropolitan University, Manchester, United Kingdom;* [4]*CSIR-Water Research Institute, Accra, Ghana*

WP 118 **Simultaneous quantitation of ultrashort-, short- and long-chain PFAS in different water matrices**; Holly Lee[1]; Simon Roberts[2]; Craig Butt[3]; Robert Di Lorenzo[1]; Sam

Lodge[4]; Cora Young[5]; Trevor VandenBoer[5]; RenXi Ye[5]; *[1]SCIEX, Concord, ON; [2]SCIEX, Golden, CO; [3]SCIEX, Framingham, MA; [4]Phenomenex, Torrance, California; [5]Department of Chemistry, York University, Toronto, ON*

WP 119 **First correlation of EOF vs. NTS for PFAS analysis. Can qualitative non-target data be indicative of PFAS contamination?**; Fabian Simon[1]; Jonathan Zweigle[2]; Christian Zwiener[3]; *[1]Georgetown University, Washington, DC; [2]University of Copenhagen, Copenhagen, Denmark; [3]University of Tübingen, Tübingen, Germany*

WP 120 **Detection and Characterization of Semi-volatile Disinfection Byproducts using Dielectric Barrier Discharge Ionization Mass Spectrometry**; Olivia A Jaye[1]; Douglas B. Collins[1]; *[1]Bucknell University, Lewisburg, PA*

WP 121 **Assessment of Adsorption of Microcystins onto Modified Corncob-based Activated Carbons using UHPLC-MS**; Yohan Chandika Yasanga Sudusingha[1]; Dragan Isailovic[1]; *[1]University of Toledo, Toledo, OH*

WP 122 **Incorporating Ultrashort-Chain Compounds into the Comprehensive Analysis of PFAS in Potable and Non-Potable Waters**; Shun-Hsin LIANG[1]; Derick Lucas[1]; *[1]Restek Corporation, BELLEFONTE, PA*

WP 123 **Physicochemical Profiling and Thermal Degradation of PFAS-Containing Aqueous Film-Forming Foams: Environmental Considerations**; Dhimiter Bello[1]; Kushal Biswas[1]; Suresh Bhandari[1]; Anila Bello[1]; Michael Ross[1]; Chuntao Wang[1]; Chani Sahabandu Hewa Sahabanduge[1]; Pengyuan Liu[1]; *[1]University of Massachusetts Lowell, Lowell, MA*

WP 124 **Characterizing the emissions of nitrogen containing gas-phase species associated with automotive brake wear using high resolution chemical ionization mass spectrometry**; Madeline Cooke[1]; Michelia Dam[1]; Lisa Wingen[1]; Véronique Perraud[1]; Adam Thomas[1]; Berenice Rojas[1]; Sanjeevi Nagalingam[1]; Michael Ezell[1]; Samuel La Salle[1]; Paulus Bauer[1]; Barbara Finlayson-Pitts[1]; James Smith[1]; *[1]University of California, Irvine, Irvine*

WP 125 **Proteomic analysis of Macrophages and Neuroblastoma cells exposed to polyfluoroalkyl substances (PFAS)**; Jocelyn Vincent[1]; Shawn King[1]; Sahar Chowdhury[2]; Saiful M Chowdhury[3]; *[1]University of Texas at Arlington, Arlington, TX; [2]Harmony Science Academy, Euless, Texas; [3]Univerisity of Texas at Arlington, Arlington, TX*

WP 126 **Novel techniques for ultra-sensitive detection of PFAS in LC-MS/MS**; Kazuhiro Kawakami[1]; Nami Iwasa[1]; Yui Higashi[1]; Riki Kitano[1]; Yuka Fujito[1]; *[1]Shimadzu Corporation, Kyoto, Japan*

WP 127 **From Industry to Tap: Quantifying PFAS in drinking water**; Serge Auger[1]; Mégane Moreau[1]; Sarah Demers[1]; Jonathan Rochon[1]; Pierre Picard[1]; Jean Lacoursière[1]; *[1]Phytronix Technologies, Quebec, QC*

WP 128 **Are Koreans Overexposed to Perfluoroalkyl Substances? Results from a Single Referral Laboratory**; JunHyung Lee[1]; Sung-Eun Cho[1]; Ahram Yi[1]; Sang Gon Lee[1]; Eun Hee Lee[1]; *[1]GC Labs, Yongin, South Korea*

WP 129 **Characterization of Biodegradable Plastic Bags Using Pyrolysis-Two-Dimensional Gas Chromatography-High-Resolution Time-of-Flight Mass Spectrometry and AI-Assisted Qualitative Analysis**; Kirk R Jensen[1]; Robert B Cody[1]; *[1]JEOL USA, Inc., Peabody, MA*

WP 130 **Untargeted Screening for Per/Poly-fluoroalkyl Substances in Ghanaian Firefighter Serum Using LC/Ion Mobility/Mass Spectrometry and Pattern Analysis**; Jeff Goshawk[1]; Russell Mortishire-Smith[1]; Andrew Tudor[1]; David Eatough[1]; Sarah Dowd[2]; Michael McCullagh[1]; Emma Marsden-Edwards[1]; David Megson[3]; Pennante Bruce-Vanderpuije[4]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Waters Corp., Milford, MA; [3]Manchester Metropolitan University, Manchester, United Kingdom; [4]Council for Scientific and Industrial Research, Accra, Ghana*

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WP 156 **Identification and characterization of dietary fiber polysaccharides in food by quantitative LC-MS/MS approach**; Nebiyu Abshiru[1]; Boris Nemzer[1, 2]; *[1]VDF FutureCeuticals Inc, Momence, Illinois; [2]University of Illinois at Urbana-Champaign, Urbana, Illinois*

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WP 165 **Rapid Analysis of Water-Soluble Vitamins in Peanut Butter Using LCMS-2050**; Jenishia Menezes[1]; Anant Lohar[1]; Shailesh Sadashiv Damale[1]; Jessin Mathai[1]; *[1]Shimadzu Middle East & Africa FZE, Dubai, United Arab Emirates*

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Technologies, Mumbai, India; [3]Agilent Technologies, Hyderabad, India; [4]Agilent Technologies, Delhi, India

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WP 169 **Visualization of Spatially Resolved Polyamine Metabolism in the Gastrointestinal Tract with Nanofiber Ingestion by MALDI-Mass Spectrometry Imaging**; Fumito TANI[1]; Mahiro OKAMOTO[1]; Maiko OKAMURA[2]; Nanata HORI[1]; Masaki HONEN[1]; Shohei OOI[1]; Takahiro KAWASE[3]; Takamitsu TSUKAHARA[3]; Kentaro MATSUMIYA[1]; Shuji YAMASHITA[2]; Masaya IKEGAWA[2]; *[1]Kyoto University, Kyoto, Japan; [2]Doshisha university, Kyotanabe City, Japan; [3]Kyoto Institute of Nutrition and Pathology, Uji-Tawara City, Japan*

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WP 175 **Peptide target selection in roasted tree nuts for a multi-allergen mass spectrometry quantification method in incurred food matrices**; Jerry C. Kahu[1]; Philip Johnson[1]; Melanie L. Downs[1]; *[1]Food Allergy Research and Resource Program, Department of Food Science and Technology, University of Nebraska-Lincoln, Lincoln, NE*

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WP 191 **Intrinsic chemistry of UIII and UIV species: gas-phase reactions of [UF2(C2H)]+ and [UF2]+ with carboxylic acids**; Samuel Lenze[1]; Michael J Van Stipdonk[1]; Theodore A Corcovilos[1]; Justin G Terhorst[1]; *[1]Duquesne University, Pittsburgh, PA*

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WP 205 **The Influence of Monovalent and Divalent Metal Ions on the Cross-Ring Fragmentation ofN-Linked Glycans by IR-MALDESI**; Makenna L. Schroder[1, 2]; Mahtab Heyrani[1, 2]; Tana V. Palomino[1, 2]; David C. Muddiman[1, 2]; *[1]Biological Imaging Laboratory for Disease and Exposure Research, Raleigh, NC; [2]North Carolina State University, Raleigh, NC*

WP 206 **Revisiting the C. elegans N-Glycome for Aging-Associated Glycosylation and Biosynthetic Pathway Reconstruction**; Myung Jin Oh[1, 2]; Yong Heum Na[1, 2]; Sungjin Kim[3]; Hyun Joo An[1, 2]; *[1]Graduate School of Analytical Science and Technology, Chungnam National University, South Korea; [2]Asia-Pacific Glycomics Reference Site, Chungnam National University, South Korea; [3]Department of Microbiology and Molecular Biology, Chungnam National University, South Korea*

WP 207 **Investigation of the correlation between glycosaminoglycans and lung cancer**; Domonkos Pál[1, 2]; Gábor Tóth[3]; Simon Sugár[3]; Kata Fügedi[3]; Dániel Szabó[3, 4]; Ilona Kovalszky[5]; Dávid Papp[4, 6]; Gitta Schlosser[6]; Tamás Tornóczky[7]; Tünde Harkó[8]; Judit Moldvay[8, 9]; László Drahos[3]; Lilla Turiák[1]; *[1]MTA-TTK Lendület (Momentum) Glycan Biomarker Research Group, HUN-REN Reasearch Centre for Natural Sciences, Budapest, Hungary; [2]Semmelweis University Doctoral School, Budapest, Hungary; [3]MS Proteomics Research Group, HUN-REN Research Centre for Natural Sciences, Budapest, Hungary; [4]Hevesy György PhD School of Chemistry, ELTE Eötvös Loránd University, Budapest, Hungary; [5]1st Department of Pathology and Experimental Cancer Research, Semmelweis University, Budapest, Hungary; [6]MTA-ELTE Lendület Ion Mobility Mass Spectrometry Research Group, ELTE Eötvös Loránd University, Budapest, Hungary; [7]Department of Pathology, Faculty of Medicine and Clinical Center, University of Pécs, Pécs, Hungary; [8]National Korányi Institute of Pulmonology, Budapest, Hungary; [9]Pulmonology Clinic, Albert Szent-Györgyi Medical School, University of Szeged, Szeged, Hungary*

WP 208 **TLR2D deficiency is associated with sex-linked compositional and structural rearrangements of membrane lipids**; Raluca Ica[1]; Mirela Sarbu[2]; Roxana Biricioiu[2, 3]; Kristina Mlinac-Jerković[4]; Svjetlana Kalanj-Bognar[4]; David E. Clemmer[5]; Alina D. Zamfir[2, 6]; *[1]National Inst for R&D in Electrochemistry and Condensed Matter, Timisoara, Romania; [2]National Institute for Research and Development in Electrochemistry and Condensed Matter, Timisoara, Romania; [3]West University of Timisoara, Timisoara, Romania; [4]Department for Chemistry and Biochemistry & Croatian Institute for Brain Research, School of Medicine, Zagreb University,, Zagreb, Croatia; [5]Indiana University, Bloomington, IN; [6]Department of Technical and Natural Sciences, "Aurel Vlaicu" University of Arad, Arad, Romania;, Arad, Romania*

WP 209 **Defining Glucose Unit Index for Isomeric Permethylated Glycans Using LC-MS on Mesoporous Graphitized Carbon Columns**; Odunayo O. Oluokun[1]; Oluwatosin Daramola[1]; Ayobami Oluokun[1]; Favour M Chukwubueze[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX*

WP 210 **Alterations in the Bisecting and Fucosylated N-Glycans in the Frontal Lobes of Parkinson's Disease Brains Determined by LC-MS/MS**; Oluwatosin E Daramola[1]; Andrew I. Bennett[1]; Judith Nwaiwu[1]; Mojibola Fowowe[1]; Sherifdeen Onigbinde[1]; Joy Solomon[1]; Isaac Lopez[1]; Hanh Minh Thu Nguyen[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX*

WP 211 **LC-MS/MS N-Glycome and Proteome Alterations in Rat Kidneys Following Chronic Glyphosate-Based Herbicide Exposure**; Favour M. Chukwubueze[1]; Cristian D. Gutierrez Reyes[1]; Jesús Chávez-Reyes[2]; Joy Solomon[1]; Vishal Sandilya[1]; Sarah Sahioun[1]; Bruno A. Marichal-Cancino[2]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX; [2]Universidad Autonoma de Aguascalientes, Aguascalientes, Mexico*

WP 212 **SerumN-glycan Profiling Identifies Candidate Glycan Biomarkers for Early Detection and Prediction of Alzheimer's Disease**; Sherifdeen B Onigbinde[1]; Joy Solomon[1]; Cristian D. Gutierrez-Reyes[1]; Oluwatosin Daramola[1]; Mojibola Fowowe[1]; Moyinoluwa Adeniyi[1]; Kelly N. DuBois[2, 3]; Kelly M. Bakulski[3]; Nicholas M. Kanaan[2, 3]; David M. Lubman[3]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX; [2]Michigan State University, College of Human Medicine, Grand Rapids, MI; [3]University of Michigan, Ann Arbor, MI*

WP 213 **Modulation of ProteinN-Glycosylation by Blue Agave Fructans in Atopic Dermatitis Using LC-MS/MS for Therapeutic Insights**; Esther O. Oji[1]; Sherifdeen B Onigbinde[1]; Cristian D. Gutierrez-Reyes[1]; Eva Salinas[2]; Marcela Rois-Carlos[2]; Daniel Cervantes-Garcia[2]; Odunayo O. Oluokun[1]; Judith Nwaiwu[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX; [2]Universidad Autonoma de Aguascalientes, Aguascalientes, Mexico*

WP 214 **Optimized LC-MS/MS Profiling of O-Glycans for Severity Assessment in Traumatic Brain Injury**; Joy O Solomon[1]; Sherifdeen B Onigbinde[1]; Odunayo O. Oluokun[1]; Oluwatosin Daramola[1]; Favour M Chukwubueze[1]; Firas Kobeissy[2]; Stefania Mondello[3]; Ava M Puccio[4]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX; [2]Center for Neurotrauma, Multiomics & Biomarkers (CNMB) Morehouse School of Medicine, Atlanta, GA; [3]Department of Biomedical and Dental Sciences and Morphofunctional Imaging, University of Messina, Messina, Italy; [4]Department of Neurological Surgery, University of Pittsburgh, Pittsburgh, PA*

WP 215 **Evaluation of the Bare Glass CE-MS ZipChip Interface for Characterizing Glycosaminoglycans**; Adam Hawkridge[1]; Nidhi Naik[1]; Morgan Cooper[1]; *[1]Virginia Commonwealth University, Richmond, VA*

WP 216 **Glycan Sequencing with Ion Mobility Mass Spectrometry**; Kevin C Hooijschuur[1]; Julia C.C. Vreugdenhil[1]; Igor R. Sweet[1]; Bernd Stahl[1, 2]; Javier Sastre Toraño[1]; Geert-Jan P.H. Boons[1, 3]; *[1]Utrecht University, Utrecht, Netherlands; [2]Danone Research & Innovation, Utrecht, Netherlands; [3]Complex Carbohydrate Research Center, University of Georgia, Athens, GA*

WP 217 **Profiling of O-glycan isomers in bovine saliva mucin (BSM) on porous carbon HPLC column**; Michael Ye[1]; Andras Z Komaromy[2]; Morten Thaysen-Andersen[2]; William Maule[1]; Egidijus Machtejevas[3]; *[1]MilliporeSigma, Bellefonte, PA; [2]School of natural science, Macquarie University, Sydney, Australia; [3]The life science business of Merck KGaA, Darmstadt, Germany*

WP 218 **Sensitive Glycosaminoglycan Disaccharide and Feature Analysis with Isotopic Labeling and HILIC-MS**; Stephanie A Archer-Hartmann[1]; Amrita Basu[1]; Mehrnoush Taherzadeh Ghahfarrokhi[1]; Ryan Joseph Weiss[1]; Parastoo Azadi[1]; *[1]Complex Carbohydrate Research Center, University of Georgia, Athens, GA*

WP 219 **Glycosaminoglycan reducing end derivatization efficiency analysis by LC-UV-vis-MS**; Morgan E Cooper[1]; Nidhi Naik[1]; Adam Hawkridge[1]; *[1]Virginia Commonwealth University, Richmond, VA*

WP 220 **Structural glycomics powered by glyPAQ reveals N-glycan alterations in COVID-19 hearts**; Melinda Wojtkiewicz[1]; Sabarinath Subramanian[1]; John Wilson[2]; Rebekah Gundry[1]; *[1]University of Nebraska Medical Center, Omaha, NE; [2]ProtiFi, LLC, Farmingdale, NY*

WP 221 **TheSynergy between DeepGlyco and GlycanFinderfor Deep CharacterizationofProteinN/O-Glycosy**; Chao Peng[1]; Ping Wu[1]; Wenting Li[1]; Lei Xin[1]; Baozhen Shan[1]; *[1]BaizhenBio Inc., Wuhan, China*

WP 222 **A complete workflow for analysis of challenging metal-sensitive released N-glycans by LC/MS**; Randall Robinson[1]; Jordy J. Hsiao[2]; Connor Flannery[2]; Tom Rice[1]; Aled Jones[1]; Oscar Potter[2]; Anne Blackwell[2]; Wendi A Hale[3]; *[1]Agilent Technologies, Folsom, CA; [2]Agilent Technologies, Santa Clara, CA; [3]Agilent Technologies, Lexington, MA*

WP 223 **Characterization and quantification of Xylooligosaccharides extracted from almond shells**; Shirin K. Pournaki[1]; Sumit Sharma[1]; Han Peng[2]; Zhiliang Fan[2]; Daniela Barile[2]; *[1]University of California, Davis, Davis, CA; [2]University of California Davis, Davis, CA*

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WP 224 **Low Detection Limit High-Throughput Surface Analysis with nAPCI-MS**; Nicole C Auvil[1]; Mark E Bier[1]; *[1]Carnegie Mellon University, Pittsburgh, PA*

WP 225 **High-throughput metabolomics of pathogens for medical countermeasure discovery using nano-DESI and 2D MS/MS on a miniature mass spectrometer**; Dalton Snyder[1]; Andrew Eller[1]; Edwin Gonzalez[1]; Scott Griffin[1]; Ann Donnelly[1]; Miranda Jacobs[1]; Andrew Houvenagle[1]; Kevin Rosenbaum[1]; Ilya Shinkeyev[1]; Kerry O'Donnell[1]; Brandon Reese[1]; Anna Leech[1]; Mitch Wells[1]; *[1]Teledyne FLIR, West Lafayette, IN*

WP 226 **Analytical considerations for developing and optimizing high throughput 96 well plate-based proteomics platforms**; Jose Navarrete-Perea[1]; Shideh Mirhadi[1]; Jiaming Li[1]; Ryan Hastings Gerkman[1]; Smaranda Bodea[1]; An Chi[1]; *[1]Merck & Co., Inc., Cambridge, MA 02115, USA, Cambridge, MA*

WP 227 **Acoustic Ejection Mass Spectrometry (AE-MS) for High-Throughput In Vitro Microsomal Stability Assays**; Ronghai Cheng; *Biogen -, Cambridge, MA*

WP 228 **Fragmentation First Experimentation**; Daniel Blair; *St Jude Children's Research Hospital, Memphis, TN*

WP 229 **Creating a Compound Library for Optimized ADE-OPI-MS Analysis of Pharmaceutical Drug Modalities**; Michael Recchia[1]; Michelle R Robinson[1]; Conor Leahy[1]; Paul Harradine[1]; *[1]Merck Research Laboratories, West Point, PA*

WP 230 **High-Throughput Chiral Analysis using DESI-MS**; Jie Li[1, 2]; Nicolás M. Morato[2, 3]; Mahdiyeh Shahi[2]; Bo Hao[1]; Zhicai Shi[1]; Karel Goossens[4]; Iulia Strambeanu[1]; R. Graham Cooks[2, 3]; *[1]Chemical Capabilities, Analytical and Purification, Global Discovery Chemistry, Johnson & Johnson, Spring House, PA; [2]Department of Chemistry, Purdue University, West Lafayette, IN; [3]Purdue Institute for Cancer Research, Purdue University, West Lafayette, IN; [4]Chemical Process Research and Development, Johnson & Johnson, Beerse, Belgium*

WP 231 **Application of magnetic nanobead affinity selection-mass spectrometry to the discovery of natural antimicrobial agents against Neisseria gonorrhoeae**; Daniel Simchuk[1]; Abhishek Chanda[1]; Aleksandra E. Sikora[1]; Tom Covey[2]; Chang Liu[2]; Richard B. Van Breemen[1]; *[1]Oregon State University, Corvallis, OR; [2]SCIEX, Concord, ON*

WP 232 **High-throughput identification and quantitation of metal contamination for high-throughput screening samples with Acoustic Ejection Mass Spectrometry**; Alandra Quinn[1]; Kenneth DiRico[1]; Simon Berritt[1]; Thomas R. Covery[2]; Jamie Tourville[1]; Brendon Kapinos[1]; Bhagyashree Khunte[1]; Pablo Trigo-Mourino[1]; Hui Zhang[1]; Matthew Troutman[1]; Chang Liu[3]; *[1]Pfizer, Groton, CT; [2]SCIEX, Concord, ON; [3]SCIEX, Concord, ontario*

WP 233 **Open Port Sampling Interface (OPSI) System for High Throughput Flow Injection Mass Spectral Analysis**; Gary J. Van Berkel[1]; Thomas R. Covey[2]; Peter Kovarik[2]; Chang Liu[2]; Scott Frederick[3]; Erik Miller[3]; *[1]Van Berkel Ventures, LLC, Oak Ridge, TN; [2]SCIEX, Concord, ON; [3]IMI Life Sciences, Palmer, Massachusetts*

WP 234 **An Ultra-High Throughput Method for 13C6-Fructose-6-Phosphate in Cells Using Acoustic Ejection Mass Spectrometry (AEMS)**; Yuanqiang Su[1]; Xinxin Wen[1]; Xiaotong Li[1]; Chunli Zhu[1]; Zhiyu Li[1]; Lili Xing[1]; Yi Tao[1]; Liang Shen[1]; *[1]WuXi AppTec, Shanghai, China*

WP 235 **Enhancing analysis efficiency in high-throughput semi-targeted intact mass spectrometry**; Juan Florez[1]; Stephen Kok[2]; Matthew Green[3]; Stephan Steigele[1]; *[1]Genedata, Basel, Switzerland; [2]Genedata, San Francisco, CA; [3]Genedata, Cambridge, United Kingdom*

WP 236 **Strategies for rapid intact mass screening analysis: Achieving one-second per well**; Matthew Green[1]; Jacob W. McCabe[2]; Juergen Kastler[3]; Alasdair Jack[1]; *[1]Genedata, Cambridge, United Kingdom; [2]Sciex, Framingham, MA; [3]Genedata, Basel, Switzerland*

WP 237 **AP-SMALDI high-throughput screening at an Exploris MX mass detector**; Julian Roth[1]; Kerstin Strupat[2]; Bernhard Spengler[1, 3]; Sabine Schulz[1, 4]; *[1]Institute of Inorganic and Analytical Chemistry, Justus Liebig University Giessen, Giessen, Germany; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [3]TransMIT GmbH, Giessen, Germany; [4]Department of Chemistry and Biology, Universität Siegen, Siegen, Germany*

WP 238 **High-Throughput Plasma Proteomics Pipeline Enhanced Biomarker Discovery in Early Detection of Non-smoking Lung Cancer**; Sung-Liang Yu[1]; Yi-Ju Chen[2]; Kun-Hao Chang[2, 3]; Jared Deyarmin[4]; Yi-Shuang Chuang[2]; Yi-Jing Hsiao[2]; Chong-Jen Yu[5]; Tabiwang Arrey[6]; Jana Richter[6]; Stephanie Samra[4]; Daniel Hermanson[7]; Gee-Chen Chang[8]; Jin-Shing Chen[9]; Pan-Chyr Yang[10]; Yu-Ju Chen[2]; *[1]Department of Clinical Laboratory Sciences and Medical Biotechnology, College of Medicine, National Taiwan University, Taipei, Taiwan; [2]Institute of Chemistry, Academia Sinica, Taipei, Taiwan; [3]Molecular Science and Technology Program, Taiwan International Graduate Program, Academia Sinica, Taipei, Taiwan; [4]Thermo Fisher Scientfic, San Jose, CA; [5]Department of Surgery, National Taiwan University Hospital, Taipei, Taiwan; [6]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [7]Thermo Fisher Scientific, San Jose, CA; [8]Department of Internal Medicine, Division of Pulmonary Medicine, Chung Shan Medical University Hospital, Taichung, Taiwan; [9]Department of Surgery, National Taiwan University Hospital and National Taiwan University College of Medicine, Taipei, Taiwan; [10]Department of Internal Medicine, National Taiwan University Hospital, Taipei, Taiwan*

WP 239 **Higher Throughput Peptide Mapping Workflows Enabled by Automation of MS Data Analysis, Review, and Reporting**; Stephen Kok[1]; Michelle English[2]; Aude Tartière[1]; Catherine Evans[3]; Nick DeGraan-Weber[1]; *[1]Genedata Inc., San Francisco, CA; [2]Genedata Inc., Boston, MA; [3]Genedata AG, Basel, Switzerland*

WP 240 **Improved Throughput of GLP-1 Agonist Using Elevated pH and New LC Packing Materials**; Peter Pellegrinelli[1]; Joshua McBee[1]; Barry Boyes[1]; *[1]Advanced Materials Technology, Wilmington, DE*

WP 241 **Simultaneous Multi-Omics Analysis by Direct Infusion Mass Spectrometry (SMAD-MS)**; Yuming Jiang[1]; Amanda Momenzadeh[1]; Ivan SALLADAY-PEREZ[2]; Jose De Jesus Munoz Estrada[1]; Anthony J. Covarrubias[2]; Jesse Meyer[1]; *[1]Cedars Sinai Medical Center, Los Angeles, CA; [2]UCLA, Los Angeles, CA*

WP 242 **Accelerating cyclic peptide hit optimisation using a novel affinity-selection mass spectrometry (ASMS) platform**; Poppy Llowarch[1]; Joseph Gault[1]; Andrea Possenti[1]; Leran Zhang[1]; Elise Bernard[1]; Hannah Bolt[1]; Jarrod Walsh[1]; Sergio Martinez Cuesta[1]; Siva Genapathy[1]; *[1]AstraZeneca, Cambridge, United Kingdom*

WP 243 **Faster Than the Speed of Life: A Rapid Screening Method for Select PFAS Compounds in Serum by RapidFire-MS**; Jennifer Cottine Hitchcock[1]; Emily Parry[2]; *[1]Agilent Technologies, Santa Clara, CA; [2]Agilent Technologies, Wilmington, DE*

WP 244 **High-Throughput Dual-Arm, Dual-Stream LC-MS/MS Bioanalysis Leveraging the LS-II Autosampler**; Jason Hulen[1]; Drew Zielonka[1]; Estelle Maes[1]; Gary Jenkins[1]; *[1]AbbVie, QTAS, North Chicago, IL*

WP 245 **Scalable High-Throughput Workflow for Simultaneous Targeted and Discovery Proteomics by Hybrid DIA MS**; Ziyue Wang[1]; Li Yang[1]; Kathrin Textoris-Taube[1]; Michal Nadler-Holly[2, 3]; Yue Xuan[2, 3]; Markus Ralser[1]; Michael Mülleder[1]; *[1]Charité University Medicine, Berlin, Germany; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [3]Thermo Fisher Scientific, Dreieich, Germany, Dreieich, Germany*

WP 246 **From Complexity to Clarity: Automating Multi-Layered Targeted Proteomics Data Analysis**; Uthpala I Seneviratne; *AstraZeneca, Waltham, MA*

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WP 247 **Triboelectric Nanogenerator-Powered Laser Ablation/Nanoelectrospray Ionization (TENG LAESI) Mass Spectrometry Imaging Ion Source**; Dmitry Leontyev[1]; Xin Ma[2]; Joseph L Corstvet[1]; Carter K Asef[1]; Rebecca Arnold[3]; John A Petros[3]; Facundo M Fernandez[1]; *[1]Georgia Institute of Technology, Atlanta, GA; [2]University of Virginia, Charlottesville, VA; [3]Emory University, Atlanta, GA*

WP 248 **MALDI mass microscopy for high throughput imaging**; Aljoscha Körber[1]; Bryn Flinders[1]; Frans Giskes[1]; Ron M. A. Heeren[1]; *[1]The Maastricht MultiModal Molecular Imaging Institute (M4i) / Maastricht University, Maastricht, Netherlands*

WP 249 **Cryo-3D MSI for Plant cells by Water Cluster Secondary Ion Mass Spectrometry (Cluster SIMS)**; Michal Ryszka[1]; Naoko Sano[1]; Paul Blenkinsopp[1]; *[1]Ionoptika Ltd, Chandlers Ford, United Kingdom*

WP 250 **High-Sensitivity MALDI MS Imaging of Lipid C=C Positional Isomers via O_2-Enhanced Oxygen Attachment Dissociation (O_2E-OAD)**; Satoshi Kasamatsu[1]; Kaoru Nakagawa[1]; Naoto Mishina[1]; Hidenori Takahashi[1]; Manami Kobayashi[2]; Kengo Takeshita[1]; Mohamed Boutaghou[3]; Noriyuki Ojima[1]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]Shimadzu corporation, Kawasaki, Japan; [3]Shimadzu Scientific Instruments, Columbia, Maryland*

WP 251 **Facilitating MALDI Imaging Sample Preparation: A High-Resolution, Reproducible, and User-Friendly Sublimation Device**; Tanja Bien[1]; Corinna Henkel[1]; Achim Buck[2]; Carla Ebner[2]; Michael Becker[2]; Jens Hoehndorf[1]; *[1]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [2]Boehringer Ingelheim, Biberach, Germany*

WP 252 **A Quality Management System Dashboard for Bruker's new GlycoTyper™ Targeted High-Throughput Glycoproteomics Platform**; Grace Grimsley[1]; Gray Huffman[1]; Steve Castellino[1]; Klaus Lindpaintner[1]; *[1]Bruker Scientific LLC, Glycobiology Solutions, Billerica, MA*

WP 253 **1,000,000 Resolving Power at 10 µm Spatial Resolution with a Prototype MALDI TIMS-FT-ICR MS**; Madeline Colley[1]; Alina Theisen[2]; Martin Dufresne[3, 4]; Lukasz G Migas[5]; David M.G. Anderson[4, 6]; Marcel Niehaus[2]; Melissa A. Farrow[3, 4]; Raf Van De Plas[4, 5, 6]; Christopher A Wootton[2]; Jeffrey M Spraggins[3, 4, 7, 8, 9, 10]; *[1]Vanderbilt University, Nashville, TN; [2]Bruker Daltonics GmbH & Co.KG, Bremen, Germany; [3]Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; [4]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [5]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [6]Department of Biochemistry, Vanderbilt University, Nashville, TN; [7]Chemical and Physical Biology Program, Vanderbilt*

University, Nashville, TN, United States 2. Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [8]Department of Biochemistry, Vanderbilt University School of Medicine, Nashville, TN; [9]Department of Chemistry, Vanderbilt University, Nashville, TN; [10]Department of Pathology, Microbiology, and Immunology, Vanderbilt University Medical Center, Nashville, TN

WP 254 **Multidirectional Analysis of Plant Alkaloids Using MS Imaging (MSI) and Oxygen Attachment Dissociation (OAD)**; Kaoru Nakagawa[1]; Hidenori Takahashi[1]; Satoshi Kasamatsu[1]; Kengo Takeshita[1]; Manami Kobayashi[1]; Noriyuki Ojima[1]; [1]*Shimadzu Corporation, Kyoto, Japan*

WP 255 **Chemical Imaging with a Spaceflight LDMS Instrument for Planetary Exploration**; Oya Kawashima[1]; Ricardo Arevalo[1]; Lucas Taft Andrews[1]; Madeline Raith[1]; Adrian Southard[2]; Ryan M. Danell[3]; [1]*University of Maryland, College Park, Maryland; [2]NASA Goddard Space Flight Center, Greenbelt, MD; [3]Danell Consulting, Inc., Winterville, NC*

WP 256 **MS Imaging with > 100 pixels/sec and HRAM: TransMIT AP-SMALDI5AF ion source and Thermo Scientific Orbitrap Astral Analyzer**; Karl Christian Schäfer[1]; Lars Liebschwager[1]; Hamish Stewart[2]; Eduard Denisov[2]; Kerstin Strupat[2]; Bernhard Spengler[1, 3]; [1]*Transmit GmbH, Giessen, Germany; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [3]Justus Liebig University, Institute of Inorganic and Analytical Chemistry, Giessen, Germany*

WP 257 **Adding molecular imaging capabilities to any LC-MS - Plug & play laser ablation setup with SICRIT® ion source**; Jan-Christoph Wolf[1]; Markus Weber[1, 2]; Ciara Conway[1, 2]; [1]*Plasmion GmbH, Augsburg, Germany; [2]Technical University of Munich, München, Germany*

WP 258 **Orbitrap HRMS imaging applications using AP/MALDI and 266nm UV laser (post-)ionization**; Gilles FRACHE[1]; Maureen Feucherolles[1]; Eugene Moskovets[2, 3]; Konstantin Novoselov[2]; [1]*Luxembourg Institute of Science and Technology (LIST), BELVAUX, Luxembourg; [2]MassTech Inc., Columbia, MD; [3]MassTech Inc, Columbia, MD*

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WP 259 **Comprehensive metabolomic analyses of PLN9RC mutant mouse hearts using MALDI MS imaging and LC-MS/MS**; Siva Swapna Kasarla[1]; Theresa Brand[2]; Joachim P. Schmitt[3]; Kristina Lorenz[1, 2]; Albert Sickmann[1, 4]; Karl W. Smith[1]; [1]*Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Dortmund, Germany; [2]Institute of Pharmacology and Toxicology, University of Würzburg, Würzburg, Germany; [3]Institute of Pharmacology, Medical Faculty and University Hospital Düsseldorf, Heinrich-Heine-University Düsseldorf, Düsseldorf, Germany; [4]Medizinische Fakultät, Medizinische Proteom-Center (MPC), Ruhr-Universität Bochum, Bochum, Germany*

WP 260 **Mapping Isomeric Cerebroside Distribution in Rat Brain via MSI with MALDI-TIMS and Signal Enhancement through On-Tissue Enzyme Treatment**; Hsi-Chun Chao[1, 2]; Marisa Asadian[1, 2]; Stanislav S. Rubakhin[1, 2]; Fan Lam[1, 2]; Jonathan Sweedler[1, 2]; [1]*Beckman Institute for Advanced Science and Technology, University of Illinois Urbana-Champaign, Urbana, IL; [2]University of Illinois Urbana-Champaign, Urbana, IL*

WP 261 **Metal Doping Strategies for IR-MALDESI Mass Spectrometry Imaging of N-Linked Glycans**; Mahtab Heyrani[1, 2]; Makenna L. Schroder[1, 2]; Tana V. Palomino[1, 2]; David C. Muddiman[1, 2]; [1]*Biological Imaging Laboratory for Disease and Exposure Research, Raleigh, NC; [2]Department of Chemistry, North Carolina State University, Raleigh, NC*

WP 262 **Deciphering the Biomolecular Distribution Profile of Gangliosides in Alzheimer's Disease Brain with MALDI MS Imaging**; Emily M. Hubecky[1]; Penghsuan Huang[1]; Kelly H. Lu[1]; Hua Zhang[2]; Andrew J. Schneider[3, 4]; Luigi Puglielli[3, 4]; Lingjun Li[1, 2]; [1]*Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [2]School of Pharmacy, University of Wisconsin-Madison, Madison, WI; [3]Department of Medicine, University of Wisconsin-Madison, Madison, WI; [4]Waisman Center, University of Wisconsin-Madison, Madison, WI*

WP 263 **Understanding Regional Molecular Alterations in Scn2a Mutated Mouse Brains using Nanospray Desorption Electrospray Ionization Mass Spectrometry Imaging**; Alyssa Moore[1]; Xiaoling Chen[1]; Emerson Hernly[1]; Yang Yang[1]; Julia Laskin[1]; [1]*Purdue University, West Lafayette, IN*

WP 264 **MALDI mass spectrometry imaging of mouse tissue fine structure at 5-10 µm spatial resolution for accurate lipid and small-molecule profiling**; Sabina Holm Skov[1, 2]; Henrik Max Jensen[2]; Ole N. Jensen[1]; [1]*University of Southern Denmark, Odense M, Denmark; [2]IFF (International N&H Denmark, ApS), Brabrand, Denmark*

WP 265 **Correlative Stimulated Raman Imaging and Nano-DESI MSI for Mapping Isomeric Triglyceride Distributions in Biological Tissues**; Xindi Tang[1]; Mushfeqa Iqfath[1]; Bin Dong[1]; Manxi Yang[1]; Frederick Nguele Meke[2]; Chi Zhang[1]; Julia Laskin[1]; [1]*Department of Chemistry, Purdue University, West Lafayette, IN; [2]Department of Medicinal Chemistry and Molecular Pharmacology, Purdue University, West Lafayette, IN*

WP 266 **Spatial lipidomic analysis of mouse epididymis through MALDI-TOF MS imaging**; Aidan J Reynolds[1]; Soo Hyun Ahn[2, 3]; Margaret G Petroff[2, 3]; Tian (Autumn) Qiu[1]; [1]*Department of Chemistry, Michigan State Univeristy, East Lansing, MI; [2]Department of Pathobiology and Diagnostic Investigation, Michigan State University, East Lansing, MI; [3]Department of Microbiology, Genetics and Immunology, Michigan State University, East Lansing, MI*

WP 267 **An approach based on ion mobility spectrometry-mass spectrometry for the separation of stereoisomers of monoterpenoid indole alkaloids in Catharanthus roseus**; Tetsuya Mori[1]; Noriko Kamiya Takeda[1]; Takashi Nirasawa[2]; Ryo Nakabayashi[2]; Mai Uzaki[1]; Yushiro Fuji[1]; Kiminori Toyooka[1]; Masami Yokota Hirai[1, 3]; [1]*RIKEN CSRS, Yokohama, Japan; [2]Bruker Japan, Yokohama, Japan; [3]Nagoya University, Nagoya, Japan*

WP 268 **Visualization of polyunsaturated fatty acid accumulation in a mouse tumor model using automated on-tissue chemical derivatization for MALDI-MSI**; Akiko Kubo[1]; Yuki Katoh[2]; Kaoru Nakagawa[3]; Francine Yanchik-Slade[4]; Manami Kobayashi[3]; [1]*Kobe University Graduate School of Medicine, Kobe, Japan; [2]Nihon University School of Medicine, Itabashi-ku, Japan; [3]Shimadzu Corporation, Kyoto, Japan; [4]Shimadzu Scientific Instruments, Columbia, Maryland*

WP 269 **Spatially mapping lipid mediator biosynthesis to immune cell populations with targeted multimodal imaging**; Matthew J. Smith[1]; Alexandra Firsova[2, 3]; Jesper Säfholm[1]; Alexandros Sountoulidis[2, 3]; Christos Samakovlis[2, 3]; Craig E. Wheelock[1]; [1]*Karolinska Institutet, Solna, Sweden; [2]SciLifeLab, KTH Royal Institute of Technology, Solna, Sweden; [3]Stockholm UNIVERSITY, Stockholm, Sweden*

WP 270 **Polyamine and Lipid Metabolism in Optic Nerve: Spatial Omics with AP/MALDI Mass Spectrometry Imaging**; Sean Meehan[1]; Caleigh Rose O'Connor[2]; Eugene Moskovets[2]; Konstantin Novoselov[2]; Nivedita Bhattacharya[2]; Sanjoy K Bhattacharya[1]; [1]*Bascom Palmer Eye Institute, Miller School of Medicine, University of Miami, Miami, Florida; [2]MassTech, Columbia, MD*

WP 271 **Comprehensive Spatial Mapping of Phospholipids with Mass Spectrometry Imaging (MSI) via Diazo-Based On-Tissue Chemical Derivatization**; Kelly Lu[1]; Wei Wilson Li[2]; Hua Zhang[2]; Andrew J. Schneider[3, 4]; Luigi Puglielli[3, 4]; Lingjun Li[1, 2]; [1]*Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [2]School of Pharmacy, University of Wisconsin-Madison, Madison, WI; [3]Department of Medicine, University of Wisconsin-Madison, Madison, WI; [4]Waisman Center, University of Wisconsin-Madison, Madison, WI*

WP 272 **MALDI Imaging Mass Spectrometry Enables Spatial Cell-type-specific Metabolomics and Lipidomics in**

Alzheimer's Disease Mouse Model and Human Brain; Jinhyeok Kim[1]; Nicholas Asiimwe[2]; Ji-Su Shin[1]; Gabbie Lagdameo[3]; Dalton Brown[3]; Laura Gomez-Isaza[1]; Juan C. Troncoso[1]; Tae-In Kam[1]; Caitlin M. Tressler[3, 4]; Valina Dawson[1]; Kristine Glunde[3, 4, 5]; Chan-Hyun Na[1]; *[1]Johns Hopkins School of Medicine, Baltimore, MD; [2]Baylor College of Medicine, Houston, TX; [3]The Johns Hopkins University Applied Imaging Mass Spectrometry Core and Service Center, Baltimore, MD; [4]The Sidney Kimmel Comprehensive Cancer Center, The Johns Hopkins University School of Medicine, Baltimore, MD; [5]Department of Biological Chemistry, The Johns Hopkins University School of Medicine, Baltimore, Maryland*

WP 273 **Imaging Mass Spectrometry Analysis of Gastric Metabolite Changes in Response to Helicobacter Pylori Infection**; Michelle L. Reyzer[1]; Gabrielle E. Fortier[1]; Mandy D. Truelock[1]; Jennifer H. Battle[1]; Timothy L. Cover[2, 3]; Kevin L. Schey[1]; Jeffrey M. Spraggins[1]; *[1]Vanderbilt University, Nashville, TN; [2]Vanderbilt Medical Center, Nashville, TN; [3]Veterans Affairs Tennessee Valley Health Care System, Nashville, TN*

WP 274 **MALDI MSI analysis of single oocytes to find changes in lipids composition between oocytes of different developmental potential**; Anna Bodzon-Kulakowska[1]; Paulina Kret[1]; Przemyslaw Mielczarek[1, 2]; Dominika Siekierska[3]; Wiesława Młodawska[3]; Piotr Suder[1]; *[1]AGH University of Krakow, Krakow, Poland; [2]Laboratory of Proteomics and Mass Spectrometry, Maj Institute of Pharmacology, Polish Academy of Sciences, Krakow, Poland; [3]University of Agriculture in Krakow, Krakow, Poland*

WP 275 **Mapping Biochemical Markers of Post-Harvest Microbial Spoilage in Table Grapes with AP/MALDI Mass Spectrometry Imaging**; Nivedita Bhattacharya[1, 2]; Caleigh Rose O'Connor[1]; Vishal Mahale[1, 2]; Eugene Moskovets[1]; Konstantin Novoselov[1]; Kaushik Banerjee[3]; Venkateswarlu Panchagnula[1]; *[1]MassTech, Columbia, MD; [2]Barefeet Analytics Private Limited, 100 NCL Innovation Park, Dr. Homi Bhabha Road, Pune, India; [3]National Reference Laboratory, ICAR-National Research Centre for Grapes, P.O. Manjri Farm, Pune, India*

WP 276 **Rapid determination of the pharmacokinetics, metabolism, elimination and tissue distribution of a PROTACs drug using UHPLC-MS/MS, HRMS and DESI Imaging**; Robert S Plumb[1]; Ian Wilson[2]; Steven Lai[3]; Andrew Leightner[3]; *[1]Waters, Milford, MA; [2]Imperial College London, London, United Kingdom; [3]Waters Corp., Milford, MA*

WP 277 **Last lipid standing: Lipid A imaging byLPS-to-Lipid A Mass Spectrometry Imaging (LLA-MSI)from FFPE tissues**; Hyojik Yang[1]; Casey E Hofstaedter[1]; Robert K. Ernst[1, 2]; Alison J. Scott[1, 2]; *[1]Department of Microbial Pathogenesis, University of Maryland School of Dentistry, Baltimore, Maryland; [2]Department of Microbiology & Immunology, University of Maryland School of Medicine, Baltimore, Maryland*

WP 278 **Uncovering Metabolic Responses to 'Candidatus Phytoplasma vitis' Infection in Grapevine Leaves Using Mass Spectrometry Imagin**; Alice Passoni[1]; Stefano Mauro Carabellese[1]; Matteo Preziati[1]; Luciana Galetto[2]; Cristina Marzachì[2]; Renzo Bagnati[1]; Enrico Davoli[1]; *[1]Istituto di Ricerche Farmacologiche Mario Negri IRCCS, Milano, Italy; [2]Istituto per la Protezione Sostenibile delle Piante, Consiglio Nazionale delle Ricerche, IPSP-CNR, Turin, Italy*

WP 279 **Isomer-Selective Imaging of Carbohydrates in Soybeans Using Ion-Mobility Coupled to Mass Spectrometry Imaging (IM-MSI)**; Emerson L Hernly[1]; Syeda Nazifa Wali[1]; Laura Wayne[2]; Kathrine Thilges[2]; Julia Laskin[1]; *[1]Purdue University, West Lafayette, IN; [2]Corteva Agriscience, Indianapolis, IN*

WP 280 **Functional validation of regio-specific brain lipogenesis modulation as an actionable target in a chronic pain model**; Alison Scott[1]; Mahadi Shahed[1]; Hayelom Mekonen[1]; Michael Keaser[1]; Joyce Da Silva[1]; Abena Ntiamoah[1]; Shelby Hanson[1]; Luis Hernandez[2]; Tialfi Bergamin De Castro[1]; Natalia Islam[1]; David Seminowicz[3]; Ohannes Melemedjian[1]; Robert Ernst[1]; Richard Traub[1]; *[1]University of Maryland, Baltimore, MD; [2]Technologico de Monterrey, Guadalajara, Mexico; [3]Western University, London, Ontario*

WP 281 **MALDI MSI Lipidomic profiles of major regions in the human heart**; Kayla M Osumi[1]; Ian Williamson[2]; Yaqi Gao[2]; Kyoungmin Kim[2]; David Lefer[3]; Lawrence S.C Czer[3]; Evan P. Kransdorf[2]; Anja Karlstaedt[2]; Elizabeth K. Neumann[1]; *[1]Department of Chemistry, University of California, Davis, Davis, CA; [2]Department of Cardiology, Smidt Heart Institute, Cedars-Sinai Medical Center, Los Angeles, CA; [3]Department of Cardiothoracic Surgery, Smidt Heart Institute, Los Angeles, CA*

WP 282 **Visualizing Local Tissue Drug Metabolism by Functional Mass Spectrometry Imaging**; Nav Raj Phulara[1]; Herana Kamal Seneviratne[1]; *[1]University of Maryland, Baltimore County, Baltimore, MD*

WP 283 **Visualizing the incorporation of deuterium-reinforced polyunsaturated fatty acids (D-PUFAs) in mouse retina using MALDI-2-MS Imaging**; Sebastian Bessler[1]; Tim Padberg[2]; Julian Zimmermann[2]; Jens Soltwisch[1]; Martin-Paul Agbaga[3]; Karsten Schmidt[4]; Peter Heiduschka[2]; Klaus Dreisewerd[1]; *[1]University of Muenster, Muenster, Germany; [2]University Hospital Münster, Münster, Germany; [3]University of Oklahoma Health Sciences Center and the Dean McGee Eye Institute, Oklahoma City, OK; [4]BioJiva LLC, San Jose, CA*

WP 284 **MALDI Imaging and Spatial SILAC Proteomics of Three-Dimensional Multicellular Spheroids Dynamically Dosed with Doxorubicin-Encapsulating Liposomes**; Arbil Lopez[1]; Joseph H Holbrook[2]; Amanda B. Hummon[1, 2]; *[1]Department of Chemistry and Biochemistry, The Ohio State University, Columbus, Ohio; [2]Ohio State Biochemistry Program (OSBP), The Ohio State University, Columbus, OH*

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WP 286 **Sequential Mass Spectrometry Imaging Workflow for Co-localization of N-glycans and Insulin Hormone in Pancreatic Islets**; Wan Jo Lee[1]; Kelly Lu[1]; Connie S Chamberlain[2]; Peter J Chlebeck[2]; Deep Kapadia[2]; Jon S Odorico[2]; Lingjun Li[1, 3]; *[1]Department of Chemistry, University of Wisconsin–Madison, Madison, WI; [2]Department of Surgery, University of Wisconsin–Madison, Madison, WI; [3]School of Pharmacy, University of Wisconsin-Madison, Madison, WI*

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WP 288 **Metabolic profiling of microenvironments directly from live bacterial colonies using capillary sampling**; Dharmeshkumar Parmar[1, 2]; Stanislav S. Rubakhin[1, 2]; Jonathan Sweedler[1, 2]; *[1]Department of Chemistry, University of Illinois Urbana-Champaign, Urbana, IL; [2]Beckman Institute for Advanced Science and Technology, University of Illinois Urbana-Champaign, Urbana, IL*

WP 289 **Spatially mapping neuropeptide isomers by MALDI trapped ion mobility MS imaging**; Timothy J Trinklein[1]; Samuel Okyem[1]; Stanislav S Rubakhin[1]; Jonathan V Sweedler[1]; *[1]University of Illinois Urbana Champaign, Champaign, IL*

WP 290 **Infrared Laser Ablation Microdissection for Localized Shotgun Lipidomics**; Kadeem O Hayes[1]; Kermit K. Murray[1]; *[1]Louisiana State University, Baton Rouge, LA*

WP 291 **Spatial Mapping of Gangliosides and Proteins in Amyloid Beta Plaques at Cellular Resolution Using Mass Spectrometry Imaging and MALDI-IHC**; Christopher Good[1]; Andrew Bowman[1]; Corinna Klein[2]; Khader Awwad[2]; Wayne Buck[1]; Junhai Yang[1]; David Wagner[1]; *[1]AbbVie, North Chicago, IL; [2]AbbVie, Ludwigshafen, Germany*

WP 292 **Gold Nanostar-Enhanced MALDI Imaging of Neurotransmitters and Metabolites in Mouse Brain Tissue Sections**; Wanyue Wang[1]; Swati Tanwar[2]; Caitlin M. Tressler[1]; Ishan Barman[2]; Kristine Glunde[1]; *[1]Johns Hopkins Applied Imaging Mass Spectrometry Core, Russell H. Morgan Department of Radiology and Radiological Science, Johns Hopkins School of Medicine, Baltimore, Maryland; [2]Department of Mechanical Engineering, Johns Hopkins University, Baltimore, Maryland*

WP 293 **Unveiling the Spatial Metabolomic Landscape of the Developing Human Brain**; Tianzhi Wu[1]; Lihua Jiang[2]; Ruiqi Jian[2]; Nannan Tao[3]; Michael Snyder[2]; Jingjing Li[1]; *[1]Department of Neurology, University of California, San Francisco, CA; [2]Department of Genetics, Stanford University, Stanford, CA; [3]Bruker Daltonics Inc, 101 Daggett Dr., San Jose, CA*

WP 294 **MALDI-MS Imaging Reveals Molecular Spatial Heterogeneity at the Gut-Lumen Interface**; Jacob Haffner[1]; Soo Hyun Ahn[2]; Tian (Autumn) Qiu[1]; *[1]Michigan State University, Department of Chemistry, East Lansing, MI; [2]Michigan State University, College of Veterinary Medicine, Department of Pathobiology and Diagnostics Investigation, East Lansing, MI*

WP 295 **High Resolution DESI imaging Single Cell Analysis**; Mark Towers[1]; Gary Harland[1]; Scarlett Ferrinho[1, 2]; Lisa Reid[1]; Lee A Gethings[1]; Preeti Mourya[2]; Shazneil Briones[2]; Olivier NF Cexus[2]; Paul Townsend[2]; Joanne Ballantyne[1]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Faculty of Health and Medical Sciences, University of Surrey, Guildford, United Kingdom*

WP 296 **Opto-proteomic Pipeline for Mass-Spectrometry Based Analysis of Sub-Cellular Regions of Interest**; Benjamin L Muselius[1]; Pauline Douglas[1]; Mariel Kleer[1]; Jennifer A Corcoran[1]; David C. Schriemer[1]; *[1]University of Calgary, Calgary, AB*

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WP 298 **Advanced Multimodal Spatially-Resolved Mass Spectrometry Methods for Untargeted Spatial Metabolomics and Untargeted Spatial Proteomics on the Same Tissue Section**; Marija Velickovic[1]; Yi-Syuan Guo[1]; Gregory W Vandergrift[1]; Dusan Velickovic[1]; Le Z Day[1]; Sarah M Williams[1]; Paul D Piehowski[1]; Christopher Anderton[2]; *[1]Pacific Northwest National Laboratory, Richland, Washington; [2]Pacific Northwest National Laboratory, Richland, WA*

WP 299 **MALDI mass spectrometry imaging for lipid profiling in coral tentacles**; Ryutaro Jacobson[1]; Sabrina L. Rosset[2, 3]; Kiran Shivaiah[2]; Thomas Cline[2]; Robert Quinn[2]; Tian (Autumn) Qiu[1]; *[1]Michigan State University Department of Chemistry, East Lansing, MI; [2]Michigan State University Department of Biochemistry and Molecular Biology, East Lansing, MI; [3]Hawai'i Institute of Marine Biology, University of Hawai'i at Manoa, Kane'ohe, HI*

WP 300 **Multiplex Deep Visual Proteomics Unveils Spatial Heterogeneity and Rare Endocrine States in Human Adult Pancreatic Islets**; Mariya Mardamshina[1]; Nicolai Dorka[1]; Marvin Thielert[2]; Frida Björklund[1]; Fredric Ballllosera[1]; Anna Martinez Casals[1]; Ferenc Kovacs[3, 4]; Peter Horvath[3, 4]; Patrick E. MacDonald[5]; Matthias Mann[2]; Emma Lundberg[1, 6]; *[1]Stanford University, Stanford, CA; [2]Max Planck Institute of Biochemistry, Martinsried, Germany; [3]Biological Research Centre, Eötvös Loránd Research Network, Szeged, Hungary; [4]Single-Cell Technologies Ltd., Szeged, Hungary; [5]University of Alberta, Edmonton, AB; [6]KTH Royal Institute of Technology, Stockholm, Sweden*

WP 301 **A Combined MALDI and IR-MALDESI MSI Approach for Enhanced Metabolomic Coverage in a Rat Model of Parkinson's Disease**; Mary F. Wang[1]; Anna Nilsson[2]; Reza Shariatagorji[2]; Ibrahim Kaya[2]; Per E. Andrén[2]; David C. Muddiman[1]; *[1]Biological Imaging Laboratory for Disease and Exposure Research (BILDER), Department of Chemistry, North Carolina State University, Raleigh, North Carolina; [2]Department of Pharmaceutical Biosciences, Spatial Mass Spectrometry, Science for Life Laboratory, Uppsala University, Uppsala, Sweden*

WP 302 **Multiomics analysis for advanced tumor typing of lung cancer using 116plex MALDI HiPLEX-IHC and released N-glycans on the neofleX**; Janina Oetjen[1]; Corinna Henkel[1]; Michael Easterling[2]; Nannan Tao[2]; Mark Lim[3]; Gargey Yagnik[3]; Andrew Yatsuhashi[3]; Kenneth Rothschild[3]; Mengze Stettler-Zhang[4, 5]; Konrad Steinestel[6]; Bernd Bodenmiller[4, 5]; *[1]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [2]Bruker Scientific, Billerica, MA; [3]AmberGen Inc., Billerica, MA; [4]University of Zurich, Zurich, Switzerland; [5]ETH Zurich, Zurich, Switzerland; [6]Bundeswehrkrankenhaus Ulm, Ulm, Germany*

WP 303 **Spatial metabolomics and lipidomics using mzmine 4**; Steffen Heuckeroth[1, 2]; Robin Schmid[1]; Carina Wolf[2, 3]; Arne Behrens[4]; Arne Fuetterer[4]; Ansgar Korf[1]; Katharina Kronenberg[5]; Corinna Brungs[6]; Henning Richter[7]; Astrid Jeibmann[8]; Uwe Karst[2]; *[1]mzio GmbH, Bremen, Germany; [2]University of Muenster, Muenster, Germany; [3]University of Bayreuth, Bayreuth, Germany; [4]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [5]University of Graz, Graz, Austria; [6]University of Vienna, Vienna, Austria; [7]University of Zurich, Zurich, Switzerland; [8]University Clinic Muenster, Muenster, Germany*

WP 304 **Cell-Specific MALDI MS Imaging Reveals Competitive Utilization of di-PUFA-Phospholipids in Biosynthesis of N-Acyl-Phosphatidylethanolamines and Ferroptotic Peroxidation in Traumatic Brain Injury**; Sviatlana N. Samovich[1]; Taha Kelestemur[1]; Alptug H. Kaynar[1]; Louis J. Sparvero[2]; Ecem Saritas[1]; Teodora M. Bratu[1]; Vladimir A. Tyurin[2]; Valerian E. Kagan[1, 2]; Hülya Bayir[1]; *[1]Department of Pediatrics, Division of Critical Care and Hospital Medicine, Redox Health Center, Vagelos College of Physicians and Surgeons, Columbia University Irving Medical Center, New York, New York; [2]Department of Environmental and Occupational Health, Center for Free Radical and Antioxidant Health, School of Public Health, University of Pittsburgh, Pittsburgh, PA*

WP 305 **Laser Ablation Inductively Coupled Plasma Mass Spectrometry Imaging for the Study of Metal Ions in Organophosphate Poisoning**; Gabriella Lagdameo[1]; Benjamin Wadsworth[2]; Samantha Carriero[2]; Natalie Dillman[3]; C Linn Cadieux[2]; Caitlin M. Tressler[1, 4]; *[1]The Johns Hopkins University Applied Imaging Mass Spectrometry Core and Service Center, Baltimore, MD; [2]United States Army Medical Research Institute of Chemical Defense, Aberdeen Proving Ground, MD; [3]Russell H. Morgan Department of Radiology and Radiological Science, The Johns Hopkins University School of Medicine, Baltimore, Maryland; [4]The Sidney Kimmel Comprehensive Cancer*

Center, The Johns Hopkins University School of Medicine, Baltimore, MD

WP 306 **Pathologists embracing novel developments of MALDI and DESI HR MS Histochemistry of FFPE tissues**; Peter D. Verhaert[1, 2]; Marco Giampa[3]; Ling Shan[4]; Dick Swaab[4]; Per E. Andren[5]; Dietmar Thal[1]; Raf Sciot[1]; Bart Ghesquière[3]; Gilles Frache[6]; *[1]Department of Imaging and Pathology, Leuven University, Leuven, Belgium; [2]ProteoFormiX, Vorselaar, Belgium; [3]Laboratory of Applied Mass Spectrometry, University of Leuven, Leuven, Belgium; [4]Netherlands Institute for Neuroscience, Amsterdam, Netherlands; [5]Department of Pharmaceutical Biosciences, Spatial Mass Spectrometry, Science for Life Laboratory, Uppsala University, Uppsala, Sweden; [6]Luxembourg Institute of Science and Technology (LIST), BELVAUX, Luxembourg*

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WP 308 **massSight: A Bayesian Framework for Automated LC-MS Feature Alignment with Dynamic Parameter Optimization and Drift Correction**; Chiraag Gohel[1]; Ali Rahnavard[1]; *[1]The George Washington University, Milken Institute School of Public Health, Washington, DC*

WP 309 **Improvements and Analysis of Kendrick Mass Defect (KMD) Algorithms: An Error Informed Approach and Uses of Circular Distance Metrics**; Cole Stapleton[1]; Christopher Joseph Shaffer[1]; Dana Reed[1]; *[1]3M, Maplewood, MN*

WP 310 **SpecCheck: Transformer-Based Quality Assessment for Immunopeptidomics Mass Spectra**; Frédérique Vilenne[1, 2]; Dirk Valkenborg[1]; *[1]Hasselt University, Diepenbeek, Belgium; [2]Flemish Institute for Technological Research, Mol, Belgium*

WP 311 **svdImpute2: An enhanced SVD-based imputation of randomly and non-randomly missing values in proteomics data**; Murat Akhmedov; *BigOmics Analytics, Lugano, Switzerland*

WP 312 **Interference of Adjacent Ion Signals in CDMS: The Effect on Charge Accuracy and Potential Correction Algorithm**; Liangxuan Fu[1]; Michael P Goodwin[1]; Dmitry Grinfeld[2]; Kyle Patrick Bowen[1]; Mike Senko[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

WP 313 **A decoy-free method to derive Posterior Error Probabilities from False Discovery Rates**; Yuqi Zheng[1]; Matthew The[2]; Lukas Käll[1]; *[1]SciLifeLab, KTH Royal Institute of Technology, Solna, Sweden; [2]TUM School of Life Sciences, Chair of Proteomics and Bioanalytics, München, Germany*

WP 314 **Predicting Immune Cell Admixture in Bulk Proteomics Data Using ProteoMixture**; Joshua P Schaaf[1]; Tamara Abulez[1]; Pang-ning Teng[1]; Brian L. Hood[1]; Kelly A. Conrads[1]; Litzi J. Tracy[1]; Allison L. Hunt[2]; Matthew D. Wilkerson[3]; Kathleen M. Darcy[1]; Neil Phippen[1]; Christopher M. Tarney[1]; Larry Maxwell[1]; Thomas P. Conrads[2]; Nicholas W. Bateman[1]; *[1]Gynecologic Cancer Center of Excellence and the Women's Health Integrated Research Center, Annandale, VA; [2]Women's Health Integrated Research Center, Women's Service Line, Inova Health System, Annandale, VA; [3]The American Genome Center, Department of Anatomy Physiology and Genetics, Uniformed Services University of the Health Sciences, Bethesda, MD, United States, Bethesda, MD*

WP 315 **Comparison of software solutions for peptide quantification by label-free mass spectrometry**; Irbaz Isaac Badshah[1]; Pedro Rodriguez Cutillas[1]; *[1]Barts Cancer Institute, Queen Mary University of London, London, United Kingdom*

WP 316 **Application of Concepts from Adaptive Retention Time Improves the Robustness of LC Peak Integration in Targeted MSn Experiments**; Philip M Remes[1]; Lilian H. Heil[1]; Cristina C. Jacob[1]; Nicholas Shulman[2]; Brendan X. MacLean[2]; Qin Fu[1]; Jihyeon Lee[3]; Jennifer Van Eyk[3]; Michael J. MacCoss[2]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]University of Washington, Seattle, WA; [3]Cedars Sinai Medical Center, Los Angeles, CA*

WP 317 **Pythia: A Fast, Sensitive, and Accurate Search Engine for Quantitative DIA Proteomics**; Seth Just[1]; Drew Nichols[1]; Lee Cantrell[1]; Jian Wang[1]; Harendra Guturu[1]; Iman Mohtashemi[1]; Theo Platt[1]; Serafim Batzoglou[1]; *[1]Seer, Inc, Redwood City, CA*

WP 318 **Unveil the Dark Matters of Proteins: Deep learning based De Novo Peptide Sequencing with Open PTM Search at State-of-the-Art Accuracy**; Zeping Mao[1]; Lei Xin[2]; Baozhen Shan[2]; *[1]University of Waterloo, Waterloo, ON; [2]Bioinformatics Solutions Inc, Waterloo, ON*

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WP 320 **Reverse spectral search reimagined: a simple but overlooked solution for annotating chimeric spectra in untargeted metabolomics**; Shipei Xing[1]; Vincent Charron-Lamoureux[1]; Haoqi Nina Zhao[1]; Yasin El Abiead[1]; Mingxun Wang[2]; Pieter C. Dorrestein[1]; *[1]University of California San Diego, San Diego, CA; [2]University of California, Riverside, Riverside, CA*

WP 321 **Expanding de novo peptide sequencing to post-translationally modified peptides**; Daniela Klaproth-Andrade[1]; Yanik Bruns[2]; Christian Nix[2]; Wassim Gabriel[3]; Mathias Wilhelm[3]; Julien Gagneur[2]; *[1]Technical University of Munich, Garching bei Muenchen, Germany; [2]Computational Molecular Medicine, School of Computation, Information and Technology, Technical University of Munich, Munich, Germany; [3]Computational Mass Spectrometry, School of Life Sciences, Technical University of Munich, Freising, Germany*

WP 322 **The Spiked Mixture Model: A New Clustering Approach for Imaging Mass Spectrometry Offers Advanced Resilience to Noise**; Paul-Louis Delacour[1]; Sander Wahls[2]; Lauren N. Emmerson[3, 4]; Madeline E Colley[3, 5]; Jeffrey M Spraggins[3, 5, 6, 7]; Lukasz G Migas[8]; Raf Van De Plas[3, 8, 9]; *[1]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [2]Karlsruhe Institute of Technology, Institute of Industrial Information Technology, Karlsruhe, Germany; [3]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [4]Chemical Physical Biology Program, Vanderbilt University, Nashville, TN; [5]Dept. of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; [6]Dept. of Biochemistry, Vanderbilt University, Nashville, TN; [7]Department of Chemistry, Vanderbilt University, Nashville, TN; [8]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [9]Department of Biochemistry, Vanderbilt University, Nashville, TN*

WP 323 **In-browser FTMS simulations: from isotopic calculations to top-down mass spectra of biotherapeutics**; Yury O. Tsybin[1, 2]; Konstantin O. Nagornov[1]; Nina A. Khristenko[2]; Michael Zasso[3]; Daniel Kostro[3]; Luc Patiny[3]; Natalia Gasilova[4]; Laure Menin[4]; Anton N. Kozhinov[1]; *[1]Spectroswiss, Lausanne, Switzerland; [2]Spectrotech, Lyon, France; [3]Zakodium, Lonay, Switzerland; [4]Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland*

WP 324 **Novor.ai – Increased precision and accuracy utilizing an AI model for de novo sequencing**; Tharan Srikumar[1]; Qixin Liu[2]; Dennis Trede[3]; Jonathan R Krieger[1]; Bin Ma[2]; George Rosenberger[4]; *[1]Bruker Ltd., Milton, ON; [2]Rapid Novor Inc,* *Kitchener, ON; [3]Bruker Daltonics GmbH & Co.KG, Bremen, Germany; [4]Bruker Switzerland AG, Fällanden, Switzerland*

WP 325 **Enhancing classification of Liquid Chromatography Mass Spectrometry data with batch effect correction using Artificial Neural Networks**; Simon J. Pelletier[1]; Mickaël Leclercq[1]; Florence Roux-Dalvai[1, 2]; Frédéric Precioso[3]; Arnaud Droit[1, 2]; *[1]Computational Biology Laboratory, CHU de Québec - Université Laval Research Center, Quebec, QC; [2]Proteomics Platform, CHU de Québec - Université Laval Research Center, Quebec, QC; [3]Université Côte d'Azur, CNRS, INRIA, I3S, Nice, France*

WP 326 **Better than WGCNA? Re-examination of protein-protein networks using alternative inference methods**; Justin Zhu[1]; Ali Bagherinia[1]; Henock M Deberneh[1]; Rovshan G Sadygov[1]; *[1]UTMB at Galveston, Galveston, TX*

WP 327 **DreamDIAlignR: improved cross-run statistical scoring in DIA using deep learning**; Mingxuan Gao[1]; Shubham Gupta[2]; Wenxian Yang[3]; Rongshan Yu[3, 4, 5]; Hannes L. Röst[1, 6, 7]; *[1]Terrence Donnelly Centre for Cellular & Biomolecular Research, University of Toronto, Toronto, ON; [2]Department of Genetics, Stanford University, Stanford, CA; [3]Aginome Scientific, Xiamen, China; [4]School of Informatics, Xiamen University, Xiamen, China; [5]National Institute for Data Science in Health and Medicine, Xiamen University, Xiamen, China; [6]Department of Molecular Genetics, University of Toronto, Toronto, ON; [7]Department of Computer Science, University of Toronto, Toronto, ON*

WP 328 **Improving the Casanovo de novo peptide sequencer**; Gwenneth Straub[1]; Melih Yilmaz[2]; Justin Sanders[2]; Wout Bittremieux[3]; William E. Fondrie[4]; William S. Noble[1, 2]; *[1]Department of Genome Sciences, University of Washington, Seattle, WA; [2]Paul G. Allen School of Computer Science and Engineering, University of Washington, Seattle, WA; [3]Department of Computer Science, University of Antwerp, Antwerp, Belgium; [4]Talus Bioscience, Seattle, WA*

WP 329 **Deep Learning Approaches for the Presence of KRAS Gene Classification in Colon Tumour based on Mass spectrometry**; Ziqi Yang[1]; Yuchen Xiang[1]; James Kinross[1]; Joram Matthias Posma[1]; Takats Zoltan[1]; Burak Temelkuran[1]; *[1]Imperial college london, London, United Kingdom*

WP 330 **Development of the Expert Algorithm for Substance Identification (EASI) to Electron Ionization Mass Spectra of Fentanyl Analogs**; Glen Paul Jackson[1]; Alexandra I Adeoye[1]; *[1]West Virginia University, Morgantown, WV*

WP 331 **Machine Learning–Based Molecular Networking and Deconvolution of Dissolved Organic Matter Tandem Mass Spectra**; Thomas V. Harwood[1]; Katherine B. Louie[1]; Suzanne M. Kosina[2]; Markus De Raad[1, 2]; Katherine T. McMahon[3, 4, 5]; Neslihan Taş[2, 6]; Nicholas J. Bouskill[6]; Terry C. Hazen[7, 8]; Shellie Bench[9, 10]; Rachel Mackelprang[11]; Fernando T. Maestre[12]; Daniel Petras[13]; Mingxun Wang[14]; Stephen J. Giovannoni[1, 15]; Trent R. Northen[1, 2]; Benjamin P. Bowen[1, 2]; *[1]The Joint Genome Institute, Lawrence Berkeley National Laboratory, Berkeley, CA; [2]Environmental Genomics and Systems Biology Division, Lawrence Berkeley National Lab, Berkeley, CA; [3]Department of Civil and Environmental Engineering, University of Wisconsin-Madison, Madison, WI; [4]Wisconsin Energy Institute, University of Wisconsin-Madison, Madison, WI; [5]Department of Bacteriology, University of Wisconsin-Madison, Madison, WI; [6]Climate and Ecosystems Division, Earth and Environmental Sciences Area, Lawrence Berkeley National Laboratory, Berkeley, CA; [7]University of Tennessee Knoxville, Knoxville, TN; [8]Oak Ridge National Laboratory, Oak Ridge, TN; [9]Fellow Health, San Leandro, CA; [10]Global Viral - Now LRC systems, Burlingame, CA; [11]Biology Department, California State University Northridge, Northridge, CA; [12]Environmental Sciences and Engineering, Biological and Environmental Science and Engineering Division, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia; [13]Department of Biochemistry, University of California Riverside, Riverside, CA; [14]Department of Computer Science and Engineering, University of California Riverside, Riverside, CA; [15]Department of Microbiology, Oregon State University, Corvallis, OR*

WP 332 **Reference based FDR control for peptide discoveries from de novo sequencing**; Justin A Sanders[1]; William Noble[1]; Uri Keich[2]; *[1]University of Washington, Seattle, WA; [2]University of Sydney, Sydney, Australia*

WP 333 **In silico characterization of biomolecules by Referenced Kendrick Mass Defect analysis**; Gillian Leach[1, 2]; Abanoub Mikael[1, 2]; Linda Nartey[1, 2]; Derek Smith[2]; Helena Petrosova[1, 2]; David R. Goodlett[1, 2]; *[1]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC; [2]UVic Genome BC Proteomics Centre, Victoria, BC*

WP 334 **Conditional use of search-engine-determined integration boundaries in Skyline 25.1**; Nicholas Shulman[1]; Michael Riffle[1]; Christine C Wu[1]; Brendan MacLean[1]; Michael J MacCoss[1]; *[1]University of Washington - Genome Sciences, Seattle, WA*

WP 335 **Deconvolution of Electrospray Spectra Using a Harmonic Product Spectrum Algorithm**; Jef Rozenski; *Rega Institutem KU Leuven, Leuven, Belgium*

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WP 336 **Features and benefits of using a slotted bandpass ion guide**; David Gordon; *Waters Corporation, Wilmslow, United Kingdom*

WP 337 **Improving the AC-ejection method for enhanced duty cycle and wide m/z range detection of ions in oTOF-MS**; Anastasios Grigoriadis[1]; Athanasios Smyrnakis[1]; Ioannis Orfanopoulos[1]; Ilias Panagiotopoulos[1]; Rafail Gioves[1]; Jonathan Krieger[2]; Vinzent Krug[3]; Benjamin Birner[3]; Oliver Raether[3]; Dimitris Papanastasiou[1]; *[1]Fasmatech Science & Technology, Chalandri, Greece; [2]Bruker, Milton, ON; [3]Bruker Daltonics, Bremen, Germany*

WP 338 **Implementation of Electron-transfer dissociation (ETD) and Electron-transfer/higher-energy collision dissociation (EThcD) on a modified Orbitrap Hybrid MS**; Peter Krueger[1]; Hanno Resemann[2]; Erik Couzijn[2]; Andreas Kühn[2]; Cong Wang[2]; Jan-Peter Hauschild[2]; *[1]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

WP 339 **Grid models using a combination of an infinite grid model and an ideal grid model in SIMION**; Robert Jackson[1]; Mark Osgood[1]; *[1]Ashwood Labs, LLC, Wilton, NH*

WP 340 **Synchronization of an oaTOF-MS and Pulsed Ion Source: Temporally Resolved Analysis via a Hexapole Ion Transfer**; Franziska Schuler[1]; Maja Hammelrath[1]; Markus Hübner[1]; Niklas Pengemann[1]; Hendrik Kersten[1]; Thorsten Benter[1]; *[1]University of Wuppertal, Wuppertal, Germany*

WP 341 **Simulation of the effect of mechanical misalignment on high m/z resolution CDMS trap solutions**; David Langridge[1]; Keith Richardson[1]; Kevin Giles[1]; *[1]Waters Corporation, Wilmslow, United Kingdom*

WP 342 **Development of a modified, compact single quadrupole mass spectrometer for quality control of oligonucleotides**; Jeff Dahl[1]; Stephen Kurzyniec[1]; Toshiya Matsubara[1]; Yoshio Takami[2]; So Kusumoto[2]; Ryo Kageyama[2]; Masaru Nishiguchi[2]; Kosuke Uchiyama[2]; Atsuhiko Toyama[1]; *[1]Shimadzu Scientific Instruments, Columbia, Maryland; [2]Shimadzu Corporation, Kyoto, Japan*

WP 343 **The Meaning of (Detector) Life**; Aditya Wakhle[1]; Antony Jones[1]; Peter Raffin[1]; David Whiteley[1]; Dane Ekers[1]; *[1]IMI Adaptas, Sydney, Australia*

WP 344 **Characterization of calibration ion sources for quantification of plasma ion densities using long path ion transfer stages**; Lena Marie Mokros[1]; Sanna Benter[1]; Niklas Pengemann[1]; Hendrik Kersten[1, 2]; Thorsten Benter[1]; *[1]Bergische Universität Wuppertal, Wuppertal, Germany; [2]Institute for Pure and Applied Mass Spectrometry (ipaMS), Wuppertal, Germany*

WP 345 **Cooling Ions to 0.4 K: New Instrumentation for Capture of Ions in He Nanodroplets**; Neil A Ellis[1]; Madeline

Schultz[1]; Miyuru M. Wellalage[1]; Nwanne D Banor[1]; Daniel A. Thomas[1]; *[1]University of Rhode Island, Kingston, RI*

WP 346 **Triple Quadrupole Mass Spectrometer Performance: A Novel Ion Guide Design for Increased Robustness**; Jason D. White[1]; Sumeet S. Chakravorty[1]; Harald Oser[1]; Michael V. Ugarov[1]; *[1]Thermo Fisher Scientific, San Jose, California*

WP 347 **High dynamic range peptide mass spectrometry using segmented precursor ions accumulation**; Maria C Panepinto[1]; Paolo Cifani[1]; *[1]Cold Spring Harbor Laboratory, Cold Spring Harbor, NY*

WP 348 **A Cryogenic Hexapole Ion Trap for Infrared Action Spectroscopy**; Neil A Ellis[1]; Madeline Schultz[1]; Daniel A Thomas[1]; *[1]University of Rhode Island, Kingston, RI*

WP 349 **Construction of A UPLC-UPC2- MS/MS Platform**; Hailong Liu[1]; Xingxing Huang[1]; Bichao Yang[1]; Haoqiang Chen[1]; Hongye Li[1]; Zhiyu Li[1]; Yi Tao[1]; Liang Shen[1]; *[1]WuXi AppTec, Shanghai, China*

WP 350 **Simplifying Sample Preparation: Python-Driven Robot Integration for Automated Normalization**; Jessica A Salguero[1]; Kes A. Luchini[1]; Tara Harvey[1]; Philip Mach[1]; *[1]Los Alamos National Laboratory, Los Alamos, NM*

WP 351 **Importance of Ion Losses in 90-Degree Curved Quadrupole Ion Guides for the Performance of a Folded-Layout Triple Quadrupole Mass Spectrometer**; Matthias Lorenz[1]; Anna Kornilova[1]; Adrian Maclean[1]; Tak Shun Cheung[1]; Hamid Badiei[1]; *[1]PerkinElmer, Woodbridge, ON*

WP 352 **A Novel Resonant RF Axial Ejection System for Reduced Ion Time of Flight Dispersion**; Nathan K. Kaiser[1]; Gordon A. Anderson[2]; Christopher L. Hendrickson[1]; Chad R. Weisbrod[1]; *[1]National High Magnetic Field Laboratory, Tallahassee, FL; [2]GAA Custom Electronics, LLC, Kennewick, WA*

WP 353 **Optimization of the Entropy-Based Wavelet Method for Removing Strong RF and AC Interferences in CSPD Linear Ion Trap Mass Spectrometer**; Minh Cong Dang[1,2,3]; Avinash A. Patil[1]; Ly Khánh Thị Lại[1]; Szu-Wei Chou[1]; Trang Kieu Thi Hoang[2]; Mhar Ian Cua Estayan[1,4]; Wen-Ping Peng[1]; *[1]National Dong Hwa University, Shoufeng, Hualien, Taiwan; [2]Vietnam National University – Ho Chi Minh City, Ho Chi Minh City, Vietnam; [3]Vietnam Atomic Energy Institute, Lam Dong, Vietnam; [4]University of Santo Tomas, Manila, Philippines*

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WP 354 **Exploring Enantiomer Separation Using Structural Mass Spectrometry Methods**; Rashi M Gupta[1]; Benjamin K Blakley[1]; Jody C May[1]; John A McLean[1]; *[1]Department of Chemistry, Center for Innovative Technology, Institute of Chemical Biology, Institute for Integrative Biosystems Research, and Education, Vanderbilt University, Nashville, TN*

WP 355 **Human Milk Oligosaccharide Sequencing by High-Resolution Cyclic Ion Mobility Separations Coupled with Tandem Mass Spectrometry**; Sanaz C Habibi[1]; Storm Bowser[1]; Gabe Nagy[1]; *[1]University of Utah, Salt Lake City, UT*

WP 356 **Advancing Untargeted Analysis of PFAS Compounds using Structures for Lossless Ion Manipulations and Mobility Aligned Fragmentation**; Heidi Sabatini[1]; Ralph Aderorho[1]; Christopher Chouinard[1]; *[1]Clemson University, Clemson, SC*

WP 357 **Ligand Conformational and Metal Coordination Isomers in Complexes of Metal Ions and Cyclic Depsipeptides**; Emmanuel Nkyaagye[1]; Hernando J. Olivos[2]; Thanh D. Do[1]; *[1]University of Tennessee, Knoxville, TN; [2]Waters, Milford, MA*

WP 358 **Unravelling the Structural Heterogeneity of Polysorbates Using High Resolution Ion Mobility (HRIM) Strategies**; Kyle E Lira[1]; Jody C May[1]; John A McLean[1]; *[1]Vanderbilt University, Nashville, TN*

WP 359 **Isolating Reduced Mass Contributions in Isotopic Shifts with High-Resolution Cyclic Ion Mobility Separations**; Noah D Roberts[1]; Gabe Nagy[1]; *[1]University of Utah, Salt Lake City, UT*

WP 360 **Ion mobility separation mass spectrometry for rapid and reliable identification of gangliosides associated to metastatic lung adenocarcinoma**; Mirela Sarbu[1]; Raluca Ica[2]; Roxana Biricioiu[2,3]; Liana Dehelean[4]; David E. Clemmer[5]; Željka Vukelić[6]; Alina D. Zamfir[1,7]; *[1]National Inst for R&D in Electrochemistry and Condensed Matter, Timisoara, Romania; [2]National Inst for R&D in Electrochemistry and Condensed Matter, Timisoara, Romania; [3]West University of Timisoara, Timisoara, Romania; [4]University of Medicine and Pharmacy Victor Babes, Timisoara, Romania; [5]Department of Chemistry, The College of Arts & Science, Indiana University, Bloomington, IN; [6]Department of Chemistry and Biochemistry, Faculty of Medicine, University of Zagreb, Zagreb, Croatia; [7]Department of Technical and Natural Sciences, Aurel Vlaicu University of Arad, Arad, Romania*

WP 361 **Exploring Amino Acid-based Complexation Methods for Differentiating Drug Enantiomers using Ion Mobility-Mass Spectrometry**; Nina A Metzger[1]; Benjamin K Blakley[1]; Jody C May[1]; John A McLean[1]; *[1]Department of Chemistry, Center for Innovative Technology, Institute of Chemical Biology, Institute for Integrative Biosystems Research, and Education, Vanderbilt University, Nashville, TN*

WP 362 **Structural Characterization of Per- and Polyfluoroalkyl Substances (PFAS) using High Precision and High Resolving Power Ion Mobility-Mass Spectrometry**; Karly B Serrano[1]; Benjamin K Blakley[1]; David C. Koomen[1]; Jody C May[1]; John A McLean[1]; *[1]Department of Chemistry; Center for Innovative Technology; Institute of Chemical Biology; Institute for Integrative Biosystems Research and Education; Vanderbilt-Ingram Cancer Center; Vanderbilt University, Nashville, TN*

WP 363 **Chemical Metabolomics - Advanced chemoselective probe-based mass spectrometric investigation of the human carbonyl-metabolome**; Alejandro Torregrosa Chinillach[1]; Weifeng Lin[1]; Maria Theodorou[1]; Wawrzyniec Haberek[1]; Nikolas Kessler[2]; Sofie Weinkouff[2]; Aiko Barsch[2]; Cristian De Gobba[2]; Matthew R. Lewis[2]; Daniel Globisch[1]; *[1]Uppsala University, Uppsala, Sweden; [2]Bruker Daltonics GmbH & Co.KG, Bremen, Germany*

WP 364 **Collision Induced Unfolding (CIU) of Native–like Proteins on a Structures for Lossless Ion Manipulations (SLIM) High Resolution Ion Mobility Instrument**; Walker N Hodges[1,2]; Jody C May[1]; Christopher Chouinard[2]; John A McLean[1]; *[1]Vanderbilt University, Nashville, TN; [2]Clemson University, Clemson, SC*

WP 365 **Tandem Ion Mobility Scanning Modes Implemented on a Cyclic Ion Mobility-Mass Spectrometer Improves Proteoform Sequence Coverage for Native Top-Down Proteomics**; Ryan K Schroeder[1]; Devin Makey[1]; Carolina Rojas Ramirez[2]; Brandon T. Ruotolo[1]; *[1]Department of Chemistry, University of Michigan, Ann Arbor, MI; [2]Department of Pathology, University of Michigan, Ann Arbor, MI*

WP 366 **Ganglioside biomarker discovery and characterization in human epilepsy by ion mobility tandem mass spectrometry**; Maria R Biricioiu[1,2]; Mirela Sarbu[1]; Raluca Ica[1]; David E. Clemmer[3]; Kristina Mlinac-Jerković[4]; Svjetlana Kalanj-Bognar[4]; Alina D. Zamfir[1,5]; *[1]National Institute for Research and Development in Electrochemistry and Condensed Matter, Timisoara, Romania; [2]West University of Timisoara, Timisoara, Romania; [3]Department of Chemistry, The College of Arts & Science, Indiana University, Bloomington, IN; [4]University of Zagreb, School of Medicine, Croatian Institute for Brain Research, Zagreb, Croatia; [5]Department of Technical and Natural Sciences, "Aurel Vlaicu" University of Arad, Arad, Romania*

WP 367 **Probing Configurational Complexity: Separation of Dimeric Diastereomers of Arylomycin derived Antibiotic Using SLIM-Ion Mobility Mass Spectrometry**; Meenakshi Goel[1]; Christopher M. Crittenden[1]; *[1]Genentech Inc., South San Francisco, CA*

WP 368 **Optimization of Ion Focusing Optics in IMS detectors**; Andrew Michael Jones[1]; Zakari Echo[1]; Phillip Rocco Miller[1]; Joshua Jonathan Whiting[1]; [1]*Sandia National Laboratories, Albuquerque, NM*

WP 369 **Characterization of bio-oils derived from biomass pyrolysis using trapped ion mobility spectrometry hyphenated with 18 T FTICR mass spectrometry**; Theo Imhoff[1, 2, 3]; Julien Maillard[2, 3]; Caroline Barrère-Mangotte[2, 3]; Mélanie Mignot[1, 3]; Christopher A Wootton[4]; Pierre Giusti[2, 3]; Carlos Afonso[1, 3]; [1]*University of Rouen-Normandy, Mont Saint Aignan, France;* [2]*TotalEnergies Research and Technology Gonfreville, Harfleur, France;* [3]*International Joint Laboratory, iC2MC: Complex Matrices Molecular Characterization, Harfleur, France;* [4]*Bruker Daltonics GmbH & Co.KG, Bremen, Germany*

WP 370 **Rapid Analysis of Acylcarnitines in Dried Blood Spots Using Fast Chromatography with Ion Mobility High Resolution Mass Spectrometry**; Sheher Mohsin[1]; Julie Cichelli[2]; Tracy Blethen[3]; [1]*Agilent Technologies, Wood Dale, IL;* [2]*Agilent Technologies, Wilmington, DE;* [3]*Agilent Technologies, Inc., Wood Dale, Il*

WP 371 **Rapid analysis of biological samples using fast LC-HRIM-QTOFMS with a flexible sample delivery system**; Sabrina M. Cramer[1]; Viktoria Kowarz[2]; Sarah M. Stow[3]; Ruwan Kurulugama[3]; Kelly Wormwood Moser[4]; Diethard Mattanovich[2]; Stephan Hann[1]; Tim Causon[1]; [1]*BOKU University, Department of Natural Sciences and Sustainable Resources, Institute of Analytical Chemistry, Muthgasse 18, 1190, Austria;* [2]*BOKU University, Department of Biotechnology and Food Science, Institute of Microbiology and Microbial Biotechnology, Muthgasse 18, 1190, Austria;* [3]*Agilent Technologies, Inc., Santa Clara, CA;* [4]*MOBILion Systems, Inc, Chadds Ford, PA*

WP 372 **Comprehensive Characterization of Steroidal Compounds using Ion Mobility-Mass Spectrometry**; Cole L Frank[1]; Breland Jones[1]; Makenna Hoover[1]; Emmaleigh Efird[1]; Selena Kingsley[2]; Christopher Chouinard[1]; [1]*Clemson University, Clemson, SC;* [2]*Lake Superior State University, Sault Ste. Marie, MI*

WP 373 **Multiplatform mass spectrometry imaging analysis of aging endocrine system**; Stanislav Rubakhin[1]; Jonathan V Sweedler[2]; [1]*Beckman Institute, UIUC, Urbana, IL;* [2]*Department of Chemistry and Beckman Institute, University of Illinois at Urbana-Champaign, Urbana, IL*

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WP 374 **Recent advancements in MARS for computer driven-analysis in stable isotope labeling studies in untargeted metabolomics**; Stefano Bonciarelli[1]; Paolo Tiberi[2]; Ismael Zamora[1]; Marta Piroddi[3]; Giovanna Ilaria Passeri[2]; Gabriele Cruciani[4]; Laura Goracci[4]; [1]*Mass Spec Analytica, Sant Cugat del Vallés, Spain;* [2]*Molecular Discovery Ltd, Borehamwood, United Kingdom;* [3]*c Molecular Horizon Srl, Bettona, Italy;* [4]*University of Perugia, Perugia, Italy*

WP 375 **AI enabled quantitation of 13C-containing cell metabolites and media components as input for metabolic flux analysis for improvements in biomanufacturing**; Jack Howland[1]; Philip Michaels[1]; Ana S. H. Costa[1]; Devesh Shah[1]; Mel Hernandez[1]; Jennifer M Campbell[1]; Sam Yenne[2]; Daniel Benjamin[2]; Eric Cumming[2]; [1]*Matterworks, Somerville, MA;* [2]*Metalytics, Cary, NC*

WP 376 **Investigating Cellular Metabolism on a modified Orbitrap Hybrid Mass Spectrometer by the simultaneous use of differently labeled elemental isotope substrates**; Ayush Midha[1]; Thomas Moehring[2]; Bashar Amer[3]; Claire Dauly[2]; Isha Jain[1]; Susan Bird[3]; Rahul Ravi Deshpande[3]; [1]*Gladstone Institute, UCSF, San Francisco, California;* [2]*Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany;* [3]*Thermo Fisher Scientific, San Jose, California*

LC/MS: SAMPLE PREPARATION I
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WP 377 **Optimizing Lipidomics Extraction and Reconstitution Methods for Comprehensive Lipid Profiling in Mouse Brain Tissue**; Rencheng Wang[1]; Minsoo Son[1]; Jaenyeon Kim[1]; Young Ah Goo[1]; [1]*Washington University School of Medicine, St. Louis, MO*

WP 378 **Automated high-throughput extraction of Per- and polyfluoroalkyl substances (PFAS) in human breastmilk**; Aryan D. Patel[1]; Catherine E. Mullins[1]; Douglas I. Walker[1]; [1]*Emory University, Atlanta, GA*

WP 379 **Innovation Development of Multidimensional Holographic Analysis Technology of the ten Mycotoxin in Pu'er tea sample of multi-mycotoxin analysis**; Shan-An Chan[1]; Yang Song[2]; Hui Zhao[3]; Limian Zhao[3]; [1]*Agilent Technologies, Inc., Taipei, Taiwan;* [2]*Agilent Technologies, Inc., Shanghai, China;* [3]*Agilent Technologies, Inc., Philadelphia, PA*

WP 380 **Comparative Evaluation of Organic Solvent- and Antibody-Based Methods for Plasma Protein Depletion**; Shruti Kale[1]; Philp To[1]; Sophia Chung[1]; Sonja Hess[1]; [1]*AstraZeneca Pharmaceuticals LP, Gaithersburg, MD*

WP 381 **Strategy for Addressing Specificity Challenges in the Quantitation of Etonogestrel in Human Plasma by LC-MS/MS**; Benjamin Charron[1]; Milton Furtado[1]; Kevork Mekhssian[1]; [1]*Altasciences, Laval, QC*

WP 382 **Interlaboratory Comparision for Per- and Polyfluorinated Alkyl Substances (PFAS) Results of multiple XAD-2, Polystyrene/Divinylbenzene, Resin Lots**; Joshua J Fera[1]; Olga Shimelis[1]; Hugh Cramer[1]; M. James Ross[1]; [1]*Millipore Sigma, Bellefonte, PA*

WP 383 **Fully automated implementation of EPA Method 1633 for LC-MS/MS analysis of PFAS in environmental samples using a customized robotic autosampler**; Marzieh Shojaei[1]; Jonathan Beck[2]; Oliver Wyss[2]; Thomi Preiswerk[2]; Tiantian Li[2]; Charles E. Maxey[3]; Cynthia M. Grim[3]; Ed George[3]; Patrick Lee Ferguson[1]; [1]*Duke University, Durham, NC;* [2]*CTC Analytics AG, Zwingen, Switzerland;* [3]*Thermo Fisher Scientific, San Jose, CA*

WP 384 **A simplified approach to optimizing the Oasis™ PRiME HLB 2 step protocol to maximize recoveries for bioanalytical/biomarker quantification**; Nikunj Tanna[1]; Chelsea Plummer[1]; [1]*Waters Corporation, Milford, MA*

WP 385 **Sample Matrix Cleanup using Protein and Phospholipid Depletion Technique (PLD) for Drugs of Abuse LC-MS/MS Analysis in Whole Blood**; Sohel Rana[1]; Kyle D. Dukes[1]; Esraa AboJasser[1]; Yuan Li[1]; Lee Williams[1]; Farah Mavandadi[1]; [1]*Biotage LLC, Charlotte, NC*

WP 386 **Proteonano(TM): a novel deep proteomics platform with picogram sensitivity and its application in gastric cancer**; Yi Wang[1]; Xiehua Ouyang[2]; Jiawei Pang[2]; Yonghao Zhang[2]; Hao Wu[2]; Wenqing Li[3]; [1]*Nanomics Biotechnology, Hangzhou, China;* [2]*Nanomics Biotechnology, Hangzhou, China;* [3]*Peking University Cancer Hospital & Institute, Beijing, China*

WP 387 **Automated Liquid-Liquid Extraction and Determination of Xylazine and Medetomidine in Plasma and Urine Samples using a Robotic Autosampler and LC-MS/MS**; Fred Foster[1]; Megan Harper-Kerr[1]; [1]*Gerstel, Inc., Linthicum, MD*

WP 388 **Automated workflow for protein digestion, tandem mass tag labeling and clean-up for multiplex LC-MS analysis**; Boren Lin[1]; Kinnari Watson[1]; [1]*Opentrons Labworks, Queens, NY*

WP 389 **Optimizing Sample Preparation for Cell Culture-Based Secretome Studies**; Jiawei Ni[1]; Ling Hao[1]; [1]*University of Maryland, College Park, MD*

WP 390 **Development and Optimization of SPE-UPLC-MS/MS Method for Trace-Level Detection of PFAS in Environmental Samples**; Deepak Timalsina[1]; Bhargavi Srija Ramisetty[2]; Brian E. Haggard[3]; Bradley J Austin[3]; Michael Zhuo Wang[2]; [1]*Department of Chemistry, University of Kansas, Lawrence, KS;* [2]*Department of Pharmaceutical Chemistry, University of Kansas, Lawrence, KS;* [3]*University of Arkansas, Fayetteville, AR*

WP 391 **Automating BSA Depletion and Peptide Desalting in LC/MS Workflows to Ensure Compatibility with Stem**

Cell and Conditioned Media Analysis; Trinh Ton[1]; Andrew Wasylyna[1]; [1]*Advanced Regenerative Manufacturing Institute (ARMI), Manchester, NH*

WP 392 **Depletion of Abundant Plasma Proteins by MOF-Based Technology for Integrated Proteomics**; Emily A. Reasoner[1]; Hsin-Ju Chan[1]; Timothy J. Aballo[1]; Kylie J. Plouff[1]; Seungwoo Noh[1]; Song Jin[1]; Ying Ge[1]; [1]*University of Wisconsin-Madison, Madison, WI*

WP 393 **Comparison of Sample Preparation Strategies for Enhanced Exosomal Surface Proteome Profiling Using S-Trap and In-Gel Digestion**; Su-Min Lee[1]; Geul Bang[1]; Jin Young Kim[1, 2]; [1]*Korea Basic Science Institute, Cheongju, South Korea;* [2]*Korea Research Institute of Bioscience and Biotechnology, Daejeon, South Korea*

WP 394 **Novel Recombinant Chymotrypsin: A Superior Complementary Protease to Trypsin for Proteomics and Crosslinking MS, Enhancing Specificity and Minimizing Missed Cleavages**; Jonathan E. Ditcham[1]; Alba Katiria González Rivera[2]; Ricardo Zenezini Chiozzi[1]; Kish Adoni[1]; Georgina H Charlton[1]; Sergei Saveliev[2]; Konstantinos Thalassinos[1]; [1]*University College London, London, United Kingdom;* [2]*Promega Corporation, Madison, WI*

WP 395 **Enhancing plasma proteome profiling through cost-effective, robust and high-throughput workflows based on hyper-porous magnetic beads**; Amy Van Graan[1]; Ireshyn S Govender[2]; Christine Wu[3]; Michael J. MacCoss[3]; Isak Gerber[1]; Justin Jordaan[1]; Previn Naicker[1]; [1]*ReSyn Biosciences, Pretoria, South Africa;* [2]*Council for scientific and industrial research, Pretoria, South Africa;* [3]*University of Washington, Seattle, WA*

WP 396 **Streamlined Analysis of Polar and Non-Polar Metabolites in Plasma Using Automated Micro-SPE LC-MS**; Laura Gisela González Iglesias[1]; Hagen M. Gegner[2]; Renzo Picenoni[2]; Guenter Boehm[2]; Gerard Hopfgartner[1]; [1]*University of Geneva, LSMS, Geneva, Switzerland;* [2]*CTC Analytics AG, Zwingen, Switzerland*

WP 397 **AUTO-SP: automated sample preparation for analyzing proteins and protein modifications**; Tung-Shing M Lih[1]; Liyuan Jiao[1]; Lijun Chen[1]; Jongmin Woo[1]; Yuefan Wang[1]; Hui Zhang[1]; [1]*Department of Pathology, Johns Hopkins University School of Medicine, Baltimore, MD*

WP 398 **A novel filter-assisted protein precipitation (FAPP) based sample pre-treatment method for LC-MS peptide mapping for biosimilar characterization**; Kritika Upadhaya; *IIT Delhi, Delhi, India*

WP 399 **Unleashing Krakatoa: Assessing a Novel Alternative Enzyme for MS-Based Proteomics**; Elizabeth M Brown[1]; Erik Nash[1]; Jennifer Roof[1]; Michael Krawitzky[2]; Hossein Fazelinia[1, 3]; Lynn A Spruce[1]; [1]*Proteomics Core Facility, Children's Hospital of Philadelphia, Philadelphia, PA;* [2]*Bruker Scientific LLC, Billerica, MA;* [3]*Department of Biomedical and Health Informatics, Children's Hospital of Philadelphia, Philadelphia, PA*

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WP 400 **C=C Bonds Positional Determination of Unsaturated Fatty Acids Using Potassium Permanganate Oxidation in Combination with Tandem Mass Spectrometry**; DANNA HU; *The Chinese University of Hong Kong, HONG KONG, Hong Kong*

WP 401 **Aziridination-assisted bifunctional tagging strategy for lipid characterization and quantification**; Erin Hirtzel[1]; Ramidi Gopal Reddy[1]; Xin Yan[1]; [1]*Texas A&M University, College Station, TX*

WP 402 **Simultaneously Determine Positional and Geometric Isomerism of Lipid C=C Bonds via Peracetic Acid-induced Chemical Derivatization and Cyclic Ion Mobility-Mass Spectrometry**; Jiahao Zhang[1, 2]; Hua Zhang[2]; Lingjun Li[1, 2]; [1]*Biophysics Graduate Program, University of Wisconsin-Madison, Madison, WI;* [2]*University of Wisconsin-Madison School of Pharmacy, Madison, WI*

WP 403 **Radical-directed dissociation of cuprate lipid ion types**; Zunaira Naeem[1]; Tingting Yan[2]; Yingchan Guo[1]; Julia R. Bonney[1]; Boone M. Prentice[1]; [1]*University of Florida, Gainesville, FL;* [2]*University of Florida, Gainesville, Florida*

WP 404 **Characterization and relative quantification of phosphatidylglycerol at the sn-isomer level via manganese adduction**; Sara Amer[1]; Haven Wilson[2]; Julia Laskin[2]; [1]*Purdue University, West Lafayette, IN;* [2]*Purdue Univeristy, West Lafayette, IN*

WP 405 **Benefits of Field Asymmetric Ion Mobility Spectrometry (FAIMS) and Kendrick Mass Defect Plots in Lipid A analysis**; Trevena N Youssef[1]; Travis D Fridgen[1]; Abanoub Mikhael[2, 3]; David R. Goodlett[2, 3]; Joseph Banoub[1, 4]; [1]*Memorial University, St. John's, NL;* [2]*University of Victoria, Victoria, BC;* [3]*University of Victoria GBC Proteomics Centre, Victoria, BC, BC;* [4]*Fisheries and Oceans Canada, St John's, NL*

WP 406 **Characterisation of triacylglycerols in milk at the double bond positional level using oxygen attachment dissociation (OAD)**; Emily G. Armitage[1]; Alan Barnes[1]; Stéphane Moreau[2]; Georgios Theodoridis[3]; Neil J. Loftus[1]; [1]*Shimadzu Corporation, Manchester, United Kingdom;* [2]*Shimadzu Europe GmbH, Duisburg, Germany;* [3]*Department of Chemistry, Aristotle University of Thessaloniki, Thessaloniki, Greece*

WP 407 **Electron Induced Dissociation of Lysophospholipids show lipid backbone specific fragment ions**; Mark J. Raftery; *Bioanalytical Mass Spectrometry, Sydney, Australia*

WP 408 **Intergrated Structrual Lipidomics Tool for Glycerophospholipids, Glycerides, and Fatty Acids Analysis**; Junhan Wu[1]; Yikun Liu[1]; Zhourui Zhang[1]; Hongzheng Zhou[1]; Shudi Guo[1]; Wenhui Pang[1]; Jiexun Bu[2]; Qiaohong Lin[3]; Wenpeng Zhang[3]; Zheng Ouyang[3]; [1]*PURSPEC Technology (China) Ltd., Suzhou, China;* [2]*PURSPEC Technology (Beijing) Ltd., Beijing, China;* [3]*Tsinghua University, Beijing, China*

WP 409 **Elevating lipid identification confidence in MS imaging using mzmine – combining on-tissue MS2 and CCS**; Lucy A. Woods[1]; Ansgar Korf[1]; Steffen Heuckeroth[1]; Robin Schmid[1]; Tomáš Pluskal[2]; Uwe Karst[3]; Heiko Hayen[3]; [1]*mzio GmbH, Bremen, Germany;* [2]*Institute of Organic Chemistry and Biochemistry of the Czech Academy of Science, Prague, Czech Republic;* [3]*Institute of Inorganic and Analytical Chemistry, University of Muenster, Muenster, Germany*

WP 410 **Determination of Fatty Acid Double Bond Position via Peracetic Acid Derivatization and Desorption Electrospray Ionization (DESI)**; Cameron J Kaminsky[1]; Hua Zhang[2]; Ally Ott[3]; Lingjun Li[2, 4]; [1]*University of Wisconsin Madison, Madison, WI;* [2]*School of Pharmacy, University of Wisconsin-Madison, Madison, WI;* [3]*Department of Chemical & Biological Engineering, University of Wisconsin-Madison, Madison, WI;* [4]*Department of Chemistry, University of Wisconsin–Madison, Madison, WI*

WP 411 **Lipid characterization in negative ion mode with ultra-violet photo-dissociation (UVPD)**; Mircea Guna[1]; Eva Duchoslav[1]; Yves Le Blanc[2]; [1]*SCIEX, Concord, ontario;* [2]*SCIEX, Concord, On, ON*

WP 412 **Phospholipid Characterization via Free Radical Directed Dissociation**; CJ Szafranski[1]; Tabia Tahsin[1]; Jinshan Gao[1]; [1]*Montclair State University, Montclair, NJ*

WP 413 **Automated Lipid A Structural Identification using Referenced Kendrick Mass Defect (RKMD) Analysis**; Abanoub Mikhael[1, 2]; Gillian Leach[2]; Linda Nartey[2]; Ian O'Keefe[3, 4]; Hyojik Yang[4]; Helena Petrosova[5]; Robert K. Ernst[4]; David R Goodlett[2, 5]; [1]*UVic Genome BC Proteomics Centre, Victoria, BC;* [2]*Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC;* [3]*Department of Biochemistry and Molecular Biology, University of Maryland – Baltimore, Baltimore, MD, USA, 21201, Baltimore, MD;* [4]*Department of Microbial Pathogenesis, University of Maryland School of Dentistry, Baltimore, Maryland;* [5]*University of Victoria GBC Proteomics Centre, Victoria, BC, BC*

WP 414 **Singular features of lipidome of Acinetobacter baumannii antibiotics persister cells by HPLC-MS/MS**

and MALDI-FTICR MS; Delphine Vergoz[1, 2]; Annick Schaumann[1]; Isabelle Schmitz[1, 2]; Carlos Afonso[3]; Emanuelle Dé[1]; Corinne Loutelier-Bourhis[2]; Stéphane Alexandre[1]; *[1]PBS, UMR 6270, University of Rouen, Mont Saint Aignan, France; [2]CARMeN, UMR 6064, University of Rouen, Mont Saint Aignan, France; [3]University of Rouen-Normandy, Mont Saint Aignan, France*

WP 415 **Development and evaluation of a high throughput and in-depth lipidomics platform using SLIM-based high resolution ion mobility spectrometry**; Xueyun Zheng[1]; Dylan H. Ross[1]; Josie G. Eder[1]; Meagan C Burnet[1]; Nubia Nieto-Pereira[1]; Kent J. Bloodsworth[1]; Jennifer E. Kyle[1]; Rachel A. Harris[2]; Daniel DeBord[2]; Ruwan Kurulugama[3]; Bryan Miller[3]; Richard D. Smith[1]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]Mobilion Systems Inc., Chadds Ford, PA; [3]Agilent Technologies, Santa Clara, CA*

WP 416 **Zero-lengthcross-linking mass spectrometry for mapping polyionic interactions between the disordered acidic tail of GPIHBP1 and LPL**; Samina Arshid[1]; Anamika Biswas[2]; Kristian Kølby Kristensen[2]; Michael Ploug[2]; Thomas J. D. Jørgensen[1]; *[1]Department of Biochemistry and Molecular Biology, University of Southern Denmark, DK–5230, Odense M, Denmark; [2]Finsen Laboratory, Copenhagen University Hospital – Rigshospitalet, Copenhagen, Denmark*

WP 417 **Isomeric discrimination by collision-/ozone-induced dissociation reveals the lipid complexity sn-onymous with triacylglycerols**; Puttandon (Arm) Wongsomboon[1]; Samuel C. Brydon[1]; David L. Marshall[1]; Berwyck L.J. Poad[1]; Stephen J Blanksby[1]; *[1]Queensland University of Technology, Brisbane, Australia*

WP 418 **Differentiation of branched-chain fatty acid isomers via charge switching derivatization**; Hannah G. Castellan[1]; Ariana E. Stratton[1]; Boone M. Prentice[1]; *[1]Department of Chemistry, University of Florida, Gainesville, FL*

WP 419 **Lipid Incorporation of 2-Fluoropalmitic Acid by CEACAM1-/- HepG2 Hepatoma Cells**; Daniel Röth[1]; Weidong Hu[1]; Patty Wong[1]; John E. Shively[1]; Markus Kalkum[1]; *[1]City of Hope, Duarte, CA*

WP 420 **Monolithic columns for improved 4D-Lipidomics analysis**; Xuejun Peng[1]; Beixi Wang[1]; Michael Krawitzky[1]; Ryo Nakabayashi[2]; Erica Marie Forsberg[1]; *[1]Bruker Scientific LLC, San Jose, California; [2]Bruker Japan, Yokohama, Japan*

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WP 421 **Development of Targeted Metabolomics to Quantify Twenty-Six Epigenetically-Relevant Metabolites in Cell Nuclei and Cytosol**; David Hidalgo Delgado[1]; Cayla Boycott[2]; Barbara Stefanska[2]; Tao Huan[1]; *[1]Department of Chemistry, University of British Columbia, Vancouver, BC; [2]Faculty of Land and Food Systems, University of British Columbia, Vancouver, BC*

WP 422 **S'Wipe: A Mass Spectrometry- Compatible Collection for High-Throughput Gut Metabolomics**; Dana Moradi[1]; Ali Lotfi[1]; Alexey V. Melnik[2, 3, 4]; Konstantin Pobozhev[2]; Hannah Monahan[2]; Evguenia Kopylova[2, 5]; Yanjiao Zhou[6]; Alexander A. Aksenov[2, 3, 4]; *[1]Department of Chemistry, University of Connecticut, Storrs, Connecticut; [2]Arome Science Inc., Farmington, Connecticut; [3]BileOmix Inc., Farmington, Connecticut; [4]Department of Chemistry, University of Connecticut, Storrs, CT; [5]Clarity Genomics Inc., San Diego, California; [6]UConn Health, Farmington, Connecticut*

WP 423 **Urinary Metabolomics for Disease Differentiation of Multiple Urological Conditions and Identification of Stable Metabolites by Chemical Isotope Labeling and LC-MS**; Yi-Ting Chen[1]; Wei-Hsuan Wang[1]; Ya-Ju Hsieh[1]; Chien-Lun Chen[2]; Liang Li[3]; Jau-Song Yu[1]; *[1]Chang Gung University, Taoyuan, Taiwan; [2]Chang Gung Memorial Hospital, Taoyuan, Taiwan; [3]University ogf Alberta, Edmonton, AB*

WP 424 **Untargeted Metabolomics Reveals Altered Metabolism in Fibrotic Livers from Fontan Associated Liver Disease Patients**; Chris Petucci[1]; Clarissa Shoffler[1]; Dina Abbasian[1]; Rasheed Sule[2]; Liming Pei[3]; *[1]Cardiovascular Institute, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA; [2]Children's Hospital of Philadelphia, Philadelphia, Pennsylvania, United States, Philadelphia, PA; [3]Department of Pathology and Laboratory Medicine, Children’s Hospital of Philadelphia, and University of Pennsylvania, Philadelphia, Philadelphia, PA*

WP 425 **Integrative Tissue and Urine Metabolomics of Amine- and Phenol-Based Metabolites in Renal Cell Carcinoma**; Hsiang-Cheng Tu[1]; Yi-Ting Chen[1]; Chien-Lun Chen[2]; Ying-Hsu Chang[2]; *[1]Chang Gung University, Taoyuan, Taiwan; [2]Chang Gung Memorial Hospital, Taoyuan, Taiwan*

WP 426 **Universal, Untargeted Detection of Bacteria in Tissues Using Metabolomics Workflows**; Wei Chen[1]; Min Qiu[2]; Petra Paizs[3]; Miriam Sadowski[4]; Toma Ramonaite[3]; Lieby Zborovsky[2]; Raquel Mejias-Luque[5]; Klaus Peter Janßen[6]; James Kinross[7]; Robert D. Goldin[3]; Monica Rebec[8]; Manuel Liebeke[4, 9]; Zoltan Takats[3, 10]; James Mckenzie[3]; Nicole Strittmatter[2]; *[1]Department of Bioscience, School of Natural Sciences, Technical University of Munich, Munich, Germany; [2]Department of Bioscience, School of Natural Sciences, Technical University of Munich, Munich, Germany; [3]Department of Metabolism, Digestion and Reproduction, Imperial College London, London, United Kingdom; [4]Department of Symbiosis, Max Planck Institute for Marine Microbiology, Bremen, Germany; [5]Institute for Medical Microbiology, Immunology and Hygiene, School of Medicine and Health, Technical University of Munich, Munich, Germany; [6]Department of Surgery, School of Medicine and Health, Technical University of Munich, Munich, Germany; [7]Department of Surgery and Cancer, Imperial College London, London, United Kingdom; [8]North West London Pathology, Imperial College Healthcare NHS Trust, London, United Kingdom; [9]Department for Metabolomics, Institute for Human Nutrition and Food Science, University of Kiel, Kiel, Germany; [10]Department of Immunomedicine, University of Regensburg, Regensburg, Germany*

WP 427 **Alteration of Metabolic Profile in Patients with Narcolepsy Type 1 (NT1)**; Md Abdul Hakim[1]; Waziha Purba[1]; Akeem Sanni[1]; Md Mostofa Al Amin Bhuiyan[1]; Farid Talih[2]; Bartolo Lanuzza[3]; Firas Kobeissy[4, 5]; Giuseppe Plazzi[6, 7]; Fabio Pizza[6, 8]; Raffaele Ferri[3]; Yehia Mechref[1]; *[1]Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX; [2]Department of Psychiatry, Faculty of Medicine, American University of Beirut, Beirut, Lebanon; [3]Sleep Research Centre, Department of Neurology IC, Oasi Research Institute-IRCCS, Troina, Italy; [4]Department of Biochemistry and Molecular Genetics, Faculty of Medicine, American University of Beirut, Beirut, Lebanon; [5]Department of Neurobiology, Center for Neurotrauma, Multiomics and Biomarkers, Neuroscience Institute, Morehouse School of Medicine (MSM), Atlanta, GA; [6]IRCCS, Instituto delle Scienze Neurologiche di Bologna, Bologna, Italy; [7]Department of Biomedical, Metabolic and Neural Sciences, University of Modena and Reggio Emilia, Modena, Italy; [8]Department of Biomedical and Neuromotor Sciences (DIBINEM), Alma Mater Studiorum, University of Bologna, Bologna, Italy*

WP 428 **Determining Novel Biomarker Candidates Associated With Cocaine Exposure Using Urine Metabolomics**; Kenichi Tamama[1]; Simmi Patel[1]; Reya Kundu[2]; Rachel K Vanderschelden[1]; *[1]Department of Pathology, University of Pittsburgh School of Medicine, Pittsburgh, PA; [2]University of Pittsburgh, Pittsburgh, PA*

WP 429 **Metabolomic Alterations in the Hippocampus of Organophosphate-Exposed Rats: Effects of Arachidonic Acid and Prediabetes Using LC-MS/MS**; Waziha Tasnim Purba[1]; Rowan E. Arida[2]; Md Mostofa Al Amin Bhuiyan[1]; Oluwatosin Daramola[1]; Judith Nwaiwu[1]; Mojibola Fowowe[1]; Favour M Chukwubueze[1]; Ahmed El-Yazbi[2]; Yehia Mechref[1]; *[1]Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, Texas; [2]Department of Pharmacology* *and Therapeutics, Faculty of Pharmacy, Alamein International University, Alamein, Egypt*

WP 430 **Metabolomic Insights into UCP1-Mediated Thermogenesis, Inflammation, and Cognitive Impairment in Prediabetic Rats Using LC-MS/MS**; Md Mostofa Al Amin Bhuiyan[1]; Alaa Y. Soliman[2]; Waziha Purba[1]; Mojibola Fowowe[1]; Oluwatosin Daramola[1]; Judith Nwaiwu[1]; Ahmed El-Yazbi[2]; Yehia Mechref[1]; *[1]Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, Texas; [2]Department of Pharmacology and Therapeutics, Faculty of Pharmacy, Alamein International University, Alamein, Egypt*

WP 431 **Determination of Urinary Organic Acid for Rare Inherited Metabolic Disease Patient Using Solid Phase Extraction and Gas Chromatography-Mass Spectrometry**; Yung-Cheng Jair[1]; Ni-Chung Lee[2]; Yi-Hsin Liu[3]; Pai-Shan Chen[1]; *[1]Institute of Toxicology, School of Medicine, National Taiwan University, Zhongzheng District, Taiwan; [2]Department of Medical Genetics, National Taiwan University Hospital, Zhongzheng District, Taiwan; [3]Department of Chemistry, National Taiwan Normal University, Wenshan District, Taiwan*

WP 432 **Rapid low-cost metabolomics testing of urine**; Ali Lotfi[1]; Alexey V Melnik[2]; Olusola Onawoga[2]; Silverio Iacono[2]; Briana M. Nosal[1]; Staci N. Thornton[1]; Manije Darooghegi Mofrad[1]; Elaine Choung-Hee Lee[1]; Ock K. Chun[1]; Alexander A. Aksenov[1]; *[1]University of Connecticut, Storrs; [2]Arome Science Inc., , CT, Farmington, CT*

WP 433 **Overcoming Clinical Metabolomics Barriers with Remote Sampling and Microchip CE-MS**; Cara L Sake[1]; Kruttika Dabke[1]; Jiajun Lei[1]; Ethan Canfield[1]; J. Will Thompson[2]; Jonathan E Katz[1, 3]; *[1]Ellison Medical Institute, Los Angeles, CA; [2]908 Devices Inc., Boston, MA; [3]USC, Los Angeles, CA*

WP 434 **Democratizing Metabolomic Studies: Remote Blood Sampling for Compound Kinetics with Pre-analytical Normalization Strategies and Sampling Site Insights**; Jiajun Lei[1]; Jonathan E Katz[1, 2]; *[1]Ellison Medical Institute, Los Angeles, CA; [2]USC, Los Angeles, CA*

WP 435 **Metabolomic Insights into the Protective Effects of Blue Agave Fructans in Atopic Dermatitis Using LC-MS/MS**; Tuli Bhattacharjee[1]; Cristian D. Gutierrez Reyes[1]; Oluwatosin Daramola[1]; Esther Oji[1]; Eva Salinas[2]; Marcela Rios-Carlos[2]; Laura E. Córdova-Dávalos[2]; Odunayo Oluokun[1]; Abiodun Adewolu[1]; Yehia Mechref[1]; *[1]Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, Texas; [2]Department of Microbiology, Universidad Autónoma de Aguascalientes, Aguascalientes, Mexico*

WP 436 **Metabolomic and Lipidomics profiling of meningioma by LC-MS/MS and machine learning with longitudinal serum analysis to facilitate biomarker discovery**; ANKIT HALDER[1]; Suhisna Dutta[2]; Sanjeeva Srivastava[2]; *[1]Indian Institute of Technology Bombay, Mumbai, India; [2]IIT Bombay, Mumbai, India*

WP 437 **Lipid Metabolomics Analysis of Fat Samples in Systemic Sclerosis Using Mass Spectrometry**; Sujun Li[1]; Haixu Tang[1]; *[1]Indiana University Bloomington, Bloomington, IN*

WP 438 **A Risk Stratification Model for GDM During Early Pregnancy Based on Metabolites and Clinical Indicators**; Ziqing Kong; *CALIBRA Scientific, Inc, Hangzhou, China*

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WP 439 **From MS2 Spectra to Molecular Structures: Unlocking Metabolomics Dark Matter with Machine Learning and Molecular Fingerprints**; Ahmad Mani-Varnosfaderani[1, 2]; Sree V. Chintapalli[1, 2]; Hailemariam Abrha Assress[1, 2]; Renny S. Lan[1, 2]; Brian D. Piccolo[1, 2]; Colin Kay[1, 2]; *[1]University of Arkansas for Medical Sciences, Little Rock, AR; [2]Arkansas Children's Nutrition Center, Little Rock, AR*

WP 440 **Metabolome Analysis of Juvenile Corals using a Comprehensive Two-Dimensional Gas Chromatography High-Resolution Time-of-Flight Mass Spectrometry**; Azusa Kubota[1]; Ayumi Kubo[1]; Masaaki Ubukata[1]; Nanami Mizusawa[2]; Ko Yasumoto[2]; *[1]JEOL Ltd., Akishima, Japan; [2]Kitasato University, Sagamihara, Japan*

WP 441 **Illuminating the Dark Matter of Metabolomics Through Molecular Community Networking**; Elizabeth A. Coler[1]; Alexey V. Melnik[1, 2, 3]; Ali Lotfi[1]; Dana Moradi[1]; Ben Ahiadu[3]; Paulo Wender Portal Gomes[4]; Abubaker Patan[5]; Pieter C. Dorrestein[5]; Stephen Barnes[6]; Vladimir Boginski[7]; Alexander Semenov[8]; Alexander A. Aksenov[1, 3, 9]; *[1]University of Connecticut, Storrs, CT; [2]Arome Science Inc., Farmington, CT; [3]BileOmix Inc., Farmington, Connecticut; [4]Universidade Federal do Para, Para, Brazil; [5]University of California San Diego, San Diego, CA; [6]University of Alabama at Birmingham, Birmingham, AL; [7]University of Central Flordia, Orlando, FL; [8]University of Florida, Gainesville, Florida; [9]Arome Science Inc., Farmington, Connecticut*

WP 442 **Investigating the Metabolic Fates of Palmitic and Linoleic Acid Revealed by Stable Isotope Labeling and Untargeted Metabolomics**; Verne T. Urquhart-Cox[1]; Nicholas S. Ly[1]; J. Rafael Montenegro-Burke[1]; *[1]University of Toronto, Toronto, ON*

WP 443 **Expanding the steroid metabolome via stable isotope tracing in 12 cell lines with stably expressed cytochrome P450 enzymes**; Shujian Zheng[1]; Joshua Mitchell[1]; Shuzhao Li[1]; *[1]The Jackson Laboratory for Genomic Medicine, Farmington, CT*

WP 444 **The Shin-MassBank project: Generation of high-quality product ion spectra from public metabolome datasets with FDR-controlled metabolite annotation**; Fumio Matsuda[1]; Ryosuke Hayasaka[2]; Taihei Torigoe[3]; Kozo Nishida[4]; Yushi Takahashi[5]; Masatomo Takahashi[3]; Takaki Oka[4]; Yuki Matsuzawa[4]; Takato Kiuchi[5]; Akiyasu C. Yoshizawa[5]; Yoshihiro Izumi[3]; Shujiro Okuda[5]; Hiroshi Tsugawa[4]; Akiyoshi Hirayama[2]; *[1]Osaka Univeristy, Suita, Japan; [2]Keio University, Tsuruoka, Japan; [3]Kyushu University, Fukuoka, Japan; [4]Tokyo University of Agriculture and Technology, Tokyo, Japan; [5]Niigata University, Niigata, Japan*

WP 445 **Mass Spectrometry-Driven Metabolomics of Pancreatic Disease: Decoding the Gut Microbiota's Metabolic Impact with Chemical Biology Tools**; Vladyslav Dovhalyuk[1]; Fan Yang[1]; Matthias Löhr[2]; Daniel Globisch[1, 2]; *[1]Uppsala University, Uppsala, Sweden; [2]Karolinska Institutet, Solna, Sweden*

WP 446 **Metabolomics Annotation Confidence Increases with Fragment Ion Mass Accuracy**; Corey D Broeckling[1]; Linxing Yao[2]; Nathan Montgomery[2]; David Heywood[3]; *[1]Colorado State University, Fort Collins, CO; [2]Colorado State University, ARC-BIO, Fort Collins, CO; [3]Waters Corporation, Wilmslow, United Kingdom*

WP 447 **Characterization of Uncommon Product Ions in a Tandem Mass Spectral Library**; Xiaoyu Yang[1]; Pedatsur Neta[1]; Dmitrii Tchekhovskoi[1]; Yuri Mirokhin[1]; Yuxue Liang[1]; Yi Liu[1]; Stephen E. Stein[1]; *[1]NIST, Gaithersburg, MD*

WP 448 **Characterization of Novel Conjugates from LC-MS/MS Data of Urine Samples**; Xinjian Yan; *National Institute of Standards and Technology, Gaithersburg, MD*

WP 449 **A Broad Range of Derivatizing Reagents for Targeting Carbonyl and Alcohol Compounds to Enhance Analytical Figures of Merit**; Jesbaniris Bas-Concepcion[1]; Christopher J Brown[2]; Jeffrey R Gilbert[2]; *[1]Corteva Agrisciences, Indianapolis, IN; [2]Corteva Agriscience, Indianapolis, IN*

WP 450 **The Remaining Discovery Potential of Untargeted Metabolomics**; Yasin El Abiead[1]; Adriano Rutz[2]; Simone Zuffa[1]; Bashar Amer[3]; Shipei Xing[1]; Corinna Brungs[4]; Robin Schmid[5]; Andres M Caraballo-Rodriguez[1]; Amir Zarrinpar[1]; Nicola Zamboni[2]; Pieter C. Dorrestein[1]; *[1]UCSD, San Diego, CA; [2]ETH Zurich, Zurich, Switzerland; [3]Thermo Fisher Scientific, San Jose, CA; [4]University of Vienna, Vienna, Austria; [5]mzio GmbH, Bremen, Germany*

WP 451 **Metabolite identification by spectral searching against predicted spectral library**; Chhavi Thakur[1]; Yuhui Hong[1];

Haixu Tang[1]; [1]*Luddy School of Informatics, Computing, and Engineering, Indiana University Bloomington, Bloomington, Indiana*

WP 452 **A workflow for the rigorous and automated identification of IROA peaks**; Michał Kaczmarek[1]; Bashar Amer[2]; Rahul R Deshpande[2]; Claire Dauly[1]; Susan S Bird[2]; Alexander Raskind[3]; Felice A de Jong[3]; Chris Beecher[3]; [1]*Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany;* [2]*ThermoFisher Scientific, San Jose, CA;* [3]*IROA Technologies LLC, Nellysford, VA*

WP 453 **Large scale combinatorial synthesis to create a MS/MS reference library for the discovery of disease associated molecules**; Abubaker Patan[1, 2]; Vincent Charron-Lamoureux[1, 2]; Shipei Xing[2, 3]; Zhewen Hu[3]; Victoria Deleray[2, 3]; Julius Agongo[2, 3]; Siegel Dionicio[3]; Pieter C. Dorrestein[2, 3]; [1]*Skaggs School Of Pharmacy And Pharmaceutical Sciences,, san diego, CA;* [2]*Collaborative Mass Spectrometry Innovation Center, University of California, San Diego, California;* [3]*Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, San Diego, CA*

WP 454 **Moving Beyond Basic ddMS2: Improving Annotation Confidence in Untargeted Metabolomics Using Higher Resolution MS and Parallel Ion Trap Experiments**; Brandon Bills[1]; Sunandini Yedla[2]; Rahul Deshpande[2]; Bashar Amer[2]; Ralf Tautenhahn[3]; Susan Bird[4]; Vlad Zabrouskov[2]; [1]*Thermo Fisher Scientific, San Jose, CA;* [2]*Thermo Fisher Scientific, San Jose, California;* [3]*ThermoFisher Scientific, San Jose, CA;* [4]*Thermo Fisher Scientific, Boston, MA*

WP 455 **Mass spectrometry-related tools expand the diversity of N-acyl lipids and their biological implications**; Helena Mannochio Russo[1]; Vincent Charron-Lamoureux[1]; Martijn Van Faassen[1, 2]; Santosh Lamichhane[1, 3]; Wilhan Nunes[1]; Victoria Deleray[1]; Abubaker Patan[1]; Pieter C. Dorrestein[1]; [1]*University of California San Diego, San Diego, CA;* [2]*University Medical Center Groningen, Department of Laboratory Medicine, Groningen, Netherlands;* [3]*University of Turku and Åbo Akademi University, Turku, Finland*

WP 456 **Mass spectral differentiation of the newly discovered acyl-homocarnitines from their isomers, acyl-carnitines**; Jaclyn Weinberg[1]; Ken H. Liu[1]; William J. Crandall[1]; Choon-Myung Lee[1]; Samuel A. Druzak[1]; André R. Cuevas[1]; Dean P. Jones[1]; [1]*Emory University, Atlanta, GA*

WP 457 **MZ2SMILES: Small Molecule Structure Prediction from MS/MS using Deep Learning Approaches**; Jiada Zhan[1]; William J Crandall[1]; Jaclyn Weinberg[1]; Dean P Jones[1]; [1]*Emory University, Atlanta, GA*

WP 458 **Enhancing untargeted metabolomics with a modified hybrid orbitrap and IROA Kit for improved metabolites annotation and normalization**; Michal Kaczmarek[1]; Bashar Amer[2]; Felice A. De Jong[3]; Chris Beecher[3]; Claire Dauly[1]; Christian Klass[1]; Allison Stewart[4]; Thomas Moehring[1]; Susan S Bird[4]; [1]*Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany;* [2]*Thermo Fisher Scientific, San Jose, CA;* [3]*IROA Technologies, LLC, Ann Arbor, Michigan;* [4]*ThermoFisher Scientific, San Jose, CA*

WP 459 **Automating Compound Integration for Efficient In-House Database Development using R**; Adam M Tisch[1]; Ewy A Mathé[1]; Djawed Bennouna[1]; [1]*NIH NCATS, Rockville, MD*

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WP 460 **Optimizing sample preparation method for urine untargeted metabolomics using UHPLC-HRMS**; Hailemariam Abrha Assress[1, 2]; Priyangi Malaviarachchi[2]; Rachael Wehrle[3]; Brittany Reed[3]; Aline Andres[2, 3]; Colin D. Kay[1, 2]; Renny S. Lan[1, 2]; [1]*Metabolomics Core, Arkansas Children’s Nutrition Center, Little Rock, AR;* [2]*University of Arkansas for Medical Sciences, Little Rock, AR;* [3]*Arkansas Children's Nutrition Center, Little Rock, AR*

WP 461 **Automating Sample Preparation for High-Throughput Metabolomic Profiling Using the MxP® Quant 500 kit and TriPlus RSH Autosample**; Gabriela Přibyl Dovrtělová[1]; Akrem Jbebli[1]; Markus Langsdorf[2]; Alice Limonciel[2]; Hagen M. Gegner[3]; Tiantian Li[3]; Thomi Preiswerk[3]; Elliott J. Price[1]; [1]*RECETOX, Masaryk University, Brno, Czech Republic;* [2]*biocrates life sciences ag, Innsbruck, Austria;* [3]*CTC Analytics AG, Zwingen, Switzerland*

WP 462 **A Standardized, Automated Workflow for Comprehensive Proteome Analysis of Large Plasma Sample Cohorts Using ENRICHplus Technology**; Measho H Abreha[1]; Kara West[2]; Zehan Hu[3]; Katrin Hartinger[3]; Ina Aretz[3]; Xaver Wurzenberger[3]; Godfred Boateng[3]; Fabian Wendt[4]; Nils Kulak[3]; [1]*PreOmics, Martinsried, Germany;* [2]*PreOmics, Billerica, MA;* [3]*PreOmics GmbH, Martinsried, Germany;* [4]*Tecan, Männedorf, Switzerland*

WP 463 **Combining background reduction and derivatization LC-MRM/MS for quantitation of dissolved free amino acids in natural water**; Jun Han[1, 2]; Jasmine Benoit[1]; Jason Bi[1]; Juncong Yang[1]; Madeleine Chan[1]; Dave Schibli[1, 2]; David R. Goodlett[1, 3]; [1]*Genome BC Proteomics Centre, University of Victoria, Victoria, BC;* [2]*Division of Medical Sciences, University of Victoria, Victoria, BC;* [3]*Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC*

WP 464 **Non-invasive Detection of Cancer Metastasis using Rapidly Freeze-Dried Droplet (RFDD) MALDI-MS and Machine Learning Analysis of Urine Metabolites**; I-Chung Lu[1]; Jeffrey Yungchuan Chao[2]; Jhih-Ling Jhang[1]; Hsin-Jung Lin[1]; [1]*Department of Chemistry, National Chung Hsing University, Taichung City, Taiwan;* [2]*Taichung Veterans General Hospital, Taichung City, Taiwan*

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WP 465 **Conformationally Selective Collision Induced Unfolding Studies of Amyloid β Peptides and their Toxic Oligomeric Complexes**; Rowan Matney[1]; Varun Gadkari[2]; [1]*University of Minnesota, Minneapolis, MN;* [2]*University of Minnesota, Minnneapolis, MN*

WP 466 **Developing a Custom SILAC Neuron Culture System to Measure Neuronal Protein Turnover**; Jamison Shih[1]; Ashley M. Frankenfield[1]; Jiawei Ni[1, 2]; Ling Hao[1, 2]; [1]*George Washington University, Washington, DC;* [2]*University of Maryland, College Park, MD*

WP 467 **Characterization of Alzheimer’s Disease biomarkers using High-Resolution Ion Mobility Mass Spectrometry**; Kimberly Youandi Kartowikromo[1]; Wael T Ismail[2]; Ahmed M Hamid[2]; [1]*Auburn University, Auburn, AL;* [2]*AUBURN UNIVERSITY, Auburn, AL*

WP 468 **Elucidating cellular and molecular features of white matter hyperintensities in Alzheimer’s disease by multimodal imaging and analysis**; Claire F Scott[1, 2]; Cody R Marshall[2, 3]; Lukasz G Migas[4]; Léonore E.M. Tideman[4]; Madeline E Colley[2, 5]; Katerina V Djambazova[1, 2]; Wilber Romero Fernandez[6]; Matthew S Schrag[6]; Raf Van De Plas[2, 4, 5]; Jeffrey M Spraggins[1, 2, 3, 5, 7, 8]; [1]*Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN;* [2]*Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN;* [3]*Chemical and Physical Biology Program, Vanderbilt University, Nashville, TN, United States 2. Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN;* [4]*Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands;* [5]*Department of Biochemistry, Vanderbilt University, Nashville, TN;* [6]*Department of Neurology, Vanderbilt University, Nashville, TN;* [7]*Department of Chemistry, Vanderbilt University, Nashville, TN;* [8]*Department of Pathology, Microbiology, and Immunology, Vanderbilt University Medical Center, Nashville, TN*

WP 469 **Comprehensive Proteomic Analysis of the zQ175 Striatum: Insights into the Soluble Proteome and Huntingtin-containing Inclusion Bodies in Huntington’s Disease**; Young June Jeon[1]; Dayeon Lee[1]; Dongyoon Shin[2, 3]; Youngsoo Kim[2]; Junho Park[2, 3]; [1]*Department of Life Sciences, CHA University, Seongnam-si, South Korea;*

[2]Proteomics Research Team, CHA Future Medicine Research Institute, Seongnam-si, South Korea; [3]Department of Medical Science, School of Medicine, CHA University, Seongnam-si, South Korea

WP 470 **Protein Dynamics in human Plasma and CSF with SILK study**; Jerome Vialaret[1]; Jacques Colinge[2]; Jana Kindermans[1]; Pierre Giroux[2]; Christophe Hirtz[1]; Sylvain Lehmann[1]; *[1]University Montpellier Hospital, Montpellier, France; [2]Montpellier University, Cancer Bioinformatics and Systems Biology, IRCM, Inserm, Montpellier, France*

WP 471 **Proteomic analyses of aging rhesus macaque brains reveal implicated pathways following inhibition of glutamate carboxypeptidase II**; Alexandra D. Steigmeyer[1]; Alexandria S. Battison[1]; Keira E. Mahoney[1]; Amy F.T. Arnsten[2]; Dibyadeep Datta[2]; Stacy A. Malaker[1]; *[1]Department of Chemistry, Yale University, New Haven, CT; [2]Department of Neuroscience, Yale University School of Medicine, New Haven, CT*

WP 472 **Aβ aggregation: A Perspective from Peptide Mass Finger Printing**; Kameswara Rao Mula[1]; Cole Hediger[1]; George Mathai[1]; Michael L Gross[1]; *[1]Washington University in St. Louis, University City, MO*

WP 473 **Deciphering Age- and Region-Specific Ganglioside Alterations in Alzheimer's Disease through a Pathway-Centered Framework**; Jae Young Yu[1, 2]; Hye Kyeong Jeong[1, 2]; Yong Heum Na[1, 2]; Jong Hyun Yoon[1, 2]; Seulah Lee[3]; Eunji Cho[3]; Jong Hyuk Yoon[3]; Hyun Joo An[1, 2]; *[1]Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, South Korea; [2]Asia Glycomics Reference Site, Chungnam National University, Daejeon, South Korea; [3]Neurodegenerative Diseases Research Group, Korea Brain Research Institute, Daegu, South Korea*

WP 474 **Development of a Multi-Dimensional Database to Define Ganglioside Neurodegenerative Disease Phenotypes in Preclinical Models and Patient Specimens using LC-HRIM-MS**; Jack P. Ryan[1]; David L. Williamson[2]; Rachel A. Harris[3]; Yao Lihang[1]; Nathan G. Hatcher[1]; Kim Ekroos[4]; Weixun Wang[2]; Daniel S. Spellman[1]; Komal D. Kedia[1]; *[1]Merck & Co., Inc., West Point, PA; [2]Merck & Co., Inc., Rahway, NJ; [3]MOBILion Systems, Inc., Chadds Ford, PA; [4]Lipidomics Consulting Ltd, Esbo, Finland*

WP 475 **Neuron type-specific proteomics reveals distinct Shank3 proteoforms in iSPNs and dSPNs lead to striatal synaptopathy in Shank3B-/- mice**; Yi-Zhi Wang; *Northwestern University, Chicago, IL*

WP 476 **Spatial lysosomal proximity labeling reveals compartmentalized lysosomal dynamics in neurons**; Wan Nur Atiqah Mazli[1]; Ashley M. Frankenfield[2]; Ling Hao[1]; *[1]University of Maryland, College Park, MD; [2]The George Washington University, Washington, DC*

WP 477 **Soluble APPβ and sAPPα Kinetic Curve Results are improved with utilization of a novel nanoflow LC-MS Platform**; Justyna A Dobrowolska Zakaria[1]; Helena Svobodova[2]; Gary Valaskovic[2]; Amanda Berg[2]; Robert Vassar[1]; *[1]Northwestern University Feinberg School of Medicine, Chicago, IL; [2]New Objective inc, LITTLETON, MA*

WP 478 **Unraveling DOI-Mediated Modulation of Neuronal Plasticity Proteins in the Medial Prefrontal Cortex: A Proteomics Approach**; Kuldeep Giri[1]; Kaden Adams[1]; Michelle Salemi[2]; Brett Phinney[2]; Christina Kim[1]; *[1]Princeton University, Princeton, NJ; [2]University of California Davis, Davis, CA*

WP 479 **Exploring the proteomic landscape in the healthy human brain across the aging spectrum**; Ernst Heinz V Pulido[1]; Katrin Schmitt[1]; Mariya Mardamshina[1]; Shoxruxxon Alimukhamedov[2]; Syed Bukhari[2]; Rong Chi[1]; Alina Isakova[2]; Tony Wyss-Coray[2, 3]; Emma Lundberg[1, 4, 5, 6]; *[1]Department of Bioengineering, Stanford University, Stanford, CA; [2]The Phil & Penny Knight Initiative for Brain Resilience, ChEM-H/Neuro Research Complex, Stanford University, Stanford, CA; [3]Department of Neurology & Neurological Sciences, Stanford University, Stanford, CA; [4]Department of Pathology, Stanford University, Stanford, CA; [5]Science for Life Laboratory, School of Engineering Sciences in Chemistry, Biotechnology and Health, KTH - Royal Institute of Technology, Stockholm, Sweden; [6]Chan Zuckerberg Biohub, San Francisco, CA*

WP 480 **Global differential proteomic analysis reveals course of TDP-43 proteinopathy**; Anna Konopka[1, 2]; Adam Karpinski[3, 4]; Daria Hajka[1]; Anna Czajkowska[1]; Malwina Wozniak[1]; Anne Sanner[5]; Agnieszka Krzyzosiak[1]; Dominic Winter[5]; Leszek Kaczmarek[6]; Ewa Bulska[2]; Witold Konopka[1]; *[1]Lukasiewicz Research Network - PORT Polish Center for Technology Development, Wroclaw, Poland; [2]Biological and Chemical Research Centre, Faculty of Chemistry, University of Warsaw, Warsaw, Poland; [3]Faculty of Chemistry, University of Warsaw, Warsaw, Poland; [4]Nencki Institute of Experimental Biology PAS, Warsaw, Poland; [5]Institute for Biochemistry and Molecular Biology (IBMB), Medical Faculty, University of Bonn, Bonn, Germany; [6]Nencki-EMBL Centre of Excellence for Neural Plasticity and Brain Disorders: BRAINCITY, Nencki Institute of Experimental Biology PAS, Warsaw, Poland*

WP 481 **Postmortem Human Medial Amygdala Proteomics Identifies Alterations by Sex and Ancestry in Post-Traumatic Stress Disorder Brains**; Tamara Abulez[1]; Joshua P Schaaf[1]; Joo Heon Shin[2]; Amy Currier[2]; Nina Rajpurohit[2]; Nicholas W. Bateman[1]; Larry Maxwell[3]; Rahul Bharadwaj[2]; Thomas P. Conrads[3]; *[1]Gynecologic Cancer Center of Excellence and the Women's Health Integrated Research Center, Annandale, VA; [2]Lieber Institute for Brain Development, Johns Hopkins Medicine Campus, Baltimore, MD; [3]Women's Health Integrated Research Center, Women's Service Line, Inova Health System, Annandale, VA*

WP 482 **Uncovering the Effects of Neuropeptide FF on human iPSC-derived Neurons Through Targeted and Global Proteomics**; Noah Smeriglio[1]; Wan Nur Atiqah Mazli[1]; Ling Hao[1]; *[1]University of Maryland, College Park, MD*

WP 483 **Unravelling Lecanemab's Therapeutic Effects in Alzheimer's Disease via TMT Proteomic Analysis**; Kritika Goyal[1]; Jörg Hanrieder[2]; Jeffrey Nicholas Savas[1]; *[1]Department of Neurology, Feinberg School of Medicine, Northwestern University, Chicago, IL; [2]Department of Psychiatry and Neurochemistry, Institute of Neuroscience and Physiology, Sahlgrenska Academy at the University of Gothenburg, Mölndal, Sweden*

WP 484 **Simultaneous Quantification of Enkephalins and Comprehensive Proteomic Analysis from a Single Mouse Spinal Cord Sample Using LC-MS**; Przemyslaw Mielczarek[1, 2]; Anna Piotrowska[3]; Joanna Bogacka[3]; Barbara Przewlocka[3]; *[1]AGH University of Krakow, Krakow, Poland; [2]Laboratory of Proteomics and Mass Spectrometry, Maj Institute of Pharmacology, Polish Academy of Sciences, Krakow, Poland; [3]Department of pain pharmacology, Maj Institute of Pharmacology, Polish Academy of Sciences, Krakow, Poland*

WP 485 **Of Peptides and Proteoforms: Insights into Body Fluid Biomarker Discovery for Alzheimer's Disease Progression using a Peptide-Centric Approach**; Dylan Nicholas T Tabang[1]; Gonzalo Blasco[2]; Patrick Van Zalm[1]; Abhay Moghekar[3]; Judith A Steen[2]; Hanno Steen[1, 2]; *[1]Department of Pathology, Boston Children's Hospital & Harvard Medical School, Boston, MA; [2]F.M. Kirby Neurobiology Center, Boston Children's Hospital & Department of Neurology, Harvard Medical School, Boston, MA; [3]Department of Neurology, Johns Hopkins University School of Medicine, Baltimore, MD*

WP 486 **Longitudinal Metabolic Alterations in Small Extracellular Vesicles from Severe Traumatic Brain Injury Patients**; Mojibola O Fowowe[1]; Oluwatosin E Daramola[1]; Odunayo O. Oluokun[1]; Ayobami O. Oluokun[1]; Moyinoluwa Adeniyi[1]; Firas Kobeissy[2]; Stefania Mondello[3]; Ava M Puccio[4]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX; [2]Center for Neurotrauma, Multiomics & Biomarkers (CNMB) Morehouse School of Medicine, Atlanta, GA; [3]Department of Biomedical* *and Dental Sciences and Morphofunctional Imaging, University of Messina, Messina, Italy; [4]Department of Neurological Surgery, University of Pittsburgh, Pittsburgh, PA*

WP 487 **N-Glycosylation Alterations in Synaptic Vesicles and Synaptosomes from the Prefrontal Cortex of Parkinson's Disease Brains**; Moyinoluwa Adeniyi[1]; Mojibola Fowowe[1]; Odunayo Oluokun[1]; Sarah Sahioun[1]; Vishal Sandilya[1]; Oluwatosin Daramola[1]; Andrew I. Bennett[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX*

WP 488 **Lipid Dysregulation in Niemann-Pick Disease Type C: New Insights from the Npc1I0161TMouse Model.**; Ralph John Emerson Javier Molino[1]; Stephanie M Cologna[2, 3]; *[1]University of Illinois Chicago, Chicago, IL; [2]Department of Chemistry, University of Illinois Chicago, Chicago, IL; [3]Laboratory of Integrative Neuroscience, University of Illinois Chicago, Chicago, IL*

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WP 489 **(Semi)-automated LC-UV-HRMS platform approach for purity analysis and impurity profiling of oligonucleotides in early drug discovery**; Kathrin Stavenhagen[1]; Manasses Jora[1]; Carina Leandersson[1]; Rebecca Rae[1]; Julien Bourquin[2]; Vahid Golghalyani[3]; Werngard Czechtizky[1]; Tomas Leek[1]; *[1]AstraZeneca, Gothenburg, Sweden; [2]Waters Corporation, Wilmslow, United Kingdom; [3]Protein Metrics, LLC, Boston, Massachusetts*

WP 490 **Development of Cell-Based In VitroAssays to Guide Optimization of Novel Small Interfering RNA (siRNA) Chemistries**; Michael M Hayashi[1]; Shuai Yan[1]; Jianzhong Chen[1]; Afrand Kamali[1]; Ethan Sanford[1]; Seongmoon Cheong[1]; Guangnong Zhang[1]; *[1]Novo Nordisk, Lexington, MA*

WP 491 **Sheath liquids and Mobile Phase Additives for enhanced LC-MS Analysis of Oligonucleotide Therapeutics**; Mollie A Glenister[1]; Jim L Stephenson[2]; Mark J Dickman[1]; *[1]The University of Sheffield, Sheffield, United Kingdom; [2]Thermo Fisher Scientific, San Jose, CA*

WP 492 **High-resolution ion mobility mass spectrometry for characterization of oligonucleotide phosphorothioate diastereomers**; Jie Du[1]; Molly S Blevins[1]; Ralph Aderorho[1, 2]; Christopher M Crittenden[1]; Tao Chen[1]; *[1]Genentech, Inc., South San Francisco, CA; [2]Clemson University, Clemson, SC*

WP 493 **Absolute quantification of epitranscriptomic modifications in S cerevisiae using a microbore LC-MSMS platform**; Robert L Ross[1]; Keeley Murphy[1]; Min Du[1]; *[1]Thermo Fisher Scientific, Lexington, MA*

WP 494 **Ultra-high-throughput, HILIC-free analysis of oligonucleotides using Acoustic Ejection Mass Spectrometry**; Jacob W. McCabe[1]; David Tinnermeier[1]; Remco Van Soest[1]; *[1]SCIEX, Frammingham, MA*

WP 495 **A rapid HRMS method for accurately quantifying oligonucleotide deamination levels**; Jonathan E Fox[1]; Jo-Anne Riley[2]; Barbara Sullivan[3]; Keith Richardson[2]; Rachelle Black[4]; Kamila Pacholarz[5]; Andrew Ray[6]; Emma Harry[7]; *[1]Waters, Wilmslow, United Kingdom; [2]Waters Corporation, Wilmslow, United Kingdom; [3]Waters Corp., Milford, MA; [4]New Modalities & Parenteral Development, Pharmaceutical Technology & Development, Operations, AstraZeneca, Macclesfield, United Kingdom; [5]Early Chemical Development, Pharmaceutical Sciences, R&D, AstraZeneca, Macclesfield, United Kingdom; [6]New Modalities & Parenteral Development, Pharmaceutical Technology & Development, Operations, AstraZeneca, Macclesfield, United Kingdom; [7]Chemical Development, Pharmaceutical Technology & Development, Operations, AstraZeneca, Macclesfield, United Kingdom*

WP 496 **Characterisation of dsRNA Biocontrols and mRNA Therapeutics using LC-MS**; Gareth R Owen[1]; Caroline A Evans[1]; Emma N Welbourne[1]; Peter M Kilby[2]; Mark J Dickman[1]; *[1]The University of Sheffield, Sheffield, United Kingdom; [2]Syngenta, Jeolott's Hill International Research Centre, Bracknell, United Kingdom*

WP 497 **Characterization of High MW Structures in siRNA Oligonucleotides by 1D- and 2D-SEC x IP-RP LCMS and Native MS**; Stilianos G. Roussis[1]; Claus Rentel[1]; *[1]Ionis Pharmaceuticals, Inc., Carlsbad, CA*

WP 498 **Fully Automated Candidate Creation Workflow for Intact Mass Mapping of Oligonucleotide Therapeutics**; A. Michelle English[1]; Stephen Kok[2]; Aude Tartière[2]; James Duffy[3]; Amy Claydon[3]; *[1]Genedata Inc., Lexington, MA; [2]Genedata Inc., San Francisco, CA; [3]Genedata, Cambridge, United Kingdom*

WP 499 **Bayesian Model for Oligo Spectrum Matching with the NucleicAcidSearchEngine**; Samuel P Wein[1, 2]; Tjeerd Dijkstra[3, 4]; Oliver Kohlbacher[2, 3, 5, 6]; *[1]University of Tübingen, Tübingen, Germany; [2]OpenMS Inc, Erie, PA; [3]Institute for Translational Bioinformatics, University Hospital Tübingen, Tübingen, Germany; [4]Dept. for Women's Health, University Hospital Tübingen, Tuebingen, Germany; [5]Institute for Bioinformatics and Medical Informatics, University of Tubingen, Tubingen, Germany; [6]Applied bioinformatics group, University of Tübingen, Tuebingen, Germany*

WP 500 **Highly Sensitive Quantification of Therapeutic Oligonucleotide in Human plasma using a Modified Orbitrap Hybrid Mass Spectrometer**; Hao Yang[1]; Markus Kellmann[2]; Heiner Koch[2]; Min Du[3]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Bremen, Germany; [3]Thermo Fisher Scientific, Lexington, MA*

WP 501 **Differentiation of Oxidized and Unoxidized Abasic Site-Hydralazine Covalent DNA Adducts Using MALDI-TOF-MS**; Tanhaul Islam[1, 2]; Lloyd W. Sumner[1]; Kent S. Gates[2]; Zhentian Lei[1]; *[1]Metabolomics Center, University of Missouri, Columbia, MO; [2]Department of Chemistry, University of Missouri, Columbia, MO*

WP 502 **Impact of charge state and ligand binding on collision cross-sections of nucleic acids in an Orbitrap mass analyzer**; Jada N Walker[1]; Noha M El Zahar[1, 2, 3]; Jennifer S Brodbelt[4]; *[1]University of Texas at Austin, Austin, TX; [2]Ain Shams University, Cairo, Egypt; [3]King Salman International University, Ras-Sedr, Egypt; [4]University of Texas - Austin, Austin, TX*

WP 503 **Glucose metabolism alters the epitranscriptome to regulate protein-RNA assemblies**; Daniel H Ramirez[1]; Carolina Bras Costa[1]; Benjamin A Garcia[1]; *[1]Washington University School of Medicine, St. Louis, MO*

WP 504 **Modification of Small Molecule Drug Methods to Confirm Drug Safety of Large Double Stranded siRNA Biotherapeutics**; Timothy Snow[1]; Limin Deng[1]; Amelie Chen[1]; Nicholas White[1]; Wenbin Liu[1]; Zamas Lam[1]; Ragu Ramanathan[1]; *[1]QPS, LLC, Newark, DE*

WP 505 **FUS Is an N1- and N6-Methyladenosine-Binding Protein**; Xiaochen Liang[1]; Ting Zhao[1]; Yinsheng Wang[1]; *[1]UC Riverside, Riversdie, CA*

WP 506 **Enhancing mRNA Production Quality: Comprehensive Charge Detection Mass Spectrometry (CDMS) Analysis of DNA Plasmid Structures**; Anisha Haris[1]; David Bruton[1]; Kevin Giles[1]; Keith Richardson[1]; Jakub Ujma[1]; Ying Qing Yu[2]; Christopher Gawlig[3]; Michael Rühl[3]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Waters, Milford, MA; [3]BioSpring Gesellschaft für Biotechnologie mbH, Frankfurt am Main, Germany*

WP 507 **Combined Ribonuclease Digestion and DIA LC-MS/MS for Enhanced sgRNA/mRNA Characterization**; Akari Ito[1]; Catalin E Doneanu[2]; Yuki Matsubara[1]; Yasuto Yokoi[1]; *[1]Mitsui knowledge, Minato, Japan; [2]Waters Corporation, Milford, MA*

WP 508 **Comprehensive evaluation of MS and LC-MS/MS based workflows for the characterisation of double stranded small interfering RNA-based (siRNA) therapeutics**; Felipe Guapo[1]; Silvia Millán-Martín[1]; Sara Carillo[1]; Ken Cook[2]; Ulrik Mistarz[2]; Jonathan Bones[1, 3]; *[1]NIBRT, Dublin, Ireland; [2]Thermo Fisher Scientific, Hemel Hempstead, United Kingdom; [3]University College Dublin, Belfield, Ireland*

WP 509 **Structural characterization of oligonucleotides by ion mobility spectrometry and UV photodissociation**; Anna L Simmonds[1]; Tiago Moreira[1]; Weijing Liu[2]; Scott Kronewitter[3]; Rosa Viner[2]; Frank Sobott[1]; *[1]University of Leeds, Leeds, United Kingdom; [2]ThermoFisher Scientific, San Jose, CA; [3]ThermoFisher Scientific, Lexington, MA*

WP 510 **Rapid Characterization of 5 Capping of mRNA using Ultra performance liquid chromatography-High Resolution Accurate Mass-Mass Spectrometer (UPLC-HRAM-MS)**; Qianqian Zhang[1]; Yun Zhang[2]; Mike Boggs[2]; *[1]MilliporeSigma, Rockville, MD; [2]MilliporeSigma, Rockville, Maryland*

WP 511 **Interaction of HIV-1 Gag protein with both the 5' and 3' regions of HIV genomic RNA**; Kaylee Grabarkewitz[1, 2, 3]; Keerthi Gottipati[4]; Jerricho Tipo[4]; Kay Choi[4]; Vicki Wysocki[2, 3, 5]; Karin Musier-Forsyth[3, 6, 7]; *[1]The Ohio State University, Columbus, OH; [2]Resource for Native Mass Spectrometry Guided Structural Biology, Columbus, OH; [3]Center for RNA Biology, Ohio State University, Columbus, OH; [4]Department Molecular and Cellular Biochemistry, Indiana University-Bloomington, Bloomington, Indiana; [5]School of Chemistry & Biochemistry, Georgia Institute of Technology, Atlanta, Georgia; [6]Ohio State University, Columbus, OH; [7]Center for Retrovirus Research, Ohio State University, Columbus, OH*

WP 512 **Evaluation of a Novel SPE Sorbent for the Extraction of Oligonucleotides from Biological Matrices Prior to UPLC-MS/MS Analysis**; Zainab Khan[1]; Steve Plant[1]; Kyle Bevan[1]; Helen Lodder[1]; Charlotte Hayes[1]; Lee Williams[1]; Geoff M Davies[1]; Adam James Senior[1]; Alan Edgington[1]; Russell Parry[1]; Lucy Richards[1]; Claire Desbrow[1]; Dan Menasco[1]; *[1]Biotage GB Limited, Cardiff, United Kingdom*

WP 513 **LCMS Analysis of Oligonucleotides on the Orbitrap Astral MS: Exploring Sensitivity Limits and Comparison of Stability in Mouse Tissue Lysosomes**; Ryan Shirey[1]; Matthew Albertolle[1]; Allice Yang[1]; Hao Yang[2]; Roberto C. Gamez[2]; Min Du[3]; *[1]Avidity Biosciences, San Diego, CA; [2]Thermo Fisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific, Lexington, MA*

WP 514 **Locked nucleic acid Vs. Peptide nucleic acid probes for use in Hybridization assays for Oligonucleotide LCMS analysis**; Chris D Hardcastle; *Aliri Bioanalytical, Millcreek, UT*

WP 515 **Characterization of peptide-oligonucleotide conjugates using an on-line nanoflow desalting method**; Thanh Nguyen[1]; Qi Zhang[2]; Natalia Tretyakova[2]; Jennifer S Brodbelt[1]; *[1]University of Texas Austin, Austin, TX; [2]University of Minnesota, Minnneapolis, MN*

PEPTIDOMICS AND IMMUNOPEPTIDOMICS
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WP 516 **Peptidomic investigation of sera from donors with breast cancer (BC) and age-matched controls to identify indicators for early BC diagnosis**; Pathea S Bruno[1]; Danielle Whitham[1]; Isabella Pelkey[1]; Kaya Johnson[1]; Brian T. Pentecost[1]; Costel C. Darie[1]; *[1]Clarkson University, Potsdam, NY*

WP 517 **Dissecting the antigen presentation pathway through subcellular peptidomics to elucidate HLA neoantigen presentation**; Ana Marcu[1]; Susan Klaeger[1]; Christopher M. Rose[1]; *[1]Genentech Inc., South San Francisco, CA*

WP 518 **Optimized Dimethyl Tagging for Endogenous Peptide Profiling in Callinectes sapidus Hemolymph Under Staphylococcus aureus Immune Challenge**; Tina C Dang[1]; Wenxin Wu[1]; Peng-Kai Liu[2]; Lingjun Li[1]; *[1]University of Wisconsin-Madison, Madison, WI; [2]University of Wisconsin - Madison, Madison, WI*

WP 519 **Multi-faceted Mass Spectrometry-Enabled Global Profiling of Glycosylated Neuropeptides in the American Lobster Homarus americanus Nervous System**; Vu Ngoc Huong Tran[1]; Angel E. Ibarra[2]; Thao U Duong[2]; GAOYUAN LU[1]; Feixuan Wu[1]; Lingjun Li[1, 2]; *[1]School of Pharmacy, University of Wisconsin-Madison, Madison, WI; [2]Department of Chemistry, University of Wisconsin-Madison, Madison, WI*

WP 520 **Uncovering the Dynamic Nature of the Feeding-Induced Crustacean Neuropeptidome Remodeling via Open Modification Searching**; Kendra G Selby[1]; Lauren Fields[1]; Lingjun Li[1, 2]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [2]School of Pharmacy, University of Wisconsin-Madison, Madison, WI*

WP 521 **Exploring the HLA-A02:01 Immunopeptidome Using Parallel Accumulation Mobility Aligned Fragmentation**; Gregory Webster[1]; Amy L. Kessler[2]; Leonard Rorrer[1]; Lauren Royer[1]; Daniel DeBord[1]; Albert J.R. Heck[2]; Fabio Marino[2]; *[1]MOBILion Systems, Inc., Chadds Ford, PA; [2]Utrecht University, Utrecht, Netherlands*

WP 522 **Increased EThcD efficiency on a modified Orbitrap Hybrid MS Instrument boosts the Identification Depth and Sequence Coverage of HLA Peptides**; Amy L. Kessler[1]; Kyle L. Fort[2]; Hanno Resemann[3]; Peter Krueger[3]; Cong Wang[3]; Heiner Koch[3]; Jan-Peter Hauschild[3]; Fabio Marino[1]; Albert J.R. Heck[1]; *[1]Biomolecular Mass Spectrometry & Proteomics, Bijvoet Center for Biomolecular Research & Utrecht Institute for Pharmaceutical Sciences, Utrecht University, Padualaan 8, 3584 CH Utrecht, Netherlands; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [3]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

WP 523 **A Novel Nanoflow LC-MS Platform for the Robust Identification of HLA Peptides from High Value Clinical Samples**; Helena Svobodova[1]; Gary Valaskovic[1]; Amanda Berg[1]; Nicholas Cheung[2]; Robert Salzler[2]; *[1]New Objective inc, LITTLETON, MA; [2]Regeneron, Tarrytown, NY*

WP 524 **Deciphering the ImmunopeptidomeofMouse andHuman Colorectal Cancerfor Neoantigen Discovery by de novo sequencing**; Chao Peng[1]; Ping Wu[1]; Haofei Miao[1]; Ling Li[1]; Wenting Li[1]; Lei Xin[1]; Baozhen Shan[1]; *[1]BaizhenBio Inc., Wuhan, China*

WP 525 **The Immunopeptidome of Malignant Peripheral Nerve Sheath Tumors Reveals Novel Non-Reference Peptides and Cancer Testes Antigens with Immunogenic Potential**; Kyle A Richards[1]; Suzanne Coleman[1]; Jessica Liebau[1]; Mitchell Hruska[1]; Tyler Jubenville[1]; Reid Wagner[1]; Subina Mehta[1]; Pratik D. Jagtap[1]; David A. Largespada[1]; Timothy J. Griffin[1]; *[1]University of Minnesota, Twin Cities, Minneapolis, MN*

WP 526 **Immunopeptide analysis with a modified Orbitrap Astral mass spectrometer maximizes peptide detection and quantitation in protein degrader applications**; Angeline Chen[1]; Gregory K. Potts[1]; James W. Sawicki[1]; Omprakash Nacham[1]; Janice Y. Lee[1]; Fernanda Salvato[2]; Amirmansoor Hakimi[2]; Ellen Casavant[2]; Tonya Pekar Hart[2]; Jon D. Williams[1]; *[1]AbbVie, Inc., North Chicago, IL; [2]Thermo Fisher Scientific, San Jose, CA*

WP 527 **Creating a Liquid Chromatography, Ion Mobility Spectrometry and Mass Spectrometry (LC-IMS-MS) Library of Human Leukocyte Antigen Immunopeptides**; Allison N Fry[1]; Chelston R. Ang[2]; Sarah N. Bennett[2]; Benjamin G. Vincent[2, 3, 4]; Paul M. Armistead[3, 4]; Erin S. Baker[1]; *[1]Department of Chemistry, University of North Carolina at Chapel Hill, Chapel Hill, NC; [2]Department of Microbiology and Immunology, University of North Carolina at Chapel Hill, Chapel Hill, NC; [3]Division of Hematology, Department of Medicine, University of North Carolina at Chapel Hill, Chapel Hill, NC; [4]Lineberger Comprehensive Cancer Center, University of North Carolina at Chapel Hill, Chapel Hill, NC*

WP 528 **Maximizing immunopeptide identification from limited pediatric solid tumor biopsy samples**; Peiyao Li[1]; Richa Kapoor[1]; Thomas De Raedt[1, 2]; Jessica B. Foster[1, 2]; John M. Maris[1, 2]; Diego M Assis[3]; Matthew Willetts[3]; Hossein Fazelinia[1]; Lynn A Spruce[1]; *[1]Children's Hospital of Philadelphia, Philadelphia, PA; [2]University of Pennsylvania, Perelman School of Medicine, Philadelphia, PA; [3]Bruker Scientific LLC, Billerica, MA*

WP 529 **Evolution of Mass Spectrometers Driving Deeper and Sensitive Immunopeptide Analysis**; Ritu Raj[1]; Jenny Ho[2];

Bryanald N Aryanto[3, 4]; Ufuk Acikbas[3]; Tiaan Heunis[3]; Andrew J Jones[3]; Yoanna Ariosa-Morejon[3]; H Irem Baymaz[3]; Sergio Regufe Da Mota[3]; Ricardo J Carreira[3]; *[1]Immunocore Ltd., Abingdon, United Kingdom; [2]Thermo Fisher Scientific, Hemel Hempstead, United Kingdom; [3]Immunocore Ltd., Abingdon, United Kingdom; [4]School of Biological Sciences, Faculty of Biology, Medicine and Health, University of Manchester, Manchester, United Kingdom*

WP 530 **Optimized Enrichment and Analysis of MHC-I Peptides for Comprehensive Immunopeptidome Profiling**; Suzanne Smith[1]; Anastasia Klenke[1]; Joanna Geddes[1]; Fernanda Salvato[2]; Ellen Casavant[2]; Tonya Pekar Hart[2]; Bhavin Patel[1]; *[1]Thermo Fisher Scientific, Rockford, IL; [2]Thermo Fisher Scientfic, San Jose, CA*

WP 531 **Identifying tumor-specific antigens derived from protein translation errors**; Kyle Hoffman; *Bioinformatics Solutions Inc, Waterloo, ON*

WP 532 **Meta-iPep: A Galaxy-based metaimmunopeptidomics bioinformatics pipeline rigorously characterizes microbial peptide antigens bound to the human leukocyte antigen (HLA) complex**; Katherine T Do[1]; Subina Mehta[1]; Reid Wagner[2]; Fengchao Yu[3]; Alexey I. Nesvizhskii[3, 4]; Timothy J. Griffin[1, 5]; Pratik Dilip Jagtap[1, 5]; *[1]Department of Biochemistry, Molecular Biology and Biophysics, University of Minnesota, Minneapolis, MN; [2]Minnesota Supercomputing Institute, University of Minnesota, Minneapolis, MN; [3]Department of Pathology, University of Michigan, Ann Arbor, MI; [4]Department of Computational Medicine and Bioinformatics, University of Michigan, Ann Arbor, MI; [5]Masonic Cancer Center, University of Minnesota, Minneapolis, MN*

WP 533 **Advancing Immunopeptidomics Profiling of Epstein Barr Virus (EBV)-transformed B-lymphoblastoid cells using timsTOF Ultra Mass Spectrometer**; Saketh Kapoor; *Yale University, New Haven, CT*

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WP 543 **High-Sensitivity Immunopeptidomics: Scalable MHC I and II Profiling from Limited Samples Reveals Dynamic Antigen Presentation**; Katherinne Herrera-Jordan[1, 2]; Joel Lanoix[1]; Eric Bonneil[1]; Chantal Durette[1]; Suzanne Smith[3]; Bhavin Patel[3]; Claude Perreault[1, 4]; Pierre Thibault[1, 5]; *[1]Institute of Research in Immunology and Cancer, Université de Montréal, Montreal, QC; [2]Molecular Biology Program, Université de Montréal, Montréal, Canada, Montréal, Quebec; [3]Thermo Fisher Scientific, Rockford, Illinois; [4]Department of Medicine, Université de Montréal, Montreal, QC; [5]Department of Chemistry, Université de Montréal, Montréal, QC*

WP 544 **Leveraging advanced mass spectrometry technology for in-depth immunopeptidome profiling**; Fernanda Salvato[1]; Nicholas Cheung[2]; Ellen Casavant[1]; Robert Salzler[2]; Tonya Pekar Hart[1]; Patience Sanderson[3]; Amirmansoor Hakimi[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Regeneron, Tarrytown, NY; [3]Thermo Fisher Scientific, San Jose, California*

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ChengKang Chiang[2]; *[1]Department of Medical Research, Hualien Tzu Chi Hospital, Buddhist Tzu Chi Medical Foundation, Hualien, Taiwan; [2]Department of Chemistry, National Dong Hwa University, Shou-Feng, Hualien, Taiwan*

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Mudbhari[1, 2]; Larry M. York[1]; Tomas A. Rush[1]; Paul E. Abraham[1]; [1]*Biosciences Division, Oak Ridge National Laboratory, Oak Ridge, TN;* [2]*UT-ORNL Graduate School of Genome Science and Technology, University of Tennessee-Knoxville, Knoxville, TN*

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Scientific, Somerset, NJ; [2]Thermo Fisher Scientific, San Jose, CA; [3]Thermo Fisher Scientfic, San Jose, CA; [4]Roche, Pharma Research and Early Development (pRED), Penzberg, Germany; [5]Genentech Inc., South San Francisco, CA

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WP 594 **Structural Implications of Post Translational Modifications in Biopharmaceutical Proteins using Ion-Mobility and Collision Induced Unfolding**; Kristine F Parson[1]; Margo Wilson[1]; Austin Culberson[2]; Carter Asef[2]; Casey Vantucci[2]; Mason Chilmonczyk[2]; Jason Barker[1]; Greg Adams[1]; *[1]FUJIFILM Diosynth Biotechnologies USA, Inc., Morrisville, NC; [2]Andson Biotech Inc., Atlanta, GA*

WP 595 **LC-MS characterization of an unexpected C-terminal HC extension in a therapeutic mAb**; Ben Zigterman; *KBI Biopharma, Louisville, CO*

WP 596 **Extending Native Protein Stability with DynaChip Rapid Online Buffer Exchange Ahead of nanoESI**; Carter Asef[1]; Casey Vantucci[1]; Austin Culberson[1]; Mason Chilmonczyk[1]; *[1]Andson Biotech, Atlanta, GA*

WP 597 **MauriceFlex Fractionation of charge variants accompanied by LC-MS and Digital SPR Analysis correlates Structure to the Function of a mAb**; Srinivasa Rao[1]; Samantha Ippoliti[2]; Ying Qing Yu[2]; Michael Piazza[3]; Chris Heger[1]; *[1]Bio-techne, San Jose, CA; [2]Waters Corp., Milford, MA; [3]Nicoya LifeSciences, Kitchener, ON*

WP 598 **Multi-attribute characterization of a bispecific molecule leveraging fast EThcD and enhanced Native MS on a modified Orbitrap Hybrid MS**; Andrew Mahan[1]; Elsa Gorre[2]; Christopher Sauer[2]; Hirsh Nanda[2]; Reiko Kiyonami[3]; Min Du[3]; Cong Wang[4]; Peter Krueger[4]; Nicole Zehethofer[4]; Heiner Koch[4]; *[1]JOHNSON AND JOHNSON, Spring House, PA; [2]Johnson & Johnson Innovative Medicine, Spring House, PA; [3]Thermo Fisher Scientific, Lexington, MA; [4]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

WP 599 **Approaches to measuring protein subunits in cellular supernatant followed by native analyses of their complexes**; Daniela Salas[1]; Nastaran Nosrat Tajoddin[1]; Tian Tian[2]; Elizabeth Hecht[2]; Anisha Haris[3]; David Bruton[4]; Keith Richardson[3]; Kevin Giles[3]; Iain Campuzano[5]; *[1]Amgen, Burnaby; [2]Amgen, South San Francisco, CA; [3]Waters Corp, Wilmslow, United Kingdom; [4]Waters Corporation, Wilmslow, United Kingdom; [5]Amgen, Thousand Oaks, CA*

WP 600 **Assessment and best practices of ion mobility in a regulatory setting for characterizing higher order structure (HOS) stability of biotherapeutics**; Mack Shih[1]; Patrick J. Faustino[1]; Xiaoming Xu[1]; Jinhui Zhang[1]; *[1]Food and Drug Administration, Silver Spring, MD*

WP 601 **Confidently identifying Isomeric Glycoforms in N-Glycopeptides by Collision-Induced Dissociation MS/MS**; Zhongqi Zhang[1]; Bhavana Shah[1]; *[1]Amgen Inc., Thousand Oaks, CA*

WP 602 **Alternative fragmentation is not enough for Top-down MS and intact protein characterization**; Rafael D Melani[1]; Linda B. Lieu[2]; Jingjing Huang[1]; Jake T. Kline[2]; David Bergen[1]; Graeme C McAlister[1]; Chirstopher Mullen[1]; Luca Fornelli[2]; *[1]Thermo Fisher Scientific, San Jose, California; [2]Oklahoma University, Norman, OK*

WP 603 **Structural characterization of multiple GLP-1 receptor agonists using electron capture dissociation**; Rachel Franklin[1]; Julie Horner-Buxton[2]; Joseph C. Meeuwsen[1]; Thomas E. Walker[3]; Mike Hare[1]; *[1]Agilent Technologies, Inc., Corvallis, OR; [2]Agilent Technologies, Santa Clara, CA; [3]Agilent Technologies, Lexington, MA*

WP 604 **Inducing Disulfide Scrambling to Confidently Identify Low-Abundance Scrambles: Could a Forced-Scrambling Assessment Benefit Disulfide Engineered Biotherapeutics?**; David R Bush; *Novartis Biomedical Research, Inc., Cambridge, MA*

WP 605 **Enabling Process Development: Multi-Attribute Monitoring (MAM) Methodology for Glycosylated Subunit Vaccine Production**; Asif Shajahan[1]; Lisa M. Jenkins[2]; Nathan Barefoot[1]; Darielys Maldonado[1]; Jeremy Wolff[1]; Jiang Rong[1]; Yanhong Yang[1]; Sylvie R Yang[1]; Lisa Kueltzo[1]; Valerie Ficca[1]; Elizabeth Scheideman[1]; Ivan Loukinov[1]; Daniel B Gowetski[1]; Kevin Carlton[1]; Jason D Gall[1]; Paula Lei[1]; *[1]Vaccine Production Program, Vaccine Research Center, National Institutes of Health, Gaithersburg, MD; [2]Laboratory of Cell Biology, Center for Cancer Research, National Cancer Institute, National Institutes of Health,, Bethesda, Maryland*

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WP 606 **Integrative structural MS and cryo-EM unravels a mechanism for Phosphodiesterase-mediated reset of Protein Kinase A signaling**; Varun Venkatakrishnan[1]; Tatiana Laremore[1]; Jean-Paul Armache[1]; Ganesh Anand[1]; *[1]Penn State University, State College, PA*

WP 607 **Integrative Structural Proteomics Combined with Computational Modeling Provides Insight Into Translational Potential of Non-Covalent PPARγ Inverse Agonist**; Kuang-Ting Kuo[1, 2]; Bilel Bdiri[3]; Yuanjun He[3]; Marcel Koenig[3]; Theodore Kamenecka[3]; Patrick Griffin[1, 2, 3]; *[1]Scripps Research, Jupiter, FL; [2]Skaggs Graduate School of Chemical and Biological Sciences, The Scripps Research Institute, Jupiter, FL; [3]Department of Molecular Medicine, The Herbert Wertheim UF Scripps Institute for Biomedical Innovation & Technology, Jupiter, FL*

WP 608 **Mass Spectrometric ITEM-FOUR Analysis Differentiates Binding Motifs of Camelid Single-Domain Antibodies and Fosters Precision Malaria Diagnostics**; Kwabena F.M. Opuni[1]; Yann G.-J. Sterckx[2]; Michael O. Glocker[3]; *[1]Department of Pharmaceutical Chemistry, School of Pharmacy, College of Health Science, Legon, Ghana; [2]Laboratory of Medical Biochemistry, Faculty of Pharmaceutical, Biomedical, and Veterinary Sciences,* *University of Antwerp, Antwerp, Belgium;* [3]*Proteome Center Rostock, Rostock, Germany*

WP 609 **Investigating the Mechanistic Origin of Irreversible Thermal Unfolding in Cytochrome c and its Implications for Thermodynamic Stability Measurements**; Evelyn H MacKay-Barr[1]; Lars Konermann[1]; [1]*University of Western Ontario, London , ON*

WP 610 **Exploring the interplay between protein conformational changes and phosphorylation in a pancreatic cancer cell and stellate cell co-culture system**; Haiyan Lu[1]; Yuan Liu[1]; Hung-Yu Chiang[2]; Hua Zhang[1]; Xudong Shi[3]; Lingjun Li[1, 2, 4]; [1]*School of Pharmacy, University of Wisconsin-Madison, Madison, WI;* [2]*Biophysics Graduate Program, University of Wisconsin-Madison, Madison, WI;* [3]*School of Medicine and Public Health, University of Wisconsin-Madison, Madison, Wisconsin;* [4]*Department of Chemistry, University of Wisconsin-Madison, Madison, WI*

WP 611 **Spider Chasing Its Prey: Mass Spectrometry and Atomic Force Microscopy Reveal Structural Features of Human Serum C4BP and Its Complexes**; Tereza Kadavá[1]; Jürgen Strasser[2]; Victor C. Yin[1]; Johannes F. Hevler[1]; Sofia Kalaidopoulou Nteak[1]; Maryam Marefat[2]; Albert J.R. Heck[1]; Johannes Preiner[2]; Leendert A. Trouw[3]; [1]*Utrecht University, Utrecht, Netherlands;* [2]*University of Applied Sciences Upper Austria, Linz, Austria;* [3]*Leiden University Medical Center, Leiden, Netherlands*

WP 612 **Limited-Proteolysis Mass Spectrometry Reveals Cognition-Associated Structural Changes in the Aged Rodent Brain**; Haley E Tarbox[1]; Audrey Branch[1]; Stephen Fried[1]; [1]*Johns Hopkins University, Baltimore, MD*

WP 613 **Investigating Conformational Heterogeneity of Various Caspase-9 Maturation States**; Trisha W Brady[1]; Jeanne A. Hardy[1]; Richard W Vachet[1]; [1]*University of Massachusetts Amherst, Amherst, MA*

WP 614 **In-blood Persulfate Radical Protein Footprinting for the Study of Protein Structural Biology in Type 2 Diabetic Mice**; Mingming Zhao[1]; Sandeep K. Misra[1]; Ajay Sharma[1]; Juliette Locklar[1]; Anter Shami[1]; Sayed Mobarak[1]; James A. Stewart, Jr. [1]; Joshua S. Sharp[1]; [1]*University of Mississippi, Oxford, MS*

WP 615 **Progesterone receptor regulatory mechanisms are informed by structural mass spectrometry and computational modeling**; Matthew David Mann[1, 2]; Min Wang[3]; Josephine Ferreon[4]; Michael P. Suess[3]; Antrix Jain[5]; Anna Malovannaya[4]; Roberto Vera Alvarez[6]; Bruce D.P Pascal[6]; Raj Kumar[7]; Dean P. Edwards[3]; Patrick R. Griffin[1, 2]; [1]*Scripps Research, La Jolla, CA;* [2]*The Wertheim UF Scripps Institute, Jupiter, FL;* [3]*Department of Molecular and Cellular Biology, Baylor College of Medicine, Houston, TX;* [4]*Verna and Marrs McLean Department of Biochemistry and Molecular Pharmacology, Baylor College of Medicine, Houston, TX;* [5]*Mass Spectrometry Proteomics Core Facility, Baylor College of Medicine, Houston, TX;* [6]*Omics Informatics LLC, Honolulu, HI;* [7]*Department of Pharmaceutical and Biomedical Sciences, Touro College of Pharmacy, Touro University, New York, NY*

WP 616 **Understanding Instability Mechanisms and Developing Stabilization Strategies for Fibroblast Growth Factor 2**; Ruolan Cheng[1]; Igor A. Kaltashov[1]; [1]*University of Massachusetts Amherst, Amherst, MA*

WP 617 **Mass Spectrometry Reveals Effects of Sequence Complexity on Structure of α-Synuclein**; Olivia E Dioli[1]; Virginia K James[1]; Robert W Newberry[1]; Jennifer S Brodbelt[1]; [1]*University of Texas at Austin, Austin, TX*

WP 618 **Native Mass Spectrometry and Hydrogen Deuterium Exchange Illuminate the Role of Hydration in Transthyretin Tetramer Structural Dynamics**; Carter Lantz[1]; Robert Rider[1]; Syuan-Ting Kuo[1]; Sangho Yun[1]; Arthur Laganowsky[1]; David Russell[1]; [1]*Texas A&M University, College Station, TX*

WP 619 **Using HDX and Variable Temperature Studies to Evaluate How Shifts in Microstate Distributions Alter SR1-ADP Binding**; Kacie Evans[1]; He (Mirabel) Sun[1]; Carter Lantz[1]; David H. Russell[1]; [1]*Texas A&M University, College Station, TX*

WP 620 **The Structural Basis for Human Topoisomerase II Liquid-Liquid Phase Separation Uncovered via Crosslinking Mass Spectrometry**; Edgar Manriquez-Sandoval[1]; Stephen Fried[1]; [1]*Johns Hopkins University, Baltimore, MD*

WP 621 **Structural Proteomics by Phospho-Probing with Multiple Kinases Enhances the Detection of Conformational Changes of Substrate Proteins**; Asato Maeda[1]; Kosuke Ogata[1]; Naoyuki Sugiyama[1, 2]; Yasushi Ishihama[1, 3]; [1]*Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, Japan;* [2]*National Cerebral and Cardiovascular Center, Suita, Japan;* [3]*National Institutes of Biomedical Innovation, Health and Nutrition, Ibaraki, Japan*

WP 622 **Differential Scanning Fluorimetry and Circular Dichroism Investigation of Protein Structural Integrity after Laser Ablation Process**; Maiah Woodring[1]; Neda Feizi[1]; Kelcey B. Hines[2]; Bismark A. Nyaaba[1]; Kermit K. Murray[3]; Touradj Solouki[1]; Jonathan Clinger[1]; [1]*Baylor University, Waco, TX;* [2]*Louisiana State University, Baton Rouge, LA;* [3]*Louisiana State University, Baton Rouge, LOUISIANA*

WP 623 **Combining Microdroplet reactions with ExD fragmentation for fast characterization of proteins and antibody subunits**; Thomas E Walker[1]; Mike Knierman[2]; Harsha P. Gunawardena[3]; Hao Chen[4]; [1]*Agilent Technologies, Lexington, MA;* [2]*Agilent Technologies, Inc., Wilmington, Delaware;* [3]*JOHNSON AND JOHNSON, Spring House, PA;* [4]*New Jersey Institute of Technology, Newark, NJ*

WP 624 **Advancing mass spectrometry-based membrane protein footprinting with benzophenone, •CF3 and bromine radicals on an FPOP platform**; Tarang Jadav[1]; Ming Cheng[1]; Don Rempel[1]; Weikai Li[1]; Michael L. Gross[1]; [1]*Washington University in St.Louis, St.Louis, MO*

WP 625 **A study of the 20S proteasome by vT-ESI-CDMS reveals evidence for decay at high temperatures**; Akalanka Gunaratne[1]; Hua Pan[1]; Nick Rommel[1]; Martin Jarrold[1, 2]; David E. Clemmer[1, 2]; [1]*Indiana University Bloomington, Bloomington, IN;* [2]*Megadalton Solutions, Bloomington, Indiana*

WP 626 **Large-scale analysis ofproteinconformationsand interactions in live cellby CXMS**; Qun Zhao[1]; Li Li Zhao[2]; Yu Xin An[2]; Jing Chen[2]; Bei Rong Zhang[2]; Yu Kui Zhang[2]; Li Hua Zhang[2]; [1]*Dalian Institute of Chemical Physics, ACS, Dalian, China;* [2]*Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China*

WP 627 **X-CEMI: An Integrative Framework for Deciphering Dynamic Protein-Protein Interactions in Living Cells**; Beirong Zhang[1]; Zhou Gong[2]; Bowen Zhong[3]; Jing Chen[3]; Zhen Liang[3]; Yukui Zhang[3]; Qun Zhao[3]; Lihua Zhang[3]; [1]*State Key Laboratory of Medical Proteomics, National Chromatographic R. & A. Center, CAS Key Laboratory of Separa-tion Science for Analytical Chemistry, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China;* [2]*Innovation Academy for Precision Measurement Science and Technology, Chinese Academy of Sciences, Wuhan, China;* [3]*Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China*

WP 628 **Development and Application of Cross-Linking and Covalent Labeling to Structure-Function Characterization of the Dark Proteome**; Ashlyn N Dollar[1]; Erika Renbarger[1]; Kymeri E Davis[1]; Ian K. Webb[1]; [1]*Indiana University Indianapolis, Indianapolis, IN*

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WP 629 **Optimization of a Chemical Proteomics-based Platform for Cellular Kinase Profiling in Early Drug Discovery**; Xianmei Cai[1]; Zachary Cook[1]; Fang Fang[1]; Anthony Paiva[1]; Brian Anderson[1]; Yuka Amako[1]; Aya Kelly[1]; Helen Pham[1]; Ashok Dongre[1]; Brian Arey[1]; Wilson Shou[1]; [1]*Bristol-Myers Squibb.Co, Lawrence, NJ*

WP 630 **Distinguishing Meaningful Occupancy From Random Noise in Cases of Complete Dropout in Chemoproteomics Screens**; Jonathon OBrien[1]; Joseph Newhall[1]; Gina Turco[1]; Eitan Angel[1]; Ramin Rad[1]; *[1]Golgi Inc., Pleasant Hill, CA*

WP 631 **Development of a mass spectrometry-based approach for the stratification of functionally relevant single amino acid variants**; Flowreen Shikwana[1]; Halime Yilmaz[1]; Jessica J. Simon[2]; Dustin J. Maly[2]; Keriann Backus[1]; *[1]University of California, Los Angeles, Los Angeles, CA; [2]University of Washington, Seattle, WA*

WP 632 **Achieving reliability in high-throughput chemoprotemics screens with few or no replicates**; Jonathon OBrien[1]; Joseph Newhall[1]; Eitan Angel[1]; Gina Turco[1]; Ramin Rad[1]; *[1]Golgi LLC, Pleasant Hill, CA*

WP 633 **Elucidating Drug-Target Interactions in Ovarian Cancer Using Energy-Based Proteomics Methods**; Julia Ekiert[1]; Chang Liu[1]; Manead Khin[1]; Joanna E. Burdette[1]; Yu Gao[1]; *[1]University of Illinois at Chicago, Chicago, IL*

WP 634 **The timsTOF Ultra 2 enables systematic understanding of ubiquitination and degradation kinetics of degrader drug targets using slice-PASEF acquisition schemes**; Uli Ohmayer[1]; Martin Steger[1]; Björn Schwalb[1]; Bachuki Shashikadze[1]; Philipp Strohmidel[2]; Lisa Abel[2]; Daniel Hornburg[3]; *[1]NEOsphere Biotechnologies GmbH, Planegg, Germany; [2]Bruker Daltonics, Bremen, Germany; [3]Bruker Corporation, San Francisco, CA*

WP 635 **Development of a Chemical Proteomics Platform Using a Phenylglyoxal-Based Probe for Comprehensive Citrullinome Profiling to Reveal PAD Catalysis Insights**; Hung-Yu (Eric) Chiang[1]; Min Ma[2]; Miyang Li[3]; Lingjun Li[2, 3]; *[1]Biophysics Graduate Program, University of Wisconsin-Madison, Madison, WI; [2]School of Pharmacy, University of Wisconsin-Madison, Madison, WI; [3]Department of Chemistry, University of Wisconsin–Madison, Madison, WI*

WP 636 **Proteomic approaches to study the role of protein degradation in proteostasis and stress response**; Elena Markeviciute[1, 2]; Dr. Syed Azmal Ali[1]; Daniel Bollack[2]; Lina-Marie Wagner[1]; Toman Borteçen[1]; Prof. Jeroen Krijgsveld[1, 2]; *[1]German Cancer Research Center (DKFZ), Heidelberg, Germany; [2]Heidelberg University, Heidelberg, Germany*

WP 637 **Probing UBE2 Family Engagement and Kinome Target Space of a Novel Bifunctional Targeted Protein Degradation Modality**; Brian D Dill[1]; Tiffany V Saunders[1]; Clifford G Phaneuf[1]; Michael A Kiebish[1]; Stephane Gesta[1]; Niven R Narain[1, 2]; Dinesh Chimmanamada[3]; Vivek Vishnudas[1]; *[1]BPGbio, Framingham, MA; [2]University of Miami, FL, Miami, FL; [3]Coorg Biosciences, Arlington, MA*

WP 638 **A Novel Label-free, Solvent-based Method for Proteome-wide Monitoring of Drug Action in Live Cells**; Dominik Steinbrunn[1, 2]; Catalina Cepeleaga[1]; Alexander Betz[1]; Melanie Holzner[1]; Stefan K Maier[1]; Götz Hagemann[1]; Stephan Sieber[2]; Hannes Hahne[1]; *[1]OmicScouts GmbH, Freising, Germany; [2]TUM School of Natural Sciences, Department Biosciences, Chair of Organic Chemistry II, Center for Functional Protein Assemblies (CPA), Technical University Munich (TUM), Garching, Germany*

WP 639 **The secret life of proteins and drugs through the lens of proteome thermal stability**; Tove Bostrom[1]; Albert Arul[2]; Brett Larsen[3]; Ryan Bomgarden[4]; Joshua Kline[5]; Amanda Lee[6]; Rafael Melani[5]; Jingjing Huang[5]; Daniel Martinez Molina[1]; Alexey Chernobrovkin[1]; *[1]Pelago Bioscience AB, Stockholm, Sweden; [2]Thermo Fisher Scientific, Somerset, NJ; [3]Thermo Fisher Scientific, Mississauga, ON; [4]Thermo Fisher Scientific, Rockford, IL; [5]Thermo Fisher Scientific, San Jose, CA; [6]Thermo Fisher Scientific, Lexington, MA*

WP 640 **Bromo-desthiobiotin tag (Br-DTB) for unbiased profiling of chemical modification sites in human proteome**; Bibhuti Bhusana Palai[1]; Daniel Ramirez[1]; Zongtao Lin[1]; Benjamin A Garcia[1]; *[1]Washington University School of Medicine, St. Louis, MO*

WP 641 **Chymotrypsin as an Alternative Proteolytic Enzyme for Profiling Drug-Peptide Interactions**; Hogeun Kwak[1]; Jeongyeon Kang[1]; Donggyun Hong[1]; Hojin Yoo[1]; Namgil Lee[1, 2]; Heejung Yang[1, 2]; *[1]Bionsight, Inc., Chuncheon, South Korea; [2]Kangwon National University, Chuncheon, South Korea*

WP 642 **Dissecting the human phosphoproteome into its kinase components with dose-resolved proteomics**; Florian P Bayer[1]; Julian Müller[1]; Nicole Kabella[1]; Miriam Abele[1, 2]; Matthew The[1]; Bernhard Kuster[1, 2, 3]; *[1]Technical University of Munich, Freising, Germany; [2]Bavarian Center for Biomolecular Mass Spectrometry (BayBioMS), Freising, Germany; [3]German Cancer Research Center (DKFZ), Heidelberg, Germany*

WP 643 **Profiling extracellular vesicle-derived RNA interaction landscape in recipient immune cells**; Zheng Zhang[1]; Yi-Kai Liu[2]; Zhuojun Luo[2]; Marco Hadisurya[2]; Meng-Ju Wu[3]; Nabeel Bardeesy[4]; W. Andy Tao[2]; *[1]Purdue University, West Lafayette, IN; [2]Purdue Univeristy, West Lafayette, IN; [3]University of Massachusetts Chan Medical School, Worcester, MA; [4]Harvard Medical School, Boston, MA*

WP 644 **Towards a comprehensive chemoproteomics platform to accelerate covalent drug discovery**; Claude Shelton[1]; Ethan S. Toriki[1]; Francisco J. Garcia[1]; Jason P. Murphy[1]; Markus E. Schirle[1]; Scott M. Brittain[1]; *[1]Novartis, Cambridge, MA*

WP 645 **Drugging the Undruggable - Mass Spectrometry-Based Proteomics Screening at Industrial Scale**; Isabella Straub[1]; Andrea Foerner[1]; Patrick Allihn[1]; Thomas Wild[1]; Aarif Nazeer Batcha[1]; Florian Flenkenthaler[1]; Nagarjuna Nagaraj[1]; Christoph Schaab[1]; Felix Oppermann[1]; Andreas Tebbe[1]; Inaki Morao[2]; Andreas Weiss[3]; *[1]Evotec International GmbH, Munich, Germany; [2]Evotec (UK) Ltd, Abingdon, United Kingdom; [3]Evotec International GmbH, Göttingen, Germany*

WP 646 **Toward a Fully Automated Proteome Integral Solubility Alteration (PISA) Workflow for Scalable Target Identification**; Keith D Rivera[1]; Amanda H Damon[1]; Isabelle Kressy[1]; Namrata D Udeshi[1]; Steven A Carr[1]; *[1]Broad Institute, Cambridge, MA*

WP 647 **Capturing rapid protein responses in live cell cysteine profiling with sample multiplexing-based chemoproteomics**; Shaoxian Li[1]; Ka Yang[2]; Bohui Li[1]; Daniel Richards[1]; Itthipun Munkong[1]; Mike Rosenblatt[3]; Qing Yu[1]; *[1]Department of biochemistry and molecular biotechnology, University of Massachusetts Chan Medical School, Worcester, MA; [2]Department of Cell Biology, Harvard Medical School, Boston, MA; [3]Promega Corporation, Madison, WI*

WP 648 **Fast Photochemical Iodination and Capture by Suzuki Captures the State-dependent Proteome**; Miranda Villanueva[1]; Elijah B Biletch[2]; Andrew P Becker[2]; Nikolas R Burton[2]; Lisa M Boatner[2]; Nithesh Perumal[2]; Joelle Darrouj[2]; Ashley R Julio[2]; Julian Whitelegge[2]; Keriann M Backus[2]; *[1]UCLA, LOS ANGELES, CA; [2]UCLA, Los Angeles, CA*

WP 649 **Lipid- and protein-directed photosensitizer proximity labeling captures the cholesterol interactome**; Andrew P Becker[1, 2]; Elijah Biletch[1, 2]; John Paul Kennelly[1, 3]; Ashley R Julio[1, 2]; Miranda Villanueva[1, 2]; Rohith T Nagari[1, 3, 4]; Daniel W Turner[2]; Nikolas R Burton[1, 2]; *[1]Department of Biological Chemistry, David Geffen School of Medicine, UCLA, Los Angeles, California 6 90095, USA, Los Angeles, CA; [2]Department of Chemistry and Biochemistry, UCLA, Los Angeles, California 90095, USA, Los Angeles, CA; [3]Department of Pathology and Laboratory Medicine, David Geffen School of Medicine, UCLA, Los Angeles, Los Angeles, California 90095, USA, Los Angeles, CA; [4]Molecular Biology Institute, UCLA, Los Angeles, California 90095, USA, Los Angeles, CA*

WP 650 **Harnessing Automation and Data Analytics for Enhanced Biomolecular Insights in Covalent Cysteine Profiling**; Praveen Kumar; *AstraZeneca, Waltham, MA*

PROTEOMICS: CLINICAL APPLICATIONS
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WP 651 **A Technical Evaluation of Plasma Proteomics Technologies**; William F. Beimers[1]; Katherine A. Overmyer[1, 2, 3]; Pavel Sinitcyn[2, 4, 5]; Noah M. Lancaster[1, 6]; Scott T. Quarmby[1, 3]; Joshua J. Coon[1, 2, 3, 6]; *[1]Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI; [2]Morgridge Institute for Research, Madison, WI; [3]National Center for Quantitative Biology of Complex Systems, Madison, WI; [4]AI Technology for Life, Department of Information and Computing Sciences, Utrecht University, Utrecht, Netherlands; [5]Biomolecular Mass Spectrometry and Proteomics, Department of Pharmaceutical Sciences, Utrecht University, Utrecht, Netherlands; [6]Department of Chemistry, University of Wisconsin-Madison, Madison, WI*

WP 652 **Orbitrap Astral provides deep coverage of cerebrospinal fluid (CSF) derived small extracellular vesicle (SEV) proteome for clinical insights**; Yunyun ZHU[1]; Lauren Schmitt[1]; Kushani Attanayake[1]; Divyanshu Dubey[2]; Patrick Vanderboom[2]; *[1]Thermo Fisher Scientific, Lexington, MA; [2]Mayo Clinic, Rochester, MN*

WP 653 **Development and validation of a targeted mass spectrometry assay to quantify fibrinogen-gamma in the High School & Beyond study**; Carly A. I. Twigg[1]; Joohyun Ryu[1]; Jesenia M. Perez[2]; Jamie Enright[3]; Eric Grodsky[4]; Chandra L. Muller[5]; Bharat Thyagarajan[1]; John Robert Warren[6]; Stefani N. Thomas[1]; *[1]Department of Laboratory Medicine and Pathology, University of Minnesota School of Medicine, Minneapolis, MN; [2]Microbiology, Immunology, and Cancer Biology Graduate Program, University of Minnesota School of Medicine, Minneapolis, MN; [3]Hamline University, St. Paul, MN; [4]Department of Sociology, University of Wisconsin-Madison, Madison, WI; [5]Department of Sociology, University of Texas at Austin, Austin, TX; [6]Department of Sociology, University of Minnesota, Twin Cities, Minneapolis, MN*

WP 654 **Assessing Biological Age in Liver Transplantation: Proteomic Markers for Predicting Graft Viability and Patient Survival**; Sadr Shaheed[1, 2]; Letizia Lo Faro[1]; Chris W Sutton[3]; Benedikt Kessler[4]; James Hunter[1]; Rutger J Ploeg[1]; *[1]Nuffield Department of Surgical Sciences, University of Oxford, Oxford, United Kingdom; [2]NIHR Oxford Biomedical Research Centre, University of Oxford, Oxford, United Kingdom; [3]Institute of Cancer Therapeutics, University of Bradford, Bradford, United Kingdom; [4]Target Discovery Institute, University of Oxford, Oxford, United Kingdom*

WP 655 **Nanoparticle-enabled plasma proteomics of a preclinical atherosclerosis model reveals common signatures with human disease**; Constance Delwarde[1]; Joan T. Matamalas[1]; Sarvesh Chelvanambi[1]; Taku Kasai[1]; Gabriel Shlayen[1]; Elena Aikawa[1]; Masanori Aikawa[1]; Sasha A. Singh[1]; *[1]Brigham and Women's Hospital/Harvard Medical Sch, Boston, MA*

WP 656 **Proteomic analysis of corneal layers after trigeminal denervation: insights into inflammation and intracellular clearance in the epithelium, stroma, and endothelium**; Pei-Shan Wu[1]; I-Lian Tsai[1]; Miao-Hsia Lin[2]; Hsin-Yu Liu[1]; *[1]Department of Ophthalmology, National Taiwan University Hospital, College of Medicine, National Taiwan University, Taipei, Taiwan; [2]Department of Microbiology, National Taiwan University College of Medicine, Taipei, Taiwan*

WP 657 **Application of High-Resolution Mass Spectrometry to Assess Plasma Proteome Stability Collected by First Responders for Sudden Cardiac Arrest Biomarker Studies**; Jihyeon Lee[1]; Kotoka Nakamura[1]; Qin Fu[1]; Kyndaron Reinier[1]; Ali Haghani[1]; Harpriya Chugh[1]; Sumeet S. Chugh[1]; Jennifer Van Eyk[1]; *[1]Cedars Sinai Medical Center, Los Angeles, CA*

WP 658 **A Comparative Assessment of Sample Preparation Methods for Biomarker Discovery from Plasma**; Angie L Mordant[1]; Aurora Cabrera[1]; Thomas S Webb[1]; Natalie Barker-Krantz[1]; Scott P Lyons[1]; Claire Critchley[2]; Yara Abdou[3]; Hyman Muss[3]; Laura E Herring[1]; *[1]Department of Pharmacology, UNC Metabolomics & Proteomics Core Facility, University of North Carolina at Chapel Hill, Chapel Hill, NC; [2]Department of Epidemiology, University of North Carolina at Chapel Hill, Chapel Hill, NC; [3]Department of Medicine, Lineberger Comprehensive Cancer Center, University of North Carolina at Chapel Hill, Chapel Hill, NC*

WP 659 **Implementation of mass spectrometry-based proteomics of clinically-relevant low-input samples as a standard service in a core facility**; Keshava Krishna Datta[1]; Ching-Seng Ang[1]; Michael G Leeming[1]; Swati Varshney[1]; Nicholas A Williamson[1]; *[1]University of Melbourne, Melbourne, Australia*

WP 660 **Rapid capillary flow chromatography coupled to data-independent mass spectrometry setup for bottom-up plasma proteomics of large cohorts**; Andreas Schmidt[1]; Raphael Schuster[1]; Stephanie Kaspar-Schoenefeld[1]; Markus Lubeck[1]; *[1]Bruker Daltonics GmbH & Co. KG, Bremen, Germany*

WP 661 **Controlling hemolysis in DIA-based blood proteomics improves biomarker reliability for tracking cirrhosis progression and early cancer detection**; Henry Unger[1, 2]; Sebastian Burbano de Lara Carrillo[1, 2]; Agustin Rodriguez Gonzalez[1]; Franziska Gödtel[1]; Katharina Büchner[1]; Leonie Wilhelm[1]; Sherin Al Aoua[3]; Piotr Zadora[1, 2]; Wolf-Dieter Lehmann[1]; Marcel Schilling[1]; Madlen Matz-Soja[2, 4]; Heike Bantel[2, 3]; Marc Schneider[5, 6]; Thomas Mulley[5, 6]; Thomas Berg[2, 4, 7]; Dominic Helm[2, 8]; Barbara Helm[1, 6]; Ursula Klingmüller[1, 2, 6]; *[1]Division Systems Biology of Signal Transduction, German Cancer Research Center (DKFZ), Heidelberg, Germany, Heidelberg, Germany; [2]Liver Systems Medicine against Cancer (LiSyM-Krebs), Germany, Heidelberg, Germany; [3]Department of Gastroenterology, Hannover Medical School (MHH), Hannover, Germany, Hannover, Germany; [4]Clinic and Polyclinic for Oncology, Gastroenterology, Hepatology and Pneumology, Leipzig University Hospital, Leipzig, Germany, Leipzig, Germany; [5]Translational Research Unit, Thoraxklinik at Heidelberg University Hospital, Heidelberg, Germany, Heidelberg, Germany; [6]German Center for Lung Research (DZL) and Translational Lung Research Center Heidelberg (TRLC), Heidelberg, Germany, Heidelberg, Germany; [7]Medical Faculty, Leipzig University, Leipzig, Germany, Leipzig, Germany; [8]Proteomics Core Facility, German Cancer Research Center (DKFZ), Heidelberg, Germany*

WP 662 **PRM-based approach for defining p16-positive head and neck squamous cell carcinoma**; David J Clark[1]; Camille Lombard-Banek[1]; Sudhanshu Abhishek[1]; Steve Sweet[1]; David Chain[1]; Lara McGrath[2]; Isabella Tilmont[1]; Ross Stewart[3]; Yeoun Jin Kim[1]; *[1]AstraZeneca, Gaithersburg, MD; [2]AstraZeneca, Waltham, MA; [3]AstraZeneca, Cambridge, United Kingdom*

WP 663 **Leveraging 4D-DIA mass spectrometry and nano-particle enrichment to capture proteomic signatures of acute myeloid leukaemia in longitudinal plasma samples**; Gethin R Thomas[1, 2]; Marcus Bantscheff[2]; Koroosh Korfi[1]; Donata DeMarco[1]; *[1]Roche Pharma Research and Early Development (pRED), Pharmaceutical Sciences (PS), Basel, Switzerland; [2]Roche Pharma Research and Early Development (pRED), 360Labs, Basel, Switzerland*

WP 664 **Benchmarking mass spectrometry- and NGS-based solutions for plasma and serum proteomics from a multiomics core facility perspective**; Tobias Kockmann[1]; Claudia Fortes[1]; Catharine Aquino[1]; Hubert Rehrauer[1]; Gino Bonazza[2]; Przemyslaw Blyszczuk[2]; Gabriela Kania[2]; Oliver Distler[2]; Ralph Schlapbach[1]; Paolo Nanni[1]; *[1]Functional Genomics Center Zurich, Zurich, Switzerland; [2]University Hospital, Zurich, Switzerland*

WP 665 **Analysis of Single Human Oocytes by Proteoform Imaging Mass Spectrometry**; Nickolas P Fisher[1]; Vijaya Kanchustambham[1]; Hannah McDowell[2]; Indira Pla[1]; Diane Saunders[2]; Jared Kafader[1]; Monica M Laronda[2, 3]; Neil Kelleher[1]; *[1]Northwestern University, Evanston, IL; [2]Stanley Manne Children's Research Institute, Ann & Robert H. Lurie Children's Hospital of Chicago; Departments of Pediatrics,* *Feinberg School of Medicine, Northwestern University, Chicago, IL; [3]Departments of Obstetrics and Gynecology, Feinberg School of Medicine, Northwestern University, Chicago, IL*

WP 666 **Clinical Results of a mCRPC Cohort with Automated MALDI Sample Preparation Utilizing the Felix Liquid Handler and Active Drier**; Amanda Weaver[1]; Avery Diercks[1]; Colin McDowell PhD[1]; Reis Pestano[1]; Ethan Barnett PhD[2]; Tatiana Erazo PhD[2]; Howard Scher MD[2]; Gary Pestano PhD[1]; *[1]Biodesix, Louisville, CO; [2]Memorial Sloan Kettering Cancer Center, New York, NY*

WP 667 **Absolute quantification of mismatch repair (MMR) proteins in formalin-fixed, paraffin-embedded (FFPE) tissue by FAIMS-PRM**; Beom-Jun Kim[1]; Steve M Sweet[1]; Camille Lombard-Banek[1]; David C Chain[1]; Christopher Richardson[1]; Stephanie Zalesak-Kravec[1]; Yeoun Jin Kim[1]; *[1]AstraZeneca, Gaithersburg, Maryland*

WP 668 **Investigating platelet proteome variability in Canadian blood donors using DIA-PASEF mass spectrometry**; Elyn Rowe[1]; Loktin Hui[2]; Xiaojing Yuan[2]; Marcus Shew[1]; Noor Ali-Mohamad[1]; Jason Rogalski[2]; James Johnson[1]; *[1]Department of Cellular and Physiological Sciences, UBC, Vancovuer, BC; [2]UBC Proteomics and Metabolomics Core Facility, Vancouver, BC*

WP 669 **Development of a prm-PASEF assay for the subtyping of Small Cell Lung Cancer in minimally invasive biopsy specimens**; Ashley R Wooten[1]; Marina K Baine[1]; Michael Krawitzky[2]; Jessica R Chapman[1]; *[1]MSKCC, New York, NY; [2]Bruker Daltonics GmbH & Co. KG, Billerica, MA*

WP 670 **High-Throughput Urinary Proteome Profiling for the Discovery of Biomarkers Associated with Neurogenic Injury and Bladder Dysfunction**; Yang Tang[1]; Shannon E. DiMartino[1]; Kyle L. Katamba[1]; Emily Morrison[1]; Abby Cotsonas[1]; Stuart B. Bauer[1, 2]; Rosalyn M. Adam[1, 2]; John W. Froehlich[1, 2]; Richard S. Lee[1, 2]; *[1]Boston children's hospital, Boston, MA; [2]Harvard Medical School, Boston, MA*

WP 671 **Sequential immunoprecipitation-mass spectrometry method to characterize the dystrophin associated protein complex in skeletal muscle**; Emily H Canessa[1]; Bukola K Ojo[1]; Rita Spathis[1]; James S Novak[2]; Kanneboyina Nagaraju[1]; Yetrib Hathout[1]; *[1]Binghamton University, Binghamton, NY; [2]Children's National Research and Innovation Campus, Washington D.C., DC*

WP 672 **A pilot study on proteomic changes of human cerebrospinal fluid of Parkinson's disease after cell therapy**; Guoting Qin[1]; Yunxin Fu[2]; Mya C. Schiess[2]; Juan D. Martinez Lemus[2]; Emily Tharp[2]; Mohanmmad Shahnawaz[2]; Tirthankar Sinha[2]; Jennifer Copeland[3]; Huamin Cai[3]; Stan Stearns[3]; Chengzhi Cai[1]; *[1]University of Houston, Houston, TX; [2]University of Texas Health Science Center at Houston, Houston, TX; [3]VICI Valco Instruments, Houston, TX*

WP 673 **Proteomic Profiling of RAR Agonist and ERK ½ Modulator in Asthma Relevant Cell Models**; Vanshika Patel[1]; Jianshi Yu[1]; Mehari Weldemariam[1]; Paul Shapiro[1]; Deepak Deshpande[2]; Maureen A Kane[1]; *[1]University of Maryland, School of Pharmacy, Department of Pharmaceutical Sciences, Baltimore, MD; [2]Center for Translational Medicine, Jane and Leonard Korman Lung Center, Thomas Jefferson University, Philadelphia, Pennsylvania*

WP 674 **Combined Olink and LC-MS/MS Analysis of Skin Tapes Provides Extensive Proteome Coverage** ; Jessica Moore[1]; Kyra Richardson[1]; Jaison Arivalagan[1]; Alejandra Stihel[1]; Tiffany Louie[1]; Dragana Noe[1]; Danielle Gutierrez[1]; *[1]Discovery Life Sciences, Huntsville, AL*

WP 675 **Identification and quantification of 4-HNE-adducted proteins to study the metabolic disorders of the ALDH2 gene mutation**; Fu-An Li[1]; Ling Hui Wang[2]; *[1]Institute of Biomedical Sciences, Academia Sinica, Taipei, Taiwan; [2]Institute of Biomedical Sciences, Academia Sinica, Taipei, Taiwan, Taipei, Taiwan*

WP 676 **DiSignEVs: High sensitivity and high throughput analysis of disease signatures in extracellular vesicles using novel nanoLC and Ultra2 timsTOF**; Ulrike Resch[1]; Florian Busch[2]; Petra Martinovic[3]; Torsten Mueller[3]; Manuel R. Bauer[2]; Mario Mirabelli[2]; Martin Schirmer[3]; Goran Mitulovic[4]; *[1]Institute of Vascular Biology and Thrombosis Research, Medical University of Vienna, Vienna, Austria; [2]Bruker Switzerland AG, Fällanden, Switzerland; [3]Bruker Daltonics GmbH & Co.KG, Bremen, Germany; [4]Bruker Daltonics, Vienna, Austria*

WP 677 **Addressing the Plasma Proteomics Needs of Large-Scale Clinical Cohorts**; Cassandra G Kempf[1, 2]; Michaela Schwaiger-Haber[3]; Ethan Stancliffe[4]; Leah P Shriver[2, 3, 5]; Gary J Patti[2, 3, 5]; *[1]Washington University in St Louis, St. Louis, MO; [2]Center for Mass Spectrometry and Metabolic Tracing, Washington University in St. Louis, St. Louis, MO; [3]Washington University in St. Louis, St. Louis, MO; [4]Panome Bio, Saint Louis, MO; [5]Washington University in St. Louis School of Medicine, St. Louis, MO*

WP 678 **Simplifying Clinical Mass Spectrometry: Coupling the SISCAPA Workflow with the Stellar Mass Spectrometer for Protein Biomarker Quantification**; Richard Yip[1]; Deanna L Plubell[2]; Andrew Hettle[1]; Morteza Razavi[1]; Andrew N Hoofnagle[2]; Michael J MacCoss[2]; Leigh Anderson[1]; *[1]SISCAPA Assay Technologies Inc., Victoria, BC; [2]University of Washington, Seattle, WA*

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WP 679 **Disruption of ClpX overcomes antifungal resistance in Cryptococcus neoformans through modified heme biosynthesis and ergosterol production**; Michael J P Woods[1]; Arianne Bermas[1]; Brianna Ball[1]; Benjamin Muselius[1]; Norris Chan[1]; Davier Gutierrez-Gongora[1]; Jason McAlister[1]; Stephan Sieber[2]; Jennifer Geddes-McAlister[1]; *[1]University of Guelph, Guelph, ON; [2]TUM School of Natural Sciences, Department Biosciences, Chair of Organic Chemistry II, Center for Functional Protein Assemblies (CPA), Technical University Munich (TUM), Garching, Germany*

WP 680 **Differential proteomic profile of neutrophils in response to tetra- and hexa-acylated lipopolysaccharides**; Jose R Pittaluga[1]; Vanya Bhushan[1]; Jiraphorn Issara-Amphorn[1]; Aleksandra Nita-Lazar[1]; *[1]Functional Cellular Networks Section, Laboratory of Immune System Biology, National Institute of Allergy and Infectious Diseases, National Institutes of Health, Bethesda, MD*

WP 681 **A proteomic investigation of the macrophage response to toll-like receptor 4 stimulation using lipid A variants**; Sung Hwan Yoon[1]; Doeun Kim[1]; Hyojik Yang[2]; Robert K Ernst[2]; Aleksandra Nita-Lazar[1]; *[1]NIH/NIAID, Bethesda, MD; [2]University of Maryland, Baltimore, MD*

WP 682 **Host protein turnover dynamics and PTM crosstalk in macrophages during Salmonella typhimurium infection.**; Sandhini Saha[1]; Aleksandra Nita Lazar[1]; *[1]National Institutes of Health, Bethesda, MD*

WP 683 **Quantitative subcellular-temporal proteomics coupled with machine learning-based computational modeling to identify changes in protein signaling networks in innate immune responses**; Vanya Bhushan[1]; Aleksandra Nita-Lazar[1]; *[1]NIH/NIAID, Bethesda, MD*

WP 684 **Pseudomonas aeruginosa adaptive lipid A structures in the Cystic Fibrosis airway and their impact within the bacterial membrane proteome**; Ian O'Keefe[1]; Casey E Hofstaedter[2]; Linda Nartey[3]; David R. Goodlett[3, 4]; Robert K. Ernst[2]; *[1]Department of Biochemistry and Molecular Biology, University of Maryland – Baltimore, Baltimore, MD, USA, 21201, Baltimore, MD; [2]University of Maryland, Baltimore, Baltimore, MD; [3]University of Victoria, Victoria, BC; [4]University of Victoria GBC Proteomics Centre, Victoria, BC, BC*

WP 685 **Investigating the Influence of RNA Replication on Host Proteome Dynamics in BHK-21 Cells**; Alyssa Cruz[1];

Joseph Loo[1]; William Gelbart[1]; Yu Chen[1]; *[1]UCLA, Los Angeles, CA*

WP 686 **Mass Spectrometry-Based Proteomic Analysis of Mycobacterium tuberculosis Isolates from Kazakhstan**; Dana Auganova[1]; Sabina Atavliyeva[1]; Akmaral Akisheva[2]; Anna Tsepke[2]; Pavel Tarlykov[1]; *[1]National Center for Biotechnology, Astana, Kazakhstan; [2]City Center for Phthisiopulmonology of the Akimat of Astana, Astana, Kazakhstan*

WP 687 **Data-Independent Acquisition (DIA) Elucidation of the sigM Dependent Regulatory Pathway in Pathogenic Mycobacterium abscessus**; Emily R. Bravo[1]; Sadie R. Schultz[1]; Jill G. Canestrari[2]; Todd A Gray[2]; Keith M. Derbyshire[2]; Matthew M Champion[1]; *[1]Department of Chemistry and Biochemistry, University of Notre Dame, Notre Dame, IN; [2]Division of Genetics, Wadsworth Center, New York State Department of Health, Albany, NY*

WP 688 **FAIMS-DIA-MS reveals plasma and liver proteome alterations following acute lymphocytic choriomeningitis viral infection**; Ibukunoluwa Sodiya[1]; Molly T. Soper-Hopper[1]; Colt Capan[1]; Emily Wolfrum[1]; Lisa Decamp[1]; Russell Jones[1]; Hyoungjoo Lee[1]; Ryan D Sheldon[1]; *[1]Van Andel Institute, Grand Rapids, MI*

WP 689 **Global Proteomic Analysis of Ebola Virions Reveals Presence of Antiviral Restriction Factors APOBEC3D, TRIM22 and TRIM5**; Jyothirmai Simhadri[1]; Andrey Ivanov[1]; Bersabeh Tigabu[2]; Namita Kumari[1]; Colette A. Pietzsch[2]; Xionghao Lin[1]; Alexander Bukreyev[2]; Sergei Nekhai[1]; *[1]Howard University, Washington, DC; [2]University of Texas Medical Branch, Galveston, TX*

WP 690 **Detection of bovine mastitis pathogens in milk using machine learning defined peptide signature and targeted proteomics**; Antoine Lacombe-Rastoll[1]; Florence Roux-Dalvai[1]; Caroline Chénard[2]; Elloise Coyle[1]; Mickaël Leclercq[1]; Marie-Hélène Lessard[3]; Steve Labrie[3]; Simon Dufour[2]; Arnaud Droit[1]; *[1]AD Lab - Proteomics and Computational Biology laboratory, CHU de Québec Université Laval Research Centre, Québec, QC; [2]Department of Pathology and Microbiology, Faculty of Veterinary Medicine, Université de Montréal, Saint-Hyacinthe, QC; [3]Department of Food Sciences and Nutrition, STELA Dairy Research Center, Institute of Nutrition and Functional Foods,Université Laval, Quebec, QC*

WP 691 **An Oncogenic Virus Remodels its Cellular Microenvironment at the Tumor-Infection Interface**; James C Kostas[1]; William Rodriguez[1]; Ileana M Cristea[1]; *[1]Princeton University, Princeton, NJ*

WP 692 **Too Hot to Handle: Stability Proteomics Reveals Antimalarial Drug Targets**; Jerzy M Dziekan[1]; Arne Alder[2]; Sachin Khurana[3]; Sofia Mortensen[4]; Holger Sondermann[4]; Tim Gilberger[2]; Alan F Cowman[3]; *[1]The Walter and Eliza Hall Institute of Medical Research, Melbourne, Australia; [2]Bernhard Nocht Institute for Tropical Medicine (BNITM), Hamburg, Germany; [3]Walter and Eliza Hall Institute of Medical Research, Melbourne, Australia; [4]CSSB Centre for Structural Systems Biology, Deutsches Elektronen Synchroton DESY, Leibniz Institute of Virology, Hamburg, Germany*

WP 693 **Precise Mycobacterial Species and Subspecies Identification Using the PEP-TORCH Peptidome Algorithm**; Duran Bao[1]; Sudipa Maity[1]; Bo Ning[1]; Seungyeon Seo[2]; Adrian Zelazny[2]; Jia Fan[1]; *[1]Tulane University, New Orleans, LA; [2]NIH, Bethesda, MD*

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WP 694 **Hypothesis-free discovery of the subcellular proteome using Microscoop©**; Chantal Hoi Yin Cheung[1]; Yi-De Chen[1]; Chia-Wen Chung[1]; Hsiao-Jen Chang[1]; Chun-Kai Huang[1]; Weng Man Chong[1]; Jung-Chi Liao[1]; Azad Gucwa[1]; *[1]Syncell Inc, Taipei, Taiwan*

WP 695 **Comprehensive workflow of spatial proteomics based on laser microdissection and high resolution mass spectrometry**; Yang Song[1]; Ji Luo[1]; Hongxu Chen[2]; Bingjie Liu[2]; *[1]SCIEX, Shanghai, China; [2]SCIEX, Beijing, China*

WP 696 **Coupling laser-induced dissociation in the visible range with mass spectrometry to improve the detection and quantification of Staphylococcus Aureus enterotoxins**; Annabelle MÉDALIN[1]; Benjamin YOUENOU[2]; Chloé DESBIOLLES[3]; Roxane PRAT[3]; Cédric BADIOU[4]; François VANDENESH[3, 4]; Jérôme LEMOINE[1]; Marion GIROD[1]; *[1]Institut of Analytical Sciences, Villeurbanne, France; [2]Centre National de Référence des Staphylocoques, LYON, France; [3]Institut des agents infectieux, LYON, France; [4]Center for Infectiology Research - UMR5308, LYON, France*

WP 697 **Development of a novel LC method to limit carryover in DIA-MS experiments on the Thermo Astral**; Brandon Harder[1]; Mrittika Bhattacharya Bacharya[1]; Rod Mathews[1]; Veronica Anania[1]; *[1]Genentech Inc., South San Francisco, CA*

WP 698 **Disease and Cell-Type-Specific Surface Protein Profiling of 100-500 Cells using an Ultrasensitive Affinity Purification Mass Spectrometry System**; Amanda C. Lorentzian[1]; Juliet M. Bartleson[1]; Terence Ho[1]; Zhichang Yang[1]; Meena Choi[1]; Tommy K. Cheung[1]; Christopher M. Rose[1]; William T. Yewdell[1]; Ying Zhu[1]; *[1]Genentech Inc., South San Francisco, CA*

WP 699 **Benchmarking Bruker timsTOF Ultra 2 for deep proteomic profiling of human tissues**; Hieu T Nguyen[1]; Yasaman Jami[1]; Hendrik Neubert[1]; *[1]Pfizer, Andover, MA*

WP 700 **Probing CAR-T interaction networks using proximity proteomics for improved immunotherapies**; Bianca Dupont[1, 2]; Tammy-Lynn Tremblay[2]; Jennifer Hill[2]; Scott McComb[1, 2]; Mathieu Lavallée-Adam[1]; Joey Sheff[1, 2]; *[1]University of Ottawa, Ottawa, ON; [2]National Research Council Canada, Ottawa, ON*

WP 701 **Cell-type Specific Proteomic Profiling of Neuronal Subtypes in Mouse Brain Using in-situ Antibody-mediated Biotinylation**; Kyungdo Kim[1]; Taekyung Ryu[1]; Chan Hyun Na[1]; *[1]Johns Hopkins School of Medicine, Baltimore, MD*

WP 702 **Enhancing Cell-Free Lysate Protein Production through Guided Proteomic Profiling**; Jana M Carpenter[1]; Conor Jenkins[1]; Katherine Rhea[1]; Elizabeth Dhummakupt[1]; Aleksandr Miklos[1]; *[1]US Army, Aberdeen Proving Ground, MD*

WP 703 **High-Throughput Characterization of Tau Proteoforms in Alzheimer's Disease Mouse Brain Using Capillary Isoelectric Focusing-Mass Spectrometry**; Reyhane Tabatabaeian Nimavard[1]; Amirhossein Sadeghi[2]; Fei Fang[2]; Hsiao Tien Chien[2]; Min Kuo[2]; Liangliang Sun[2]; *[1]Michigan State University, East Lansing, MI; [2]Michigan State university, EAST LANSING, MI*

WP 704 **Multi-Draw: Revolutionizing Lyophilization-Free LC-MS Proteomics with Large Volume Injections**; Runsheng Zheng[1]; Odeta Dembovskytė[2]; Dennis Koehler[3]; Christopher Pynn[3]; Claudio De Nardi[3]; Alec Valenta[3]; Wim Decrop[3]; Lukas Taujenis[2]; Martin Samonig[3]; *[1]Thermo Fisher Scientific, Germering, Germany; [2]Thermo Fisher Scientific, Vilnius, Lithuania; [3]Thermo Fisher Scientific, Germering, Germany*

WP 705 **SynchroSep-MS: Parallel LC Separations for Multiplexed Proteomics**; Noah M. Lancaster[1, 2]; Bingnan Zhao[1, 2]; Li-Yu Chen[1, 2]; Benton J. Anderson[1, 2]; Katherine A. Overmyer[1, 2, 3]; Scott T. Quarmby[1, 2]; Mitchell D. Probasco[3]; Joshua J. Coon[1, 2, 3]; *[1]University of Wisconsin-Madison, Madison, WI; [2]National Center for Quantitative Biology of Complex Systems, Madison, WI; [3]Morgridge Institute for Research, Madison, WI*

WP 706 **Multidrug Proteasome Inhibition to Stabilize the Mycobacterial Small Proteome**; Hannah A. Marietta[1]; Emily R. Bravo[1]; Matthew M Champion[1]; *[1]University of Notre Dame, Notre Dame, IN*

WP 707 **Investigating USP18 inhibitor mode of action with SEC-MS**; Yingrong Xu[1]; Feng Wang[1]; Masaya Yamaguchi[1]; Agustin Casimiro-Garcia[2]; Graham West[1]; *[1]Pfizer Inc., Groton, CT; [2]Pfizer Inc., Cambridge, MA*

WP 708 **Rapid Monoclonal Antibody Characterization Using cVSSI-Based Direct Infusion DIA-MS for Peptide Mapping and PTM Analysis**; Herbi Yuliantoro[1]; Olanrewaju Awoyemi[2]; Amanda DeVor[2]; Stephen Valentine[1]; Peng Li[1]; *[1]West Virgina University, Morgantown, WV; [2]West Virginia University, Morgantown, WV*

WP 709 **Development of a Thiol Exchange- and Mass Spectrometry-Based Proteomic Method for Thermodynamic Measurements of Protein Folding Stability**; Yueqi Chen[1]; Jhih-Hao Ho[1]; Michael C. Fitzgerald[1]; *[1]Duke University, Durham, NC*

WP 710 **Simple in-cell processing enables deep proteome profiling of plant leaf**; Deji Adekanye[1]; Yu Yanbao[2]; Jeffrey Caplan[2]; *[1]University of Delaware, Newark, DE, DE; [2]University of Delaware, Newark, DE*

WP 711 **Development and Application of a Sub-Minute Gradient Capillary LC/MS/MS for Robust and High Throughput Proteomics**; Kosuke Ogata[1]; Ayana Tomioka[1]; Ryota Tomioka[1]; Hiroto Kakiuchi[1]; Eisuke Kanao[1, 2]; Koshi Imami[3]; Naoyuki Sugiyama[4]; Yasushi Ishihama[1, 2]; *[1]Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, Japan; [2]National Institutes of Biomedical Innovation, Health and Nutrition, Ibaraki, Japan; [3]RIKEN Center for Integrative Medical Sciences, Yokohama, Japan; [4]National Cerebral and Cardiovascular Center, Suita, Japan*

WP 712 **From the Bronze Age to nuclear medicine: unravelling the high resolution mass spectrometry in proteomics**; Marta Benazzi[1]; Serena Arpaia[1]; Carmen Domìnguez Castillo[1]; Enrica Frasca[1]; Sebastiano Maria Salomone Micocci[1]; Simonetta Geninatti Crich[1]; Sonja Visentin[1]; Claudio Medana[1]; Claudio Cavazzuti[2]; Beatrice Demarchi[1]; Federica Dal Bello[1]; *[1]University of Turin, Torino, Italy; [2]University of Bologna, Bologna, Italy*

WP 713 **Analysis of the global histone modification landscape in mouse tissue using nano C18-monolithic column and timsTOF HT**; Bella Bruszel[1]; Domenico Marano[1]; Gaia Novarino[2]; Armel Nicolas[1]; Petra Martinovic[3]; Mario Mirbelli[4]; Goran Mitulovic[5]; *[1]Institute of Science and Technology Austria, Maria Gugging, Austria; [2]Institute of Sceince and Technology Austria, Maria Gugging, Austria; [3]Bruker Daltonik GmbH, Bremen, Germany; [4]Bruker Switzerland AG, Fällanden, Switzerland; [5]Bruker Daltonics, Vienna, Austria*

WP 714 **Developing an Adapted SP3 Digest Protocol to Detect Adhesive Proteins**; Sarah C Beno[1]; Neda Feizi[1]; Bismark A. Nyaaba[1]; Touradj Solouki[1]; *[1]Baylor University, Waco, TX*

WP 715 **Batch-Specific Imputation Facilitates the Correction of Batch Effect in DIA Proteomics Data Evidenced by Controlled Quantitative Experiments**; Shichen Shen[1]; Yeoun Jin Kim[1]; Andrew Chambers[1]; *[1]AstraZeneca, Gaithersburg, MD*

WP 716 **Expediting Deep Proteome Sequencing and Splicing Variant Discovery Using Orbitrap Astral**; Li-Yu Chen[1, 2]; Katherine A. Overmyer[2, 3, 4]; Scott T. Quarmby[2, 4]; Michael Rosenblatt[5]; Alba Katiria González Rivera[5]; Joshua J. Coon[1, 2, 3, 4]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [2]Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI; [3]Morgridge Institute for Research, Madison, WI; [4]National Center for Quantitative Biology of Complex Systems, Madison, WI; [5]Promega Corporation, Madison, WI*

WP 717 **Experimental Characterization of Automated Emitter Position Optimization Strategies for a New Low-Flow Ion Source and Cartridge**; Joshua A Silveira[1]; Katherine Walker[1]; Matt Tsai[1]; Gary A Schultz[2]; Cornelia Boeser[1]; Eloy R. Wouters[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Munson Technology, Ithaca, NY*

WP 718 **Accelerating the verification of predictive biomarkers of PARP inhibitor resistance in ovarian cancer using highly multiplexed PRM assays**; Jolene M. Duda[1]; Trudy J. Philips[2]; Qingling Li[3]; Cristina Jacob[3]; Stephanie N. Samra[3]; Stefani N. Thomas[4]; *[1]University of Minnesota, Department of Biochemistry, Molecular Biology, and Biophysics, Minneapolis, MN; [2]University of Minnesota, Molecular Pharmacology and Therapeutics Graduate Program, Minneapolis, Minnesota; [3]Thermo Fisher Scientific, 355 River Oaks Pkwy, San Jose, California; [4]University of Minnesota, Department of Laboratory Medicine and Pathology, Minneapolis, MN*

WP 719 **Adaptive Focused Acoustics (AFA™) Technology for Optimized Tissue Processing in Global Proteomics**; Juan Wang; *AstraZeneca, Waltham, MA*

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WP 720 **Cell-to-cell proteome changes induced by Bcl-2-overexpression in single TNBC-cells. Deep single-cell proteome coverage complemented with 5-minute SCP for accurate quantitation**; Stanislau Stanisheuski[1]; Jacob Porter[2]; Andrew Emili[2]; Siva Kolluri[1]; Claudia S. Maier[1]; *[1]Oregon State University, Corvallis, OR; [2]Oregon Health & Science University, Portland, OR*

WP 721 **5-Minute Single Cell Proteomics**; Stanislau Stanisheuski[1]; Sima Ziyaee[1]; Hyo Sang Jang[2]; Alex Eddins[1]; Liping Yang[1]; Claudia S. Maier[1]; *[1]Oregon State University, Corvallis, OR; [2]HP Inc., Corvallis, OR*

WP 722 **Comparison of static-nanospray- and liquid chromatography-mass spectrometry for single-cell metabolomics applied to infectious diseases, utilizing a modified hybrid Orbitrap MS**; Abigail Cook[1]; Rahul Deshpande[2]; Susan Bird[2]; Dany Beste[1]; Melanie Bailey[1]; *[1]University of Surrey, Guildford, United Kingdom; [2]Thermo Fisher Scientific, San Jose, CA*

WP 723 **Balancing Sensitivity and Throughput in Single-Cell Proteomics using Low-Nanoflow LC-MS**; Runsheng Zheng[1]; Manuel Matzinger[2]; Rupert Mayer[2]; Alec Valenta[3]; Christopher Pynn[3]; Wim Decrop[3]; Dominic Hoch[4]; Martin Samonig[3]; Karl Mechtler[2]; *[1]Thermo Fisher Scientific, Germering, Germany; [2]Institute of Molecular Pathology, Vienna, Austria; [3]Thermo Fisher Scientific, Germering, Germany; [4]Thermo Fisher Scientific, Reinach, Switzerland*

WP 724 **Improving the Limit of Quantification for Single-Cell Proteomics by Novel Acquisition Strategies on a Modified Orbitrap Astral Mass Spectrometer**; Jakob Woessmann[1]; Arrey Tabiwang[2]; Benjamin Furtwängler[1]; Hamish Stewart[2]; Johannes Petzoldt[2]; Valdemaras Petrosius[1]; Eugen Damoc[2]; Vlad Zabrouskov[3]; Bo Porse[4]; Erwin Schoof[1]; *[1]Technical University of Denmark, Kongens Lyngby, Denmark; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [3]Thermo Fisher Scientific, San Jose, CA; [4]Finsen Laboratory, Copenhagen, Denmark*

WP 725 **Novel integration of capillary sampling with inductively coupled plasma and liquid chromatography mass spectrometry for sub-cellular proteomics and metallomics**; Melanie Bailey[1, 2]; Dany Beste[1]; Phil Blower[2]; Abigail Cook[1]; Davison Claire[1]; Pedro Arragon Fernandez[3]; Emily Fraser[1, 2]; Nicholas Locker[4]; Sneha Pinto[1]; Erwin Schoof[3]; Matt Spick[1]; Monica Felipe Sotelo[1]; Kasia Wulfmeier[2]; *[1]University of Surrey, Guildford, United Kingdom; [2]Kings College London, London, United Kingdom; [3]Technical University of Denmark, Kongens Lyngby, Denmark; [4]Pirbright Institute, Surrey, United Kingdom*

WP 726 **Using Desorption Electrospray Ionization Mass Spectrometry Imaging (DESI-MSI) for Single-cell Metabolomics Studies**; Nathan Colwell[1]; Dan Chen[1]; Zhibo Yang[1]; *[1]University of Oklahoma, Norman, OK*

WP 727 **Differential ion mobility single-cell proteomics provides new insights into thymic epithelial cell maturation and differentiation**; Eric Bonneil[1]; Sylvie Brochu[1]; Lilian Heil[2]; Michael Belford[3]; Cornelia Boeser[4]; Jean-Jacques Dunyach[4]; Claude Perreault[1, 5]; Pierre Thibault[1, 6]; *[1]Institute for Research in Immunology and Cancer of the Université de Montréal, Montréal, QC; [2]ThermoFisher Scientific, San Jose, CA; [3]Thermo Fisher Scientfic, San Jose, CA; [4]Thermo Fisher Scientific, San Jose, CA; [5]Department of Medicine, Université de Montréal, Montreal, QC; [6]Department of Chemistry, Université de Montréal, Montréal, QC*

WP 728 **Multicolumn low-flow nanoLC-MS platform for high-throughput label-free single-cell proteomics**; Chao Wang[1]; Hsien-Jung Lavender Lin[1]; Siqi Huang[1]; Thy Truong[2]; Xiaofeng Xie[2]; Ryan Kelly[1, 2]; [1]*Brigham Young University, Provo;* [2]*MicrOmics Technologies LLC, Spanish Fork, UT*

WP 729 **Application of single-cell mass spectrometry to prove if intracellular drug levels are heterogenous between cells infected with Trypanosoma cruzi**; Luis Ernst[1]; Deepti Bhusal[2]; Shakya Wije Munige[2]; Laura-Isobel McCall[1]; Zhibo Yang[2]; [1]*San Diego State University, San Diego, CA;* [2]*University of Oklahoma, Norman, OK*

WP 730 **Quantification of Mixed-Species Samples at Low Input Levels Using Narrow-Bore Columns with Integrated Emitters**; Thy Truong[1]; Xiaofeng Xie[1]; Ryan Kelly[1]; [1]*MicrOmics Technologies LLC, Spanish Fork, UT*

WP 731 **Low-input and single cell proteomics sample analysis with a novel ion source and cartridge column**; Martins Jansons[1]; Jeff Op De Beeck[2]; Joshua Silveira[3]; Katherine Walker[3]; Runsheng Zheng[4]; Cornelia Boeser[3]; Amirmansoor Hakimi[3]; [1]*Thermo Fisher Scientific, Vilnius, Lithuania;* [2]*Thermo Fisher Scientific, Ghent, Belgium;* [3]*Thermo Fisher Scientific, San Jose, CA;* [4]*Thermo Fisher Scientific, Germering, Germany*

WP 732 **Large-scale simultaneous measurement of single-cell proteomics and transcriptomics reveals functional subtypes in stem cell transition states**; Marvin Thielert[1]; Enes Ugur[1]; Maximilian Zwiebel[1]; Marc Oeller[1]; Constantin Diekmann[2]; Sophia Steigerwald[1]; Tim Heymann[1]; Christoph Ziegenhain[2]; Matthias Mann[1]; [1]*Max Planck Institute of Biochemistry, Martinsried, Munich, Germany;* [2]*Karolinska Institutet, Solna, Sweden*

WP 733 **Probing DNA Damage Response at the Single-Cell Level Using the Thermo Orbitrap Astral Mass Spectrometer**; Georgina H Charlton[1]; Jonathan Ditcham[1]; Riccardo Zenezini Chiozzi[1]; Jenny Ho[2]; Konstantinos Thalassinos[1]; [1]*University College London, London, United Kingdom;* [2]*Thermo Fisher Scientific, Hemel Hempstead, United Kingdom*

WP 734 **Single Plaque Proteomics Reveal the Composition and Dynamics of the Amyloid Microenvironment in Alzheimer's Disease**; Ju Wang[1]; Mengqi Chu[1]; Jay Michael Yarbro[1]; Ping-chung Chen[1]; Aijun Zhang[2]; Him Shrestha[1]; Yingxue Fu[1]; Zuo-fei Yuan[1]; Zhiping Wu[1]; Haiyan Tan[1]; Xusheng Wang[2]; Anthony A High[1]; Yun Jiao[1]; Junmin Peng[1]; [1]*St Jude Children's Research Hospital, Memphis, TN;* [2]*University of Tennessee Health Science Center, Memphis, TN*

WP 735 **Evaluation of Liquid Chromatographic and Mass Spectrometric Methods for Ultra-deep Quantitative Proteomic Analysis of Single Cells**; Diego M Assis[1]; Yuefan Wang[2]; Jongmin Woo[2]; Zhenyu Sun[2]; Matt Albano[1]; Daniel Hornburg[3]; Hui Zhang[2]; Matthew Willetts[1]; [1]*Bruker Scientific LLC, Billerica, MA;* [2]*Johns Hopkins University, Department of Pathology, Baltimore, Maryland;* [3]*Bruker Scientific LLC, San Jose, California*

WP 736 **Highly sensitive and comprehensive analysis of single-cell phospholipids by direct infusion nanoESI mass spectrometry**; Takuma Yanagisawa[1, 2]; Eiji Sugiyama[1]; Yuta Terui[3]; Masafumi Iharada[3]; Hironori Takai[3]; Iwao Sakane[4]; Susumu Y. Imanishi[1]; Kenichiro Todoroki[2]; Hajime Mizuno[1]; [1]*Faculty of Pharmacy, Meijo University, Nagoya, Japan;* [2]*University of Shizuoka, Shizuoka, Japan;* [3]*Yokogawa Electric Corporation, Musashino, Japan;* [4]*Central Research Institute, ITO EN, Ltd., Makinohara, Japan*

WP 737 **Improving shotgun lipidomic approaches for single cell analysis using single and multipass cyclic ion mobility strategies**; Nyasha C Munjoma[1]; Sean Wu[2, 3]; Scarlet Ferrinho[4, 5]; Lee Gethings[6]; Olivier NF Cexus[4]; Paul Townsend[7]; Emma Marseden-Edwards[5]; [1]*Waters, Wilmslow, United Kingdom;* [2]*Waters Corporation, Parsippany, NJ;* [3]*Waters Corporation, Milford, MA;* [4]*University of Surrey, Guildford, United Kingdom;* [5]*Waters Corporation, Wilmslow, United Kingdom;* [6]*Waters Corporation, Wilmslow, United Kingdom;* [7]*University of Stirling, Stirling, United Kingdom*

WP 738 **Optimising the Single Cell Pipeline using a Multi-Reflecting Q-Tof Platform**; Scarlet Ferrinho[1]; Lee A Gethings[2]; Roy Martin[3]; Richard Lock[4]; Robert S Plumb[3]; Olivier NF Cexus[1]; Paul Townsend[5]; [1]*University of Surrey, Guildford, United Kingdom;* [2]*Waters, Wilmslow, United Kingdom;* [3]*Waters Corporation, Milford, MA;* [4]*Waters Corporation, Wilmslow, United Kingdom;* [5]*University of Sterling, Sterling, United Kingdom*

WP 739 **Investigating Sex Dimorphism in Astrocytic Responses to Human Coronavirus 229E Using Single-Cell Proteomics**; Shuxin Chi[1]; Jason Rogalski[2]; Huan Zhong[1]; Leonard J Foster[1]; [1]*University of British Columbia, Vancouver, BC;* [2]*UBC Proteomics and Metabolomics Core Facility, Vancouver, BC*

WP 740 **High-throughput single-cell proteomics: rapid separations combined with Orbitrap Astral enable measurement throughput of >2000 TMT-labeled single cells per day**; Sachini N Moratuwage[1]; Chao Wang[2]; Ryan Kelly[2]; [1]*Brigham Young University, Provo, UT;* [2]*Brigham Young University, Provo*

WP 741 **Integrating CellenONE-Automated Single-Cell Sample Preparation and Spray-capillary CE-FAIMS-MS Top-down Proteomics**; Samin Anjum[1]; Zhitao Zhao[2]; Trishika Chowdhury[1]; Ahmed Mohamed Amin Abdelhamed[1, 3]; Kellye A. Cupp-Sutton[1]; Si Wu[1]; [1]*The University of Alabama, Tuscaloosa, AL;* [2]*University of Oklahoma, Norman, OK;* [3]*Ain Shams University, Cairo, Egypt*

WP 742 **Streamlined Bottom-Up Single-cell protocol for deep Proteome analysis**; Mai A. Atallah[1]; Zhitao Zhao[2]; Kellye A. Cupp-Sutton[1]; Si Wu[1]; [1]*University of Alabama, Tuscaloosa, AL;* [2]*University of Oklahoma, Norman, OK*

WP 743 **Imaging Mass Spectrometry Implicates Glycolipids as Mediators of RPE Migration in Age-Related Macular Degeneration**; Zhen Wang[1]; David M.G. Anderson[1]; Jeffrey D Messinger[2]; Christine A Curcio[2]; Kevin L. Schey[1]; [1]*Vanderbilt University, Nashville, TN;* [2]*University of Alabama at Birmingham, Birmingham, AL*

WP 744 **Evaluation of prioritized peptide acquisition for multiplexed single-cell proteomics on a modified Orbitrap Astral mass spectrometer**; Benjamin Furtwängler[1]; Julia Kraegenbring[2]; Martin Zeller[2]; Bernard Delanghe[2]; Christopher Rathje[2]; Eduard Denisov[2]; Eugen Damoc[2]; Johannes Petzoldt[2]; Christian Hock[2]; Hamish Stewart[2]; Erwin Schoof[1]; [1]*Technical University of Denmark, Kongens Lyngby, Denmark;* [2]*Thermo Fisher Scientific, Bremen, Germany*

WP 745 **Probing the proteome of differentiating human skin keratinocytes using single nuclei proteoform imaging**; Jared Kafader[1]; Vijaya Kanchustambham[1]; Indira Parada[1]; Pei Su[1]; Tian Xu[1]; Nickolas Fisher[1]; Michael Hollas[1]; Paulina Markiv[1]; Michael Caldwell[1]; Xiaomin Bao[1]; Neil Kelleher[1]; [1]*Northwestern University, Evanston, IL*

WP 746 **Robust identification of up to 6,600 proteins from a single HeLa cell using a modified Orbitrap Astral mass spectrometer**; Ivo A. Hendriks[1]; Ulises H. Guzman[1]; Martin Rykær[1]; Sara C. Buch-Larsen[1]; Maico Y. Lechner[1]; Hamish Stewart[2]; Johannes Petzoldt[2]; Arne Kreutzmann[2]; Tabiwang Arrey[2]; Eugen Damoc[2]; Christian Hock[2]; Jesper V. Olsen[1]; [1]*Novo Nordisk Foundation Center for Protein Research, University of Copenhagen, Denmark;* [2]*Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

WP 747 **Optimized single-cell proteomics methodology enables identification of up to 1,500 proteins from very small peripheral blood mononuclear cells**; Sara C. Buch-Larsen[1]; Ivo A. Hendriks[1]; Maico Y. Lechner[1]; Martin Rykar[1]; Jesper V. Olsen[1]; [1]*Novo Nordisk Foundation Center for Protein Research, University of Copenhagen, Denmark*

STABLE ISOTOPE LABELING
748-762

WP 748 **Serine Octamer Clusters, Peptide Synthesis, and Homochirality Explored with MS**; Brison A Shira[1]; R. Graham Cooks[1]; [1]*Purdue University, West Lafayette, IN*

WP 749 **The Study of SILAC Labeled Peptide Using High-Resolution Ion Mobility**; Hoang Kim Ngan Thai[1]; Marla Popov[2]; Ron Orlando[1]; [1]*University of Georgia, Athens, GA;* [2]*GlycoScientific, Athens, GEORGIA*

WP 750 **Improving analysis of metabolite stable isotope labeling using GC-MS/MS**; David A Scott; *Sanford Burnham Prebys Medical Discovery Institute, La Jolla, CA*

WP 751 **Stable Isotope-Labelled Multiplexed DXT Reagents Facilitate Deep DIA Proteomics**; Egor Vorontsov[1]; Harald Legner[1]; Nikolai Woellmer[1]; Jan Christoph Leichert[1]; Gomathi Ayyasamy[1]; Stephanie Ballweg[1]; Karsten Kuhn[1]; Ian Pike[1]; [1]*Proteome Sciences, Frankfurt am Main, Germany*

WP 752 **Wide-isolation window PRM for stable isotope tracing metabolomics**; Abigail E. Ellis[1]; Rahul Deshpande[2]; Susan Bird[3]; Ryan D Sheldon[1]; [1]*Van Andel Institute, Grand Rapids, MI;* [2]*Thermo Fisher Scientific, San Jose, CA;* [3]*Thermo Fisher Scientfic, San Jose, CA*

WP 753 **Fructose metabolism during sperm activation**; Melanie Balbach; *Michigan State University, East Lansing, MI*

WP 754 **Novel Electroosmotic Flow-Based Probe Enables Online LC-MS Measurement of Leu-Enkephalin Hydrolysis Rate in Rat Hippocampus**; Tingyuan Xu[1]; Stephen Weber[1]; [1]*Department of Chemistry, University of Pittsburgh, Pittsburgh, PA*

WP 755 **Characterization of newly synthesized histone acetylation sites using LC-MS/MS**; Hannah Mathew[1]; Rashmi Karki[1]; Francisca Nathalia De Luna Vitorino[1]; Benjamin A Garcia[2]; [1]*Washington University School of Medicine Dept. of Biochemistry and Molecular Biophysics, St. Louis, MO;* [2]*Washington University School of Medicine, St. Louis, MO*

WP 756 **Stable isotope labelling of cancer-derived extracellular vesicles lipidome in cancer metabolism**; Erika Dorado[1]; Yuchen Xiang[1]; Zoltan Takats[1]; [1]*Imperial College London, Division of Systems Medicine, London, United Kingdom*

WP 757 **Linear model determines protein turnover from a single labeled sample**; Henock M Deberneh[1]; Rovshan G. Sadygov[2]; [1]*UTMB at Galveston, Galveston, TX;* [2]*University of Texas Medical Branch, Galveston, TX*

WP 758 **Barcoding for Isobaric Tagging of Carboxylic Acids and Amines Metabolites**; BRIANA Mwinkom TENGAN[1]; Micheal Ambruster[2]; Julius Agongo[3]; James Edwards[1]; [1]*Saint Louis University, Saint Louis, MO;* [2]*University of Michigan, Ann Arbor, Michigan;* [3]*University of California San Diego, San Diego, CA*

WP 759 **Profiling isoprenoid metabolism during sporulation in Bacillus subtilis via stable isotope labeling and high-resolution mass spectrometry**; Joshua Baccile[1]; Dillon McBee[2]; Zackary Hulsey[2]; [1]*The University of Tennessee, Knoxville, TN;* [2]*The University of Tennessee Knoxville, Knoxville, TN*

WP 760 **18O-water labelling enables protein turnover measurements in embryogenesis.**; Edward Cruz[1]; Argit Marishta[1]; Alex Johnson[1]; Felix Keber[1]; Michael Neinast[1]; Aleigha Reynolds[1]; Joshua Rabinowitz[1]; Eric Wieschaus[1]; Martin Wuhr[1]; [1]*Princeton University, Princeton, NJ*

WP 761 **Cystic fibrosis neutrophils exhibit metabolic reprogramming including enhanced glycolysis, pentose phosphate pathway, and citric acid cycle activity**; Kathryn M. Crotty[1, 2]; James T. Lyles[1, 2]; Joshua D. Chandler[1, 2]; [1]*Department of Pediatrics, Emory University School of Medicine, Atlanta, GA;* [2]*Children's Healthcare of Atlanta, Emory University, Atlanta, GA*

WP 762 **Sipros 5 Significantly Enhances Proteomic Isotope Probing in DDA Orbitrap and Narrow-Window DIA Astral Mass Spectrometry Analyses**; Yi Xiong[1]; Chongle Pan[1]; [1]*University of Oklahoma, Norman, OK*

THURSDAY POSTERS

THURSDAY POSTERS

Set-up for all Monday posters
6:30 - 9:00 am

ALL POSTERS PRESENT
10:30 - 12:00 pm AND 1:00 - 2:30 pm

Remove all Monday posters
2:30 - 3:00 pm

Ambient Ionization: Fundamentals and Instrumentation 001-012
Biomarkers: Quantitative Analysis II 013-039
Disease Biomarkers 040-058
Education: Teaching MS 059-063
Elemental Analysis 064-070
Energy: Petroleum, Biofuels, and Algae 071-082
Environmental: General III 083-120
Exposomics 121-136
Fundamentals: Ion Activation/Dissociation 137-155
Fundamentals: Unconventional Approaches in MS 156-168
H/D Exchange: Hardware, Software and Methodology 169-184
High Throughput MS II 185-206
Imaging MS: Pharmaceuticals, Metabolites, Lipids, and Glycans II 207-232
Imaging: Spatially-Resolved Omics II 233-254
Informatics: Protein ID and Quantification 255-270
Informatics: Workflow and Data Management 271-300
Instrumentation: Mini/Portable/Fieldable MS 301-318
Instrumentation: New Developments in Mass Analyzers and Ion Detection 319-333
Ion Mobility: Applications II 334-356
Ion Mobility: FAIMS/DMS 357-362
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LC/MS: Chromatography and Software 372-386
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Microorganisms and the Microbiome 478-517
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Proteins: General and Membrane 620-628
Proteomics: New Approaches II 629-651
Proteomics: Tissue 652-675
Single Cell MS II 676-698
Small Molecules: Qualitative and Quantitative Analysis 699-740
Synthetic Polymers and New Materials 741-754
Toxicology 755-763

AMBIENT IONIZATION: FUNDAMENTALS AND INSTRUMENTATION
001-012

ThP 001 **Development of a Conductive Emitter for Dynamic Spray Mass Spectrometry**; Alexander P Zumock[1]; Purva S. Damale[1]; Abraham Badu-Tawiah[1]; *[1]The Ohio State University, Columbus, OH*

ThP 002 **Microdroplet reaction controlled through electrospray ionization source conditions**; Daniel D Hu[1, 2]; Jesbaniris Bas-Concepcion[1]; Mike D Knierman[3]; Christopher J Brown[1]; *[1]Corteva Agriscience, Indianapolis, IN; [2]University of Notre Dame, Notre Dame, IN; [3]Agilent Technologies, Santa Clara, CA*

ThP 003 **Rapid Determination of 15 Herbicides in Blood and Soil by Direct Analysis in Real-Time Tandem Mass Spectrometry**; Yuan Zhou[1]; Ying Zhang[2]; Xiaolong Hou[3]; Chenyu Xue[2]; Wenfang Zhang[2]; Jing Qiao[2]; Hua Liu[2]; Xiaokun Duan[4]; *[1]Shanxi Medical University, Shanxi, China; [2]Forensic Science Service of Beijing Public Security Bureau, Key Laboratory of Forensic Toxicology, Ministry of Public Security, Beijing, China; [3]People's Public Security University of China, Beijing, China; [4]ASPEC Technologies, Beijing, China*

ThP 004 **The Effect of Onset Voltage of Capillary Vibrating Sharp-Edge Spray Ionization (cVSSI) on Droplet Size Production**; Amanda DeVor[1]; Olanrewaju Adedayo Awoyemi[1]; Herbi Yuliantoro[1]; Stephen J Valentine[1]; Peng Li[1]; *[1]West Virginia University, Morgantown, WV*

ThP 005 **Rapid detection of illicit materials: A new simplified prototype system using Thermal desorption Mass Spectrometry and improved targeted processing software**; David Douce[1]; Scott Campbell[2]; John Moncur[2]; Lance Hiley[3]; Peter Luke[3]; Ryan M Bain[4]; *[1]Waters (MS Technologies), Wilmslow, United Kingdom; [2]SpectralWorks, Runcorn, United Kingdom; [3]Mass Spec Analytical, Bristol, United Kingdom; [4]Bureau of Alcohol, Tobacco, Firearms and Explosives, Beltsville, MD*

ThP 006 **DESI mass spectrometry for imaging of complex mixtures via a 3D printable framework**; Kevin J Zemaitis[1]; Fiona M Ellsworth[2]; Dusan Velickovic[1]; Carter C Bracken[1]; Gregory W Vandergrift[1]; Richard E Marinos[2]; Christopher Anderton[1]; Troy D Wood[2]; William Kew[1]; *[1]Pacific Northwest National Laboratory, Richland, Washington; [2]University at Buffalo, Buffalo, NY*

ThP 007 **Design of an In-line Nanospray Source for Agilent Triple-Quadruple MS with an Etched Glass Tip with Application to Forensic Toxicology**; Mehdi Moini[1]; Brian A. Eckenrode[2]; Edward Bentil[2]; *[1]Picolytics, McLean, VA; [2]George Mason University, Manassas, VA*

ThP 008 **Ion mobility separation of steroid isomers via N-acyl imidazole derivatization enabled on a MALDESI source**; Paul Zerebinski[1]; Andrews Ruano[1]; Ruwan T. Kurulugama[2]; Sarah M. Stow[2]; Richard A. Yost[1]; Timothy J. Garrett[1, 3]; Boone M. Prentice[1]; *[1]University of Florida, Department of Chemistry, Gainesville, FL; [2]Agilent Technologies, Santa Clara, CA; [3]University of Florida, College of Medicine, Department of Pathology, Immunology, and Laboratory Medicine, Gainesville, FL*

ThP 009 **Real-Time and Retrospective Detection of Chemical Warfare Agent Simulants Using VOC Sampling and SESI-HRMS**; Ana Ballester-Caudet[1]; Guillermo Vidal-de-Miguel[2]; Diego García-Gómez[3]; *[1]University of Salamanca, Salamanca, Spain; [2]Fossiliontech, Parque Científico de la Universidad de Salamanca, C. Adaja, 10, 37185 Villamayor, Salamanca, Spain; [3]University of Salamanca, Salamanca, Spain*

ThP 010 **Investigating femto-electrospray Ionization by ultra-fast Current, Ion Transmission, and Signal-to-Noise Ratio Measurement**; Kanwal Jeet[1]; Ian Ferraro[1]; TOLULOPE IDIAT OGUNSANYA[1]; Anyin Li[1]; *[1]University of New Hampshire, Durham, NH*

ThP 011 **Characterization of Textile Dyes and Their Wastewaters: A Fabric Spray Mass Spectrometry Approach**; Alison M

Trettin[1]; Nelson R. Vinueza[1]; *[1]North Carolina State University, Raleigh, NC*

ThP 012 **Panoptic Mass Spectrometry: A Novel High-Throughput Ion Source for All States of Matter**; Keerthana Ravi[1]; Dmytro Kulyk[1]; Anju Sheregar[1]; Abraham Badu-Tawiah[1]; *[1]The Ohio State University, Columbus, OH*

BIOMARKERS: QUANTITATIVE ANALYSIS II
013-039

ThP 013 **Developing a Microfluidic Paper-Based Analytical Device for the Early Prediction of Severe Acute Pancreatitis using Mass Spectrometry Based Immunoassays**; Ruth M Speidel[1]; Ella Warner[1]; Jona Kozyr-Verni[1]; Rob Huttner[1]; Sophie Miller[1]; Georgios Papachristou[2]; Peter Lee[2]; Abraham Badu-Tawiah[1]; *[1]Ohio State University, Columbus, OH; [2]Wexner Medical Center Ohio State University, Columbus, OH*

ThP 014 **Proteomic Analysis of Plasma-Derived Extracellular Vesicles in Exercised Mouse and Human**; Yanqi Tan[1, 2]; Alexander Fliflet[2, 3]; Marni Boppart[2, 3]; Jonathan Sweedler[1, 2]; *[1]Department of Chemistry, University of Illinois Urbana-Champaign, Urbana, IL; [2]Beckman Institute for Advanced Science and Technology, University of Illinois Urbana-Champaign, Urbana, IL; [3]Department of Health and Kinesiology, University of Illinois Urbana-Champaign, Urbana, IL*

ThP 015 **Development and qualification of an LC-MS/MS method for quantification of MUC5AC and MUC5B mucins in spontaneous sputum**; Weiwen Sun[1]; Si Mou[2]; Catherine Huntington[3]; Hellen Killick[3]; Ian Christopher Scott[3]; Aoife Kelly[3]; Monica Gavala[1]; Jessica Holmen Larsson[3]; Mani Deepika Vakkalanka[4]; Neil E Alexis[5]; Walter Wiley[4]; Aaron Wheeler[4]; Kumar Shah[4]; Moucun Yuan[4]; William Mylott Jr. [4]; Kevin Contrepois[2]; Anton I. Rosenbaum[2, 6]; *[1]AstraZeneca, Gaithersburg, MD; [2]AstraZeneca, South San Francisco, CA; [3]AstraZeneca, Cambridge, United Kingdom; [4]PPD Laboratory Services (a part of Thermo Fisher Scientific), Richmond, VA; [5]University of North Carolina at Chapel Hill, Chapel Hill, NC; [6]Vera Therapeutics, Brisbane, CA*

ThP 016 **Selective and sensitive quantitation of 18 steroids in human serum using Thermo Scientific™ Stellar™ mass spectrometer**; Jingshu Guo[1]; Lauren Bishop[1]; Courtney Patterson[1]; Alan Atkins[1]; Kerry Hassell[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

ThP 017 **From cytoplasm to lumen: mapping the free pools of protein subunits of three photosynthetic complexes using quantitative mass spectrometry**; Anna M. Williams[1]; Philip J. Jackson[2]; Steven M. Theg[3]; Terry M. Bricker[4]; C. Neil Hunter[2]; Haijun Liu[1]; *[1]Saint Louis University, Saint Louis, MO; [2]University of Sheffield, Sheffield, United Kingdom; [3]University of California Davis, Davis, CA; [4]Louisiana State University, Baton Rouge, LOUISIANA*

ThP 018 **Urinary Proteomic Insights into the Genetic Drivers of Pediatric Chronic Pancreatitis**; Katelyn B. Brusach[1, 2]; Vineet Garlapally[3, 4]; Madalyn G. Moore[2, 5]; Maisam Abu-El-Haija[3, 4]; Brian C. Searle[2, 6]; *[1]Veterinary Clinical Sciences, The Ohio State University College of Veterinary Medicine, Columbus, Ohio; [2]Pelotonia Institute for Immuno-Oncology, The Ohio State University, Columbus, Ohio; [3]Department of Pediatrics, College of Medicine, University of Cincinnati, Cincinnati, Ohio; [4]Ohio Division of Pediatric Gastronenterology, Hepatology, and Nutrition, Cincinnati Children's Hospital Medical Center, Cincinnati, Ohio; [5]Department of Chemistry and Biochemistry, The Ohio State University, Columbus, Ohio; [6]Department of Biomedical Informatics, The Ohio State University, Columbus, Ohio*

ThP 019 **Rapid Biotyper assay for antimicrobial resistance susceptibility of ESKAPEE pathogens using deuterium labeling**; Josiah J. Rensner[1]; Vy T Tat[1]; Paul Lueth[1]; Bryan Bellaire[1]; Young Jin Lee[1]; *[1]Iowa State University, Ames, IA*

ThP 020 **A Simple and Sensitive LC-MS/MS Method for 1-Myristyl Lysophosphatidic Acid (LPA14:0) and 1-Oleoyl Lysophosphatidic Acid (LPA18:1) Quantification in Human Serum**; Nazanin Mokhtarpour[1]; Tian-Sheng Lu[1]; Guangchun Zhou[1]; Shuyu Hou[1]; *[1]Medpace, Cincinnati, OH*

ThP 021 **Towards Multiplexed Detection of disease-associated RNA Biomarker using Ambient Mass Spectrometry**; Anju M Sheregar[1]; Rachel M. Robertson[1]; Ayesha Seth[1]; Keerthana Ravi[1]; Venkat Gopalan[1]; Abraham K. Badu-Tawiah[1]; *[1]The Ohio State University, Columbus, OH*

ThP 022 **Affinity Capture LC-MS for Biomarker Discovery: Overcoming ELISA Limitations in Tracking Complement Protein Complexes Across Species in Alzheimer's Disease**; Luis F Schachner[1]; Cong Wu[2]; Jianhui Zhu[3]; Tiffany Wong[2]; Racquel Corpuz[2]; Tiffany Wu[2]; Bill Meilandt[2]; Anne Biever[2]; Jesse Hanson[2]; Cosme Sandoval[2]; Johnny Gutierrez[2]; John Chen[3]; John Tran[2]; *[1]Genentech, Inc., South San Francisco, CA; [2]Genentech Inc., South San Francisco, CA; [3]NovaBioAssays, Woburn, MA*

ThP 023 **Contemporary high-performance oxalate quantification by novel hydrophilic-interaction chromatography and high-end triple quadrupole detection technology**; Robert MacNeill[1]; Ebru Selen[2]; Spundana Malla[1]; Sridhar Swarna[1]; Eshani Galermo[2]; Rahul Baghla[2]; *[1]Pharmaron, Exton, PA; [2]Sciex, Redwood City, CA*

ThP 024 **Determination of Alcohol Use Biomarker Phosphatidylethanol (PEth) in Clinical Samples by a Novel, High-Throughput LC-MS/MS Method with Liquid-Liquid Extraction**; Evan Jones[1]; Tian-Sheng Lu[1]; Shuyu Hou[1]; *[1]Medpace, Cincinnati, OH*

ThP 025 **Novel Treatment of Direct Microglia Replacement Reduces Psychosine in Brain and Spinal Cord of Krabbe Disease Mice**; Clarissa Shoffler[1]; William Aisenberg[2]; Chris Petucci[1]; Frederick Bennett[3]; *[1]Cardiovascular Institute, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA; [2]Department of Psychiatry, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA; [3]Department of Psychiatry, Perelman School of Medicine, University of Pennsylvania and Division of Neurology, Department of Pediatrics, Children's Hospital of Philadelphia, Philadelphia, PA*

ThP 026 **Reframing the use of kinobeads to bioanalysis: a case study demonstrating adaptation of a discovery workflow to endogenous protein bioanalysis**; Soumya Kandi[1]; Qin C Ji[1]; William J Housley[2]; Justin M Reitsma[3]; Paul L Richardson[3]; David B Duignan[4]; Mary J Saltarelli[5]; Gary J Jenkins[1]; *[1]AbbVie, QTAS, North Chicago, IL; [2]AbbVie: Bioresearch Center, Discovery Immunology, Worcester, MA; [3]AbbVie, Discovery - DDST, North Chicago, IL; [4]AbbVie: Bioresearch Center: QTAS, Worcester, MA; [5]AbbVie, QTAS, South San Francisco, CA*

ThP 027 **Application of a Slotted Bandpass Ion Guide to Increase Robustness in Tandem Quadrupole LC-MS/MS Bioanalysis**; Robert S Plumb[1]; Noelle Elliot[2]; Peter Hancock[2]; *[1]Waters, Milford, MA; [2]Waters, Wilmslow, United Kingdom*

ThP 028 **Quantification of zebrafish frataxin in intact zebrafish by UHPLC-MRM/MS utilizing a fully labeled [C-13,N-15]-zebrafish frataxin internal standard**; Teerapat Rojsajjakul[1]; Wonwook Do[2]; Robert B Wison[2]; Ian A. Alexander Blair[1]; *[1]University of Pennsylvania, Perelman School of Medicine, Philadelphia, PA; [2]Children's Hospital of Philadelphia, Philadelphia, Pennsylvania, United States, Philadelphia, PA*

ThP 029 **Correlations of plasma glycosaminoglycan disaccharides and clinical outcome and coagulation parameters in sepsis patients**; Max Kravitz[1, 2]; Bianca Silva[3]; Ryan Burke[1, 2]; Nathan I Shapiro[1, 2]; Eric P Schmidt[2, 4]; Kaori Oshima[2, 4]; *[1]Department of Emergency Medicine, Beth Israel Deaconess Medical Center, Boston, MA; [2]Harvard Medical School, Boston, MA; [3]Agilent Technologies, Lexington, MA; [4]Department of Medicine, Massachusetts General Hospital, Boston, MA*

ThP 030 **Multiplexed Detection of Disease Biomarkers Using Isobaric Peptide Probes via Mass Spectrometry-Based Immunoassay**; Stephanee Joy B Zerrudo[1]; Ayesha Seth[1];

Santosh Raman Acharya[1]; Hianka J. C. De Carvalho[1]; Abraham K. Badu-Tawiah[1]; *[1]The Ohio State University, Columbus, OH*

ThP 031 **Absolute Quantification of Amino Acids and Amine-Containing Metabolites via Surrogate Analyte Approach and Dansyl Derivatization Coupled with LC-MS/MS**; Jasim M Al-Rufaye[1]; Liang Li[2, 3]; *[1]University of Alberta, Edmonton, AB; [2]University of Alberta, Faculty of Science, Chemistry Department, Edmonton, AB; [3]The Metabolomics Innovation Centre (TMIC), University of Alberta, Edmonton, AB*

ThP 032 **Statistical learning on a large-scale chemical perturbation screen in cancer cell lines reveals novel drug mechanism of actions**; CHUWEI LIN[1]; Devin Schweppe[1]; *[1]University of Washington, Seattle, WA*

ThP 033 **Rapid preparation of human plasma for targeted proteomic analysis**; Raphaela M. De Oliveira[1]; Chao Wang[1]; Ken Triggs[1]; Garrett Haynie[1]; Ryan T. Kelly[1]; *[1]Brigham Young University, Provo, UT*

ThP 034 **Combining sensitivity, selectivity, speed and resolution: Utilization of ToF-MRM for the quantification of peptide biomarkers in human glioblastoma**; Matthew E Daly[1]; Lance Nicolaysan[2]; Lee A Gethings[1]; Chris Hughes[1]; Richard Lock[1]; Nelofer Syed[3]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Waters Corporation, Milford, MA; [3]Imperial College London, London, United Kingdom*

ThP 035 **Direct Analysis of Native Hepcidin-25 and Sequential Digestion Using Trypsin Alternatives for Quantitative Biomarker Measurement**; Ewa Sokol-Blond[1]; Michael Hall[1]; Zeinab Mokhtari[1]; Joe Palandra[1]; Anson Pierce[1]; Mike Baratta[1]; *[1]Takeda Development Center Americas Ltd., Cambridge, MA*

ThP 036 **DIA-MS Analysis of Extracellular Vesicle Enriched Urine Identifies Candidate Pancreatic Cancer Biomarkers**; Kaitlin Lowran[1]; Rita Rosati[1]; Bo Hyun Lee[1]; Anna Lokshin[2]; Paul Stemmer[1]; *[1]Wayne State University, Detroit, MI; [2]University of Pittsburgh, Pittsburgh, PA*

ThP 037 **Quantitative Global Proteomics of FFPE Tumors develops Dimethylated G3BP1(R460) as a Robust Pharmacodynamic Biomarker in MTAP-Deficient Tumors Following PRMT5 Inhibition**; Anqi Tu[1]; Steve Sweet[1]; Stephanie Zalesak-Kravec[1]; Libby Wiseman[2]; Jelena Urosevic[2]; Alan Barnicle[2]; Joanna Loizou[2]; Yeoun Jin Kim[1]; Andrew Chambers[1]; *[1]AstraZeneca, Gaithersburg, MD; [2]AstraZeneca, Cambridge, United Kingdom*

ThP 038 **Comprehensive and Sensitive UPLC-MS/MS Analysis for Urinary Porphyrins**; Mitesh Bhatt[1]; Akash Shah[1]; Bhaumik Trivedi[2]; Nitin Satish Shukla[2]; Devika Tupe[2]; Nitish Ramchandra Suryawanshi[2]; Samruddha Chavan[2]; Siddhesh Ghadi[2]; Ramesh Manigiri[2]; Jitendra Kelkar[2]; Pratap Rasam[2]; *[1]Neuberg Supratech Reference Laboratories, Ahmedabad, India; [2]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India*

ThP 039 **Mass Spectrometry-based Optimization of Immunohistochemistry for Clinical Biomarker Assay Development**; Andrew Kunihiro[1]; Sudhanshu Abhishek[1]; Christopher Richardson[1]; Shichen Chen[1]; Camille Lombard-Banek[1]; Beom-Jun Kim[1]; Stephanie Zalesak-Kravec[1]; Steve Sweet[1]; Ana Hidalgo-Sastre[2]; Nicolas Damond[2]; Hadassah Sade[2]; Mark Gustavson[1, 2]; Marlon Rebelatto[1]; Nicolas Giraldo[1]; David Chain[1]; Yeoun Jin Kim[1]; *[1]AstraZeneca Pharmaceuticals LP, Gaithersburg, MD; [2]AstraZeneca Computational Pathology GmbH, Munich, Germany*

DISEASE BIOMARKERS
040-058

ThP 040 **Uncovering APOE Genotype and Sex Specific Differences in Bone Marrow from Distinct Skeletal Sites with Lipidomics**; Sarah G. Clark[1]; Charles A. Schurman[2]; Kenneth A. Wilson[2]; Lisa M. Ellerby[2]; Birgit Schilling[2]; Erin S. Baker[1]; *[1]University of North Carolina at Chapel Hill, Chapel Hill, NC; [2]Buck Institute for Research on Aging, Novato, CA*

ThP 041 **Determination of oxidized phospholipids on human very low-density lipoproteins by capillary electrophoresis-mass spectrometry**; Mine-Yine Liu[1]; Chao-Jung Chen[2]; Chiz-Tzung Chang[3]; Wen-Chien Chiu[1]; Zhi-Ru Lin[1]; *[1]National Changhua University of Education, Changhua, Taiwan; [2]China Medical University, Taichung, Taiwan; [3]China Medical University Hospital, Taichung, Taiwan*

ThP 042 **Proteomics of hiPSC model for investigating monogenic diabetes pathogenesis and oportunities for patient cohort studies**; Ksenia Kuznetsova[1, 2]; Lucas Unger[1]; Rachel Anand Nethala[1]; Bente Berg Johansson[1]; Simona Chera[1]; Alisa Manning[2, 3, 4]; Marc Vaudel[1, 5]; *[1]Mohn Center of Diabetes Precision Medicine, faculty of Medicine, University of Bergen, Bergen, Norway; [2]Broad Institute of MIT and Harvard, Cambridge, MA; [3]Department of Medicine, Massachusetts General Hospital, Boston, MA; [4]Department of Medicine, Harvard Medical School, Boston, MA; [5]The Norwegian Institute of Public Health, Oslo, Østland, Norway, Oslo, Norway*

ThP 043 **Association of external exposome with metabolome in early childhood allergic rhinitis**; HAEUN SONG[1]; Mi Jeong Kim[1]; Hyo Yeong Lee[1]; Su Jung Kim[1]; Hyun Ju Yoo[1]; *[1]ASAN Medical center, SEOUL, South Korea*

ThP 044 **Population based proteomics: Platelet data for elucidating mechanisms of cardiovascular diseases**; Yu-Heng Hsieh[1]; Fiorella A. Solari[1]; Albert Sickmann[1]; *[1]Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Dortmund, Germany*

ThP 045 **Host and Microbial Signatures for Ovarian Cancer Detection: An Omics Study**; Subina Mehta[1]; Ashley Petersen[1]; Kristin Boylan[1]; Amy P.N. Skubitz[1]; Pratik D. Jagtap[1]; Timothy J. Griffin[1]; *[1]University of Minnesota, Twin Cities, Minneapolis, MN*

ThP 046 **Large-scale Proteomic Mapping of the Molecular Pheno-Conversion from Normal Human Coronary Artery to Advanced Atherosclerotic Plaque**; Jennifer Van Eyk[1]; Sarah Parker[2]; Austin Lyle Seale[3]; Chunhong Mao[4]; Saeed Seyedmohammad[2]; James Hixson[5]; Christopher I. Murray[2]; Richard Vander Heide[6]; Jun Qu[7]; Yue Wang[8]; David Herrrington[3]; *[1]Cedars Sinai Medical Center, Los Angeles, CA; [2]Cedars Sinai Medical Center, West Hollywood, CA; [3]Wake Forest School of Medicine, Winston-Salem, NC; [4]University of Virginia, Charlottesville, VA; [5]University of Texas Health Science Center at Houston, Houston, TX; [6]Marshfield Medical Center, Marsfield, Wisconsin; [7]University at Buffalo, Buffalo, NY; [8]Virginia Institute of Technology, Blacksburg, VA*

ThP 047 **Proteome Alterations in Microvesicles Reveal Key Molecular Signatures of Breast Cancer Brain Metastases**; Ayobami O. Oluokun[1]; Mojibola Fowowe[1]; Odunayo O. Oluokun[1]; Waziha Purba[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX*

ThP 048 **Targeted metaproteomics to detect key early diagnostic host and microbial peptide candidates from precancerous oral leukoplakia patients**; Beverly Wuertz[1]; Andrew Rajczewski[2]; Monica Kruk[1]; Paul D Piehowski[3]; Ruben Shrestha[4]; Subina Mehta[2]; Matthew Willetts[5]; Timothy J. Griffin[1]; Frank Ondrey[2]; Pratik Dilip Jagtap[6]; *[1]University of Minnesota, Twin Cities, Minneapolis, MN; [2]University of Minnesota, Minnneapolis, MN; [3]Pacific Northwest National Laboratory, Richland, Washington; [4]Bruker Daltonics Inc, 101 Daggett Dr., San Jose, CA; [5]Bruker Scientific LLC, Billerica, MA; [6]University of Minnesota, Minneapolis, MN*

ThP 049 **Capture Scheduled Retention Time Window Shift in Large Scale of Peptide Quantitation Using a Modified OrbitrapTMHybrid Mass Spectrometer**; Qingling Li[1]; Stephanie N. Samra[1]; Jared Deyarmin[1]; Markus Kellmann[2]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

ThP 050 **Discovery of novel biomarkers in multiple sclerosis phenotypes through deep proteomic profiling of human brain tissue**; Bo Yang[1]; Sean Ryan[1]; Lilu Guo[1]; Timothy Hammond[1]; Hendrik Wesseling[1]; Bailin Zhang[1]; *[1]Sanofi, Cambridge, MA*

ThP 051 **Deep Serum Proteomic Profiling in Low-Volume Mouse Serum Identifies Candidate Biomarkers of Physical**

Dysfunction Driven by Senescent Cell Transplantation; Elikanah Olusayo Adegoke[1]; Alexandra Montesinos[1]; Tomas Pierce, [1]; Reema Banarjee[1]; Mansi Shrivastava[1]; Bradley Olinger[1]; Amit K Dey[1]; Nathan Basisty[1]; *[1]NIH National Institute of Aging, Baltimore, MD*

ThP 052 **Identifying Tumor-Specific MBLN1 Splicing Variants in Glioblastoma Using Integrated Long-Read Transcriptomics and High-Resolution Proteomics**; Gautam Ghosh[1, 2]; Jae-Guen Yoon[3]; Ariana E. Shannon[2, 4]; George M. Sun[3]; Hwahyung Lee[3]; Parvinder Hothi[3]; Damien B. Wilburn[1]; Charles S. Cobbs[3]; Brian C. Searle[2, 4]; *[1]Ohio State Biochemistry Program (OSBP), The Ohio State University, Columbus, OH; [2]Pelotonia Institute for Immuno-Oncology, The Ohio State University, Columbus, Ohio; [3]Swedish Neuroscience Institute, Seattle, WA; [4]Department of Biomedical Informatics, The Ohio State University, Columbus, Ohio*

ThP 053 **Plasma Proteomics Using Mag-Net and Proteograph XT Enrichment Enables Multi-Faceted Biomarker Discovery with Complementary Protein and Peptide Coverage**; Blake L Tsu[1]; Stefanie N Kairs[1]; Sangtae Kim[1]; Goo Jun[2]; Craig L Hanis[2]; Eric L Brown[2]; Christine C Wu[3]; Michael J MacCoss[3]; Christopher A. Barnes[1]; *[1]NGeneBioAI, San Diego, CA; [2]Department of Epidemiology, School of Public Health, UTHealth Houston, Houston, TX; [3]University of Washington - Genome Sciences, Seattle, WA*

ThP 054 **Uncovering dysregulated lipid metabolism in Frontotemporal Dementia by lipidomics**; Yohannes Ambaw[1]; Alissa L Nana[2]; Peter A. Ljubenkov[3]; Shubham Singh[4]; Adam L. Boxer[3]; William W. Seeley[5]; Tobias C. Walther[4]; Robert V. Farese, Jr. [4]; *[1]Cell Biology Program, Sloan Kettering Institute, Memorial Sloan Kettering Cancer Center, New York, United States, New York, 10065; [2]Department of Neurology, Memory and Aging Center, University of California, San Francisco,, San Francisco, CA, , USA, 94158; [3]Department of Neurology, Memory and Aging Center, University of California San Francisco, San Francisco, 94158; [4]Cell Biology Program, Sloan Kettering Institute, Memorial Sloan Kettering Cancer Center, New York, United States, New York, 10065, United States, New York, 10065; [5]Department of Neurology, Memory and Aging Center, University of California,, San Francisco, CA, , USA, 94158*

ThP 055 **Development of a quantitative MRM assay from skin swabs rich in sebumfor early diagnosis of Parkinson’s Disease**; Katherine Hollywood[1, 2]; Minhui Zhu[1, 3]; Caitlin Walton-Doyle[1, 3]; Thomas D Hoare[1, 3]; Eleanor Sinclair[1, 3]; Michael Morris[1, 4]; Perdita Barran[1, 3]; *[1]Manchester Institute of Biotechnology, University of Manchester, Manchester, United Kingdom; [2]Department of Chemistry, University of Manchester, Manchester, United Kingdom; [3]Department of Chemistry, The University of Manchester, Manchester, United Kingdom; [4]Waters Corporation, Wilmslow, United Kingdom*

ThP 056 **Lipidomic signatures of spatially distinct atherosclerotic plaques in hyperlipidemic mice**; Ujjalkumar Subhash Das[1]; Robin Joshi[1]; Soon Yew Tang[1]; Elizabeth J Hennessy[1]; Garret A FitzGerald[1]; *[1]University of Pennsylvania, Perelman School of Medicine, Philadelphia, PA*

ThP 057 **Optimizing pTau217 Detection in Cerebrospinal Fluid: A Comparative Study of Mass Spectrometry Platforms**; Elyssa N Baker[1, 2, 3]; Evgeniy V Petrotchenko[1, 2]; Christoph H. Borchers[1, 2, 3, 4, 5]; *[1]Lady Davis Institute McGill University, Montréal, QC; [2]Segal Cancer Proteomics Centre, Jewish General Hospital, Montreal, QC; [3]Division of Experimental Medicine, McGill University, Montreal, QC; [4]Gerald Bronfman Department of Oncology, Montreal, QC; [5]Department of Pathology, McGill University, Montreal, QC*

ThP 058 **Development of Dried Blood Spot-based Quality Assurance Materials for Psychosine and an LC-MS/MS Method for Their Characterization**; Christian D Freeman[1, 2]; Samyukta Sah[2]; Austin Pickens[2]; Samantha L. Isenberg[2]; Elya Courtney[2]; Timothy Lim[2]; Rachel Lee[2]; Carla Cuthbert[2]; Konstantinos Petritis[2]; *[1]Oak Ridge Institute for Science and Education, Oak Ridge, TN; [2]Division of Laboratory Sciences, National Center for Environmental Health, Centers for Disease Control and Prevention, Atlanta, GA*

EDUCATION: TEACHING MS
059-063

ThP 059 **Turning the Tide Toward Equity: Gender Disparities in Scientific Publishing in Biomedical Mass Spectrometry**; Chiara Chie[1]; Amitesh Sahoo[1]; David Muddiman[2]; Juhi Samal[3]; *[1]University of Alabama at Birmingham, College of Arts and Sciences, Birmingham, AL; [2]Department of Chemistry, North Carolina State University, Raleigh, NC; [3]Department of Biomedical Engineering, University of Alabama at Birmingham, Birmingham, AL*

ThP 060 **Qualitative and Quantitative Analysis of Structural Isomer Flavonoids using UPLC-Orbitrap MS**; Kylie Robertson[1]; Kayleigh Klein[1]; Ken Fiffick[1]; Jamie Humphries[2]; Bidisha Sengupta[1]; Michael A Janusa[1]; *[1]Stephen F Austin State University, Nacogdoches, TX; [2]Thermo Fisher Scientific, San Jose, CA*

ThP 061 **Method Development and Validation of Pesticides by UPLC-MS/MS**; Kadin Green[1]; Kayleigh Klein[1]; Kylie Robertson[1]; Jamie Humphries[2]; Michael A Janusa[1]; *[1]Stephen F Austin State University, Nacogdoches, TX; [2]Thermo Fisher Scientific, San Jose, CA*

ThP 062 **Method Development for PFAS Analysis in Drinking Water Using UPLC-MS/MS**; Ken Fiffick[1]; Lilly Burton[1]; Michael A Janusa[1]; Jamie Humphries[2]; *[1]Stephen F Austin State University, Nacogdoches, TX; [2]Thermo Fisher Scientific, San Jose, CA*

ThP 063 **Signal Lost? Pressure Spiking? A Global Resource to Support LC-MS Troubleshooting**; Melanie Odenkirk[1]; Jessica E. Prenni[1]; *[1]Colorado State University, Fort Collins, CO*

ELEMENTAL ANALYSIS
064-070

ThP 064 **The impact of geographical origin and interannual on stable isotopes and multi-elemental fingerprinting in tobacco for traceability**; Lili Cui[1, 2]; Shulei Han[1, 2]; Yaning Fu[1, 2]; Hongjuan Wang[1, 2]; Yushan Tian[1, 2]; Xiao Li[1, 2]; Huan Chen[1, 2]; Hongwei Hou[1, 2]; *[1]China National Tobacco Quality Supervision and Test Center, Zhengzhou, China; [2]Beijing Life Science Academy, Beijing, China*

ThP 065 **Arsenic Speciation in Rice and Rice Products Using LC-ICP-MS: A Sensitive and Reliable Approach by Shimadzu**; Anant Lohar[1]; Sampath Pulletikurthi[1]; Shailesh Damale[1]; Kumar Raju[1]; *[1]Shimadzu Middle East & Africa FZE, Dubai, United Arab Emirates*

ThP 066 **Minerals may decrease the bioaccessibility of provitamin A carotenoids in sorghum grain**; David Zapata Carvajal[1]; Rae McDowell[1]; Davina H. Rhodes[1]; *[1]Department of Horticulture and Landscape Architecture, Colorado State University, Fort Collins, CO*

ThP 067 **Measurement of Metals in Tissue SamplesUsing LA-ICP-MSand an Organic Matrix-Based Standard**; Tetsuo Kubota[1]; Bert Woods[1]; Koichi Tsuneyama[2]; Yuki Sugiura[3]; Patrick Simmons[1]; *[1]Agilent Technologies, Santa Clara, CA; [2]Tokushima University, Tokushima, Japan; [3]Kyoto University, Kyoto, Japan*

ThP 068 **Laser ablation of silicate rock pressed powders as an efficient trace-element analysis method**; Nathan Dalleska[1]; Oliver D Wilner[2]; Paul D Asimow[2]; Claire E Bucholz[2]; *[1]Caltech, Pasadena, CA; [2]California Institute of Technology, Pasadena, CA*

ThP 069 **Elemental Showdown: Unveiling the Digestive Duel Between Open and Microwave Methods for ICP-MS Analysis of food**; Jacqueline Michelle Chaparro[1, 2]; John Chris Evans[1]; Macy J Gruszczynski[1]; Jessica E. Prenni[1]; *[1]Colorado State University, Department of Horticulture and Landscape Architecture, Fort Collins, CO; [2]Colorado State University, ARC-BIO, Fort Collins, CO*

ThP 070 **Impact of Metal Content on Asphaltene Characterization: ICP-MS-Informed Interpretation of EPR, Ion Mobility,**

Mass Spectrometry, and NMR Data; Bismark A Nyaaba[1]; Sahil Makhani[1]; Thanuja M Thilakarathna[1]; Patrick J Farmer[1]; Touradj Solouki[1]; *[1]Baylor University, Waco, TX*

ENERGY: PETROLEUM, BIOFUELS, AND ALGAE
071-082

ThP 071 **Bio-oil green carbon input evaluation inserted in delayed coking viaESI(-)-Orbitrap HRMS**; Natã Carlos Lira Madeira[1]; Nathália dos Santos Pontes[1]; Adriana Moret Borges[2]; Andrea de Rezende Pinho[2]; Raquel Vieira Santana Da Silva[1]; Gabriela Vanini[1]; Débora de Almeida Azevedo[1]; *[1]Universidade Federal do Rio de Janeiro, Rio de Janeiro, Brazil; [2]PETROBRAS, Rio de Janeiro, Brazil*

ThP 072 **Reaction Mechanisms for Fast Pyrolysis of Polystyrene by Using a Pyroprobe Integrated With an Ion Trap Mass Spectrometer**; Tanya Sharma[1]; Kumari Anshu[1]; Tuong Nguyen[1]; Annika Little[1]; Sonal K. Thengane[2]; Hilkka I Kenttamaa[1]; *[1]Purdue University, West Lafayette, IN; [2]Indian Institute of Technology, Roorkee, India*

ThP 073 **A Study on Rapid Analysis of Pyrolysis Oil Using the Blank Tube Field Ionization Method**; Takao Fukudome[1]; Takaya Satoh[1]; Masaaki Ubukata[1]; *[1]JEOL Ltd., Akishima, Japan*

ThP 074 **Developments of online FT-ICR MS for the study of natural and synthetic polymer pyrolysis**; Théo Voellinger[1]; Sébastien SCHRAMM[1]; Frédéric AUBRIET[1]; *[1]Université de Lorraine, LCP-A2MC, Metz, France*

ThP 075 **Evaluating the composition of effluents from the co-processing of different pyrolytic products and fossil streams in the delayed coking process**; Vinicius B. Pereira[1]; Natã Carlos Lira Madeira[1]; Yasmin Guimarães Pedro[1]; Nathália dos Santos Pontes[1]; Adriana Moret Borges[2]; Andrea de Rezende Pinho[2]; Gabriela Vanini[1]; Raquel Vieira Santana Da Silva[1]; Débora de Almeida Azevedo[1]; *[1]Federal University of Rio de Janeiro, Rio de Janeiro, Brazil; [2]PETROBRAS, Rio de Janeiro, Brazil*

ThP 076 **A New Window into Complex Organic Matter Analysis with FTMS: Demonstrating the Benefits of Asymmetric Apodization**; David P A Kilgour[1]; Pablo Batista Oliveira[2, 3]; Lilian Valadares Tose[2]; Kevin J. D. Fouque[3]; Konstantin O. Nagornov[4]; Anton N. Kozhinov[4]; Helena Osterholz[5]; C. Logan Mackay[6]; Yury Tsybin[4]; Francisco Fernandez-Lima[2, 3]; *[1]Vibrat-Ion Ltd, Aberystwyth, United Kingdom; [2]Department of Chemistry and Biochemistry, Florida International University, Miami, FL; [3]Institute of Environment, Florida International University, Miami, FL; [4]Spectroswiss, EPFL Innovation Park, Lausanne, Switzerland; [5]Marine Chemistry, Leibniz Institute for Baltic Sea Research, Warnemünde, Rostock, Germany; [6]Rosalind Franklin Institute, Didcot, United Kingdom*

ThP 077 **Integrating FT-ICR MS/MS Structural Elucidation with Custom Algorithms for Predicting Asphaltene Stability**; Lidya C. Silva[1]; Jussara Roque[2]; João Victor Ataide Oliveira[2]; Carla Cristina Bise Viegas[3]; Bruno Charles Do Couto[3]; Iris Medeiros Jr[3]; Boniek Gontijo[2]; *[1]UFG, Goiânia, Brazil; [2]UFG, Goiânia, Brazil; [3]PETROBRAS, Rio de Janeiro, Brazil*

ThP 078 **Characterization of Brazilian crude oils from Búzios field using ESI(±)-Orbitrap HRMS and chemometric techniques**; Mônica C. Santos[1]; Victor G. K. Cardoso[1]; Iasmim A. Souza[1]; Thamara A. Barra[1]; Dayane M. Coutinho[1]; Clarisse L. Torres[1]; Daniel S. Dubois[2]; Joelma P. Lopes[2]; Gabriela Vanini[1]; Francisco R. Aquino Neto[1]; Débora de Almeida Azevedo[1]; *[1]Universidade Federal do Rio de Janeiro, Rio de Janeiro, Brazil; [2]PETROBRAS, Rio de Janeiro, Brazil*

ThP 079 **Characterization of bio-oils derived from biomass pyrolysis using liquid chromatography hyphenated with 18 T FTICR mass spectrometer**; Theo Imhoff[1, 2, 3]; Julien Maillard[2, 3]; Marie hubert-Roux[1, 3]; Maxime SUEUR[1, 2, 3]; Caroline Barrère-Mangotte[2, 3]; Mélanie Mignot[1, 3]; Pierre Giusti[2, 3]; Carlos Afonso[1, 3]; *[1]University of Rouen-Normandy, Mont Saint Aignan, France; [2]TotalEnergies Research and Technology Gonfreville, Harfleur, France; [3]International Joint Laboratory, iC2MC: Complex Matrices Molecular Characterization, Harfleur, France*

ThP 080 **Removal of Naphthalic acid form crude oil using Biochar-MOF nanocomposite detected by LC-HRMS/MS**; Temesgen G Kebede[1]; Sol Sauna Nety[1]; Simiso Dube[1]; Mathew M Nindi[2]; *[1]University of South Africa, Johannesburg, South Africa; [2]UNISA, Florida Park, Roodepoort, South Africa*

ThP 081 **Mass Spectrometry, Synchronous Fluorescence, and NMR Studies of Asphaltene Fractionation: Influence of Metal Ions on Macromolecular Aggregations**; Thanuja M Thilakarathna[1]; Bismark A. Nyaaba[1]; Sahil Makhani[1]; Patrick J Farmer[1]; Touradj Solouki[1]; *[1]Baylor University, Waco, TX*

ThP 082 **Biofuel extraction by NH3 from microalgal feedstock (II)**; Takashi Ted Nohmi; *HysafeNohmi, Setagaya-Ku, Japan*

ENVIRONMENTAL: GENERAL III
083-120

ThP 083 **New Pollutant Screening of Environmental Samples Using High-Resolution GC/Q-TOF and Accurate Mass Spectral Library of Emerging Environmental Pollutants**; Kong Ye; *Agilent Technologies (China), Beijing, China*

ThP 084 **Low Flow Liquid Chromatography Method for Nontargeted Analysis of Per- and Polyfluoroalkyl Substances by 21 tesla FT-ICR Mass Spectrometry**; Lydia Babcock-Adams[1]; Robert Young[2]; Huan Chen[1]; William Bahureksa[3]; Wenchao Lu[2]; Emily Hughes[4]; John Kornuc[5]; Chad R. Weisbrod[1]; Kristina Hakansson[1]; Christopher L Hendrickson[1]; Jens Blotevogel[2]; Amy McKenna[1, 6]; *[1]National High Magnetic Field Laboratory, Tallahassee, FL; [2]CSIRO, Adelaide, Australia; [3]New Mexico State University, Las Cruces, NM; [4]Florida State University, Tallahassee, FL; [5]Naval Facilities Engineering Systems Command, Washington D.C., DC; [6]Colorado State University, Fort Collins, CO*

ThP 085 **Targeted LC-MS/MS analysis of PFAS in the Utah Provo River Basin**; Junhan Chen[1]; Jonah Riggs[1]; Christopher Tracy[2]; Zane Sandall[2]; Roger G. Harrison[2]; *[1]Brigham Young University, Provo, UT; [2]Brigham Young University, Provo*

ThP 086 **Expansion of an AI-Driven absolute quantification platform to the prediction of water treatment metabolic degradants**; Chris Brown[1]; Jack Howland[2]; Chris Bianca[1]; Baljit K. Ubhi[2]; *[1]Corteva Agrisciences, Indianapolis, IN; [2]Matterworks, Somerville, MA*

ThP 087 **Characterization of Pyroplastic Samples Gathered Following the Largest Recorded Maritime Spill of Microplastics: The Sinking of the M/V X-Press Pearl**; Douglas M Stevens[1]; Christopher M Reddy[2]; Bryan D James[2, 3]; Robert K Nelson[2]; Sarah Dowd[1]; Michael McCullagh[4]; Russell Mortishire-Smith[4]; Jeff Goshawk[4]; Andrew Tudor[4]; Frank L Dorman[1, 5]; *[1]Waters Corp., Milford, MA; [2]Woods Hole Oceanographic Institution (WHOI), Woods Hole, Massachusetts; [3]Northeastern University, Boston, MA; [4]Waters Corporation, Wilmslow, United Kingdom; [5]Dartmouth College, Hanover, NH*

ThP 088 **Community Odor Perceptions are Associated with Ambient BTEX Concentrations Following Landfill Remediation in Bristol, VA and TN**; Marie J Andales[1]; Xiaoying Li[1]; Joshua Rudd[2]; Tim Hilbert[3]; Patrick Ryan[4]; Joel Kellogg[5]; Becky Evenden[5]; Candace Brancato[3]; Christine Kim[3]; Erin Hayes[3]; John Volckens[1]; *[1]Colorado State University, Department of Mechanical Engineering, Fort Collins, CO; [2]King University, Bristol, TN; [3]University of Kentucky, Lexington, KY; [4]University of Cincinnati, Cincinnati, OH; [5]HOPE Bristol, Bristol, TN*

ThP 089 **Comprehensive Analysis of Ultra-Short to Long-Chain PFAS Using Multimode Chromatography-Mass Spectrometry for Environmental and Commercial Non-Targeted Analysis (NTA)**; Tanya Napolitano[1]; Beryl Zijie[2]; *[1]Shodex, New York, NY; [2]Claros Technologies, Minneapolis, MN*

ThP 090 **Resolving the Single-Particle Composition of Water-Soluble Organics, PAHs, and Inorganics in Wildfire Aerosols**; Johannes Passig[1]; Ellen I. Rosewig[1]; Mika Ihalainen[2]; Anni Hartikainen[2]; Markus Somero[2]; Olli Sippula[2]; Pasi YLI-PIRILÄ[2]; Kerneels Jaars[3]; Pieter VanZyl[3]; Kajar

Koster[4]; Stefan Siebert[5]; Saara Peltokorpi[6]; Angela Buchholz[6]; Hao Liqing[6]; Annele Virtanen[6]; Ville Vakkari[7]; Sven Ehlert[8]; Andreas Walte[8]; Ralf Zimmermann[1]; *[1]University of Rostock, Chair of Analytical Chemistry and Dept. of Life, Light and Matter, Rostock, Germany; [2]Department of Environmental and Biological Sciences, University of Eastern Finland, Kuopio, Finland; [3]Atmospheric Chemistry, Chemical Resource Beneficiation, North-West University, Potchefstroom, South Africa; [4]5Department of Environmental and Biological Sciences, University of Eastern Finland, Joensuu, Finland; [5]Unit of Environmental Sciences and Management, North-West University, Potchefstroom, South Africa; [6]Department of Technical Physics, University of Eastern Finland, Kuopio, Finland; [7]Finnish Meteorological Institute, Helsinki, Finland; [8]Photonion GmbH, Schwerin, Germany*

ThP 091 **Accurate Mass Full Spectral Monitoring and Analysis of Both the Analyte and Reference Standard with Ion Chromatography – Mass Spectrometry**; Jayesh Gandhi[1]; Sue D'Antonio[2]; John Wright[2]; Yongdong Wang[3]; *[1]Metrohm, Pasadena, TX; [2]Agilent Technologies, Santa Clara, CA; [3]Cerno Bioscience, Las Vegas, NV*

ThP 092 **Understanding the Reaction Networks of Criegee Intermediates Formed in Complex Reactive Environments: Ozone-assisted Oxidation Reaction ofAcyclic and Endocyclic Alkenes**; Denisia M. Popolan-Vaida[1]; Alec C. DeCecco[1]; Yitong Zhai[1]; Arden M. Floyd[1]; Zachary Clarke[1]; Nils Hansen[2]; Ahren W. Jasper[3]; *[1]University of Central Florida, Orlando, FL; [2]Sandia National Laboratories, Livermore, CA; [3]Argonne National Laboratory, Lemont, IL*

ThP 093 **Simultaneous Quantification of Pesticide Residues in Olive Oil via LC-MS/MS and GC-MS/MS Using a Streamlined, Automatable cSPE Clean-up Workflow**; Anant Lohar[1]; Shailesh Sadashiv Damale[1]; Jessin Mathai[1]; Lucy Richards[2]; Russell Parry[2]; Lee Williams[2]; Geoff M Davies[2]; *[1]Shimadzu Middle East & Africa FZE, Dubai, United Arab Emirates; [2]Biotage GB Limited, Cardiff, United Kingdom*

ThP 094 **Detection and Quantitation of PFAS in Sea Foam from Southeastern North Carolina**; Jeffrey Enders[1]; Rebecca A. Weed[1]; Emily Donovan[2]; Drake Phelps[1]; Grace Campbell[1]; Katlyn May[1]; Erin S. Baker[3]; *[1]North Carolina State University, Raleigh, NC; [2]Clean Cape Fear, Leland, NC 28479; [3]University of North Carolina at Chapel Hill, Chapel Hill, NC*

ThP 095 **Analysis of anabaenopeptins and microcystins by LC-MS and native fluorescence detection**; Buddhima N. Peiris[1]; Sharmila I. Thenuwara[2]; Judy A. Westrick[2]; Dragan Isailovic[1]; *[1]University of Toledo, Toledo, OH; [2]Wayne State University, Detroit, MI*

ThP 096 **MALDI TIMS MSI Detection of Polystyrene Nanoplastics in Whole-Body Murine Tissue**; Karina Ariel Vargas[1]; Amy L Parkhurst[1]; Fawaz G. Haj[1]; Elizabeth Kathleen Neumann[1]; *[1]UC Davis, Davis, CA*

ThP 097 **Monitoring the estrogen-inducible proteins in Lake trout (Salvelinus namaycush) from Great Lakes upon exposure to environmental contaminants**; Taniya Modhishika Jayaweera[1]; Krishan S Weraduwage[1]; Bernard Crimmins[2, 3]; Sujan Fernando[3]; Thomas M Holsen[3]; Costel C. Darie[1]; *[1]Biochemistry & Proteomics Laboratories, Department of Chemistry & Biochemistry,Clarkson University, Potsdam, NY; [2]AEACS, New Kensington, PA; [3]Department of Civil and Environmental Engineering, Clarkson University, Potsdam, NY*

ThP 098 **Advanced characterization of dissolved organic matter by trapped ion mobility coupled to 18 T Fourier transform ion cyclotron mass spectrometry**; Antoine Duhamel[1, 2]; Helene Lavanant[1, 2]; Emilien Varea[3]; Florence Portet-Koltalo[1, 2]; Christopher A Wootton[4]; Jingyi Zeng[5]; Jean-Philippe Croué[5]; Carlos Afonso[1, 2]; *[1]Normandie Université, CNRS, CARMeN UMR 6064 and FR 3038, Université de Rouen Normandie, Rouen, France; [2]International Joint Laboratory, iC2MC: Complex Matrices Molecular Characterization, Harfleur, France; [3]Normandie Univ, CNRS CORIA UMR 6614, UNIROUEN, INSA Rouen, Rouen, France; [4]Bruker Daltonics GmbH & Co.KG, Bremen, Germany; [5]IC2MP (UMR CNRS 7285), Université de Poitiers, Poitiers, France*

ThP 099 **Two-dimensional ion chromatography coupled with Orbitrap mass spectrometry for measuring nitrate stable isotope ratios in environmental matrices**; Allyson Girard[1]; J. David Felix[1]; Hussain Abdulla[1]; *[1]Texas A&M University-Corpus Christi, Corpus Christi, TX*

ThP 100 **Investigation of the dysregulated proteins in fishes from the Great Lakes exposed or not to environmental contaminants**; Krishan S Weraduwage[1]; Taniya Jayaweera[1]; Bernard Crimmins[2, 3]; Sujan Fernando[3]; Thomas M Holsen[3]; Costel C. Darie[1]; *[1]Biochemistry & Proteomics Laboratories, Department of Chemistry & Biochemistry, Clarkson University, Potsdam, NY 13699-5810; [2]AEACS, New Kensington, PA; [3]Department of Civil and Environmental Engineering, Clarkson University, Potsdam, NY*

ThP 101 **Time-Resolved Extraction of Metals and Characterization of Asphaltenes Using Inductively Coupled Plasma-Mass Spectrometry (ICP-MS) and Nuclear Magnetic Resonance (NMR)**; Sahil Makhani[1]; Bismark A. Nyaaba[1]; Thanuja M Thilakarathna[1]; Patrick J Farmer[1]; Touradj Solouki[1]; *[1]Baylor University, Waco, TX*

ThP 102 **Demonstration of LC-MS/MS performance for EPA 1633A: robustness and sensitivity for PFAS analysis in water, soil and tissues**; Om k Shrestha[1]; Patricia Faulkner[2]; Hannah Kruelle[2]; Toshiya Matsubara[3]; Eishi Imoto, [3]; Kathleen K Luo[3]; Ruth Marfil-Vega[3]; Christine Ratcliff[2]; Jonathan Thorn[2]; *[1]Shimadzu Scientific Instruments, Columbia, MD; [2]Eurofins Lancaster laboratories Environmental Testing, LLC, Lancaster, PA; [3]Shimadzu Scientific Instruments, Columbia, Maryland*

ThP 103 **Dual Confirmation of EPA Method 8330 explosives using a DUIS-equipped Single Quadrupole LCMS-2050 and PDA for Tandem Detection**; Valeria Zerda Pinto[1]; Ethan R Hain[1]; Sarah A Monti[1]; Lihini Mendis[1]; Ruth Marfil-Vega[1]; Chistopher T Gilles[1]; Landon A Wiest[1]; *[1]Shimadzu Scientific Instruments, Columbia, MD*

ThP 104 **Development of an ultra-high performance liquid chromatography mass spectrometry method to determine the persistence of insensitive munitions in blowflies**; Alexis T Zieminski[1]; Sarah N Dowling[1]; Hannah Zimmerman-Federle[1]; Kelsie Svara[1]; Katharine Jensen[1]; Nicholas E Manicke[1]; Christine Picard[1]; *[1]Indiana University Indianapolis, Indianapolis, IN*

ThP 105 **Enhanced Analysis of explosives listed in EPA Method 8330B using APCI-LC-MS/MS**; Valeria Zerda-Pinto[1]; Sarah A. Monti[1]; Ethan R Hain[1]; Lihini Mendis[1]; Ruth Marfil-Vega[1]; Landon A Wiest[1]; Christopher T. Gilles[1]; *[1]Shimadzu Scientific Instruments, Columbia, MD*

ThP 106 **High-Resolution Mass Spectrometry and Computational Approaches to Identify Transformation Products and Toxicity Risks**; Arzu Tugce Guler[1, 2, 3]; Zhenyu Tian[4, 5]; Madison H. McMinn[4, 5]; Yuqiao Tang[6, 7]; *[1]Institute for Experiential AI at Northeastern University, Boston, MA; [2]Boston children's hospital, Boston, MA; [3]Department of Pathology, Harvard Medical School, Boston, MA; [4]Department of Chemistry and Chemical Biology, College of Science, Northeastern University, Boston, MA; [5]Barnett Institute for Chemical and Biological Analysis, College of Science, Northeastern University, Boston, MA; [6]The Institute for Experiential AI, Northeastern University, Boston, MA; [7]Department of Bioinformatics, College of Science, Northeastern University,, Boston, MA*

ThP 107 **Metabolic signatures of air pollution exposure in children: a multi-ethnic study**; Xiangping Lin[1]; Xinyue Zhang[1]; Maya M. Kasowski[2]; Mary Margaret Johnson[3]; Kari Christine Nadeau[3]; Michael Snyder[1]; *[1]Department of Genetics, Stanford University, Stanford, CA; [2]Department of Pathology, Stanford University, Stanford, CA; [3]Department* *of Environmental Health, Harvard T.H. Chan School of Public Health, Massachusetts, Boston*

ThP 108 **Precise characterization of the presence and fate of “hidden” plastic breakdown products in water**; Changzhi Shi[1]; Mingliang Fang[1]; *[1]Fudan University, Shanghai, China*

ThP 109 **PFAS exposure alters the metabolism of plant growth promoting bacteria Pseudomonas protegens at environmentally relevant concentrations**; Amanda May; *University of Tennessee, Knoxville, TN*

ThP 110 **Effect of Mobile Phase Additives on Supercritical Fluid Chromatography-Mass Spectrometry for Enhanced PFAS Detection**; Karla M Rios Bonilla[1]; Luis A Colón[1]; Diana S Aga[1]; *[1]University at Buffalo, Buffalo, NY*

ThP 111 **Improved Analysis of N-Nitrosamines by Atmospheric Pressure Chemical Ionization Liquid Chromatography Tandem Mass Spectrometry**; Lihini Tharanga Mendis[1]; Ethan R Hain[1]; Sarah Monti[1]; Valeria Zerda-Pinto[1]; Ruth Marfil-Vega[1]; Landon Wiest[1]; Christopher T. Gilles[1]; William Lipps[1]; *[1]Shimadzu Scientific Instruments, Columbia, MD*

ThP 112 **Enhancing Confidence Levels of Emerging Contaminants Suspect Screening using Ion Mobility Spectroscopy and COSMO-RS**; Dulan H Edirisinghe[1]; Jonathan Antle[1]; John Michael N Aguilar[1]; Tristan Vick[1]; Alexander Hoepker[2]; Joshua S Wallace[1, 2]; Scott M Simpson[3]; Diana S Aga[1, 2]; *[1]Department of Chemistry, University at Buffalo, Amherst, NY; [2]Research and Education in Energy, Environment and Water (RENEW) Institute, University at Buffalo, State University of New York, Buffalo, NY; [3]Department of Chemistry, St Bonaventure University., St Bonaventure, NY*

ThP 113 **Considerations for Improved EPA Method 533 Accuracy and Precisionfor the Analysis of PFAS in a Production Laboratory Environment**; Paulina Michaud; *Phenomenex, Torrance, CA*

ThP 114 **Comprehensive Characterization of Compound Biomarkers of Modern and Ancient Greenland Sediment using Feature-Based Molecular Network (FBMN) Approach**; John Michael N Aguilar[1]; Liezel Mari M. Abaya[2]; Joshua S. Wallace[2, 3]; Elizabeth K. Thomas[4]; Diana S. Aga[2, 3]; *[1]Department of Chemistry, University at Buffalo, Amherst, NY; [2]Department of Chemistry, University at Buffalo, Buffalo, NY; [3]Research and Education in Energy, Environment and Water (RENEW) Institute, University at Buffalo, State University of New York, Buffalo, NY; [4]Department of Earth Science, University at Buffalo, Buffalo, NY*

ThP 115 **Perfluoroalkyl Substances (PFAS) Analysis in Drinking Water, Sediments, and Food Samples byQuEChERSSPE and LC-MS/MS**; Bryan Tackett[1]; Syljohn Estil[2]; Agustin Pierri[3]; *[1]Phenomenex, Torrance, CA; [2]Sanitation Districts of Los Angeles County-San Jose Creek Water Quality Laboratory, Whittier, CA; [3]Weck Laboratories, Hacienda Heights, CA*

ThP 116 **THE DETECTION OF MERCURY IN INVASIVE CARP TISSUE USING INDUCTIVELY COUPLED PLASMA: ARE CARP A VIABLE FISHMEAL SOURCE IN AQUAFEED?**; Yahminiy Ganesh[1]; Phoebe Anne Zito[1]; Stephanie Archer[2]; Edward Osborn[1]; Morris Joseph Bonton III[1]; Robert Bourgeois (WLF) [3]; Abigail Host[4]; Abigail Bockus[5]; Gibson Gaylord[5]; *[1]UNO, New Orleans, LA; [2]Louisiana Universities Marine Consortium, New Orleans, LOUISIANA; [3]LDWF Biologist DCL-B Aquatic Invasive Species Coordinator Fisheries Permit Manager LDWF, Baton Rouge, LOUISIANA; [4]University of Alaska Fairbanks - College of Fisheries & Ocean Sciences, Alaska, Alaska; [5]Bozeman Fish Technology Center Bozeman, MT, Bozeman, Montana*

ThP 117 **To Develop a Derivatized Method for Aldehyde Capture and Characterization by High-Performance Liquid Phase Coupled with Tandem Mass Spectrometry**; Shih-Shin Liang; *Kaohsiung Medical University, Kaohsiung, Taiwan*

ThP 118 **Near real-time PFAS screening with EPA 1633 confirmation on the same DART/LC-QqQ instrument**; Nihari Perera[1]; Samuel Putnam[2]; *[1]Bruker, San Jose, CA; [2]Bruker Scientific LLC, Billerica, MA*

ThP 119 **OTC ChemTracer: Advanced Membrane Inlet Laser-Photoionization Mass Spectrometry (MI-PIMS) for Real-Time Detection of Organic Contaminants in Marine Environments**; Sven Ehlert[1]; Carolin Schwarz[2]; Johannes Passig[1, 2]; Dorothee Niethammer[3]; Christian Menhard[3]; Andreas Walte[1]; Ralf Zimmermann[2]; *[1]Photonion GmbH, Schwerin, Germany; [2]University of Rostock, Chair of Analytical Chemistry and Dept. of Life, Light and Matter, Rostock, Germany; [3]InnoLas Laser GmbH, Krailling, Germany*

ThP 120 **LC-MS analysis of the partitioning of PFOS by bacterial species in liquid medium**; Dagmar Leary[1]; Christopher J. Katilie[1]; Jaimee R Compton[1]; Brian J. Eddie[1]; Lina J Bird[1]; *[1]Naval Research Laboratory, Washington, DC*

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ThP 121 **Machine Learning-Guided Identification of Halogenated Compounds from Nontargeted High-Resolution Mass Spectrometry Data**; Tingting Zhao[1, 2]; Qiming Shen[2]; Xing-Fang Li[2]; Tao Huan[1]; *[1]University of British Columbia, Vancouver, BC; [2]The University of Alberta, Edmonton, AB*

ThP 122 **Broad chemical space sample preparation for sensitive high-throughput targeted exposomics**; Yunyun Gu[1]; Maren Kirchner[1]; Caroline H Johnson[2]; Benedikt Warth[1]; *[1]University of Vienna, Vienna, Austria; [2]Yale University, New Haven, CT*

ThP 123 **Exploration of environmental contaminants in human seminal plasma, blood and urine and their association with semen quality: an exposomic approach**; Pablo Gago Ferrero[1]; German Cano-Sancho[2]; Daniel Gutiérrez-Martín[1]; Elena Sanchez-Resino[3]; Maria Fernández De La Puente Cervera[3]; Albert Salas-Huetos[3]; Maria Angeles Martinez[3]; Nancy Babio[3]; Jordi Salas-Salvado[3]; Ruben Gil-Solsona[1]; Montse Marquès[1]; *[1]IDAEA-CSIC, Barcelona, Spain; [2]LABERCA, Oniris, INRAE,, nantes, France; [3]Universitat Rovira I Virgili, Tarragona, Spain*

ThP 124 **Lipid Perturbations due to Wildfire Smoke Exposure**; Haley C. Jostes[1]; Amie M. Solosky[1]; Jessie R. Chappel[1]; Celeste Carberry[1]; Elise Hickman[1]; Julia E. Rager[1]; Erin S. Baker[1]; *[1]UNC- Chapel Hill, Chapel Hill, NC*

ThP 125 **Occupational exposure assessment of printer-emitted nanoparticles using urine and serum metabolomics analysis**; Chani Sahabandu Hewa Sahabandu[1]; Kushal Biswas[1]; Dhimiter Bello[1]; Pengyuan Liu[1]; *[1]University of Massachusetts Lowell, Lowell, MA*

ThP 126 **Quantification of PFAS in plasma: a faster way to monitor human exposure**; Sarah Demers[1]; Mégane Moreau[1]; Serge Auger[1]; Jonathan Rochon[1]; Pierre Picard[1]; Jean Lacoursière[1]; *[1]Phytronix Technologies, Quebec City, QC*

ThP 127 **Untargeted identification of pesticides metabolites to study their effects on metabolic and Parkinson diseases**; Emilien L Jamin[1, 2]; Romain Vuillaume[1, 2]; Carla Orlandi[1, 2]; Nicolas Loiseau[1, 3]; Anne Fougerat[1, 3]; Clemence Rives[1, 3]; Laurence Gamet-Payrastre[1, 3]; *[1]Toxalim (Research Center in Food Toxicology), Toulouse university, INRAE, ENVT, INP-Purpan, Toulouse, France; [2]MetaboHUB-MetaToul, National Infrastructure of Metabolomics and Fluxomics, Toulouse, France; [3]Toxicology and Integrative Metabolism, UMR1331 Toxalim (Research Centre in Food Toxicology), Toulouse University, INRAE, ENVT, INP-Purpan, Toulouse, France*

ThP 128 **Proteomic analysis of human cells exposed to Mono-n-butyl Phthalate (MnBP) using DIA-MS**; Hwangkyo Jeong[1]; Seungyoon Seo[1]; Sujeong Yu[1]; Seung-Hwa Lee[2]; Soo-Jong Hong[3]; Hosub Im[4]; Jeonghun Yeom[1]; *[1]Prometabio Research Institute, prometabio co., ltd., Hanam-si, South Korea; [2]Department of Medicine, University of Ulsan College of Medicine, Seoul, South Korea; [3]Department of Pediatrics, Childhood Asthma Atopy Center, Humidifier Disinfectant Health Center, Asan Medical Center, University of Ulsan College of Medicine,, Seoul, South Korea; [4]Institute for Life & Environmental Technology, Smartive Corporation, Hanam-si, South Korea*

ThP 129 **Higher-Throughput Chemical Exposomics in Human Serum with Phospholipid Removal and LC – Orbitrap HRMS Analysis**; Solveig Thiele[1]; Bénilde Bonnefille[1, 2]; Bashar Amer[3]; Susan S Bird[3]; Tabiwang Arrey[4]; Nicolaie Eugen Damoc[4]; Stefano Papazian[1, 2]; Jonathan W Martin[1, 2]; *[1]Department of Environmental Science, Exposure and Effects Unit, Science for Life Laboratory, Stockholm University, Stockholm, Sweden; [2]National Facility for Exposomics, Metabolomics Platform, Science for Life Laboratory, Stockholm University, Solna, Sweden; [3]ThermoFisher Scientific, San Jose, CA; [4]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

ThP 130 **An untargeted GCxGC-MS approach to investigate exposome in healthy aging**; Elettra Barberis[1]; Ameya Barde[1]; Simona Fenizia[2]; Elia Amede[2]; Marcello Manfredi[3, 4]; *[1]Department of Sciences and Technological Innovation, University of Piemonte Orientale, Alessandria, Italy; [2]Department of Translational Medicine, University of Piemonte Orientale, Novara, Italy, Novara, Italy; [3]University of Piemonte Orientale, Novara, Italy; [4]IRCCS Policlinico San Donato, Institute of Molecular and Translational Cardiology, Milan, Italy*

ThP 131 **ToxCCS: A Multidimensional ToxCast Reference Database for High-Throughput Human Exposome Analysis**; Ryan Nguyen[1]; Xingzhu Liu[1]; Reuben A. Santoso[1]; Amogh Bantwal[1]; Dylan H. Ross[2]; Ryan P. Seguin[1]; Libin Xu[1]; *[1]University of Washington, Seattle, WA; [2]Pacific Northwest National Laboratory (PNNL), Richland, WA*

ThP 132 **Evaluation of Changes in HSA-Cys34 Adductomics Profiles in Repeat Blood Samples Using Intra-Class Correlation Coefficient**; Fariba Tayyari[1]; Zhu Zou[1]; Yeunook Bae[2]; Aishwarya Jala[1]; James L Burke[1]; Kwang-Youn A Kim[1]; Siyuan Dong[1]; William E Funk[1]; *[1]Northwestern University, Chicago, IL; [2]Illinois State University, Normal, IL*

ThP 133 **Rubber Match?: Determination of confounding factors for 1,3-Butadiene Adduct Formation Arising from Genetic Variation and Endogeno**; Erik J Moran[1]; Gleb Vecherkov[1]; Natalia Tretyakova[1]; *[1]University of Minnesota, Twin Cities, Minneapolis, MN*

ThP 134 **Nontargeted Screening of Endocrine Disruptors in Urine: Linking Environmental Exposure to Ovarian Malignancies**; Zan Rekar[1, 2]; Helena Plesnik[1, 2]; Stefanela Stevanovic[3]; Irma Virnat Klun[3, 4]; Senka Imamovic Kumalic[3, 4]; Mateja Sladic[3, 4]; Milena Horvat[1, 2]; Tina Kosjek[1, 2]; *[1]Jozef Stefan Institute, Ljubljana, Slovenia; [2]Jozef Stefan International Postgraduate School, Ljubljana, Slovenia; [3]University of Ljubljana, Ljubljana, Slovenia; [4]University Medical Centre Ljubljana, Ljubljana, Slovenia*

ThP 135 **Mapping the Untargeted Exposome An Exposome Wide Association Study in the HHEAR Cohorts Reveals Associations Between the Untargeted Exposome Disease**; Dillon Lloyd[1]; Chirag Patel[2]; *[1]Harvard University, Boston, MA; [2]Harvard Medical School, Boston, Massachusetts*

ThP 136 **IDSL-SpecDB - A database of mass spectra (MS2) generated using machine learning methods for metabolomics and exposomics**; Tuan Nguyen[1]; Dinesh Barupal[1]; *[1]Icahn School of Medicine at Mount Sinai, New York, NY*

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ThP 137 **Top-Down Characterization of Protein Anions Using Ultraviolet Photodissociation and Activated-Electron Photodetachment**; Hanlin Ren[1]; Jennifer S. Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX*

ThP 138 **Charge Detection Mass Spectrometry Analysis of Thermally Activated Native Protein Complexes**; Anisha Haris[1]; Jakub Ujma[1]; Kevin Giles[1]; David Bruton[1]; Keith Richardson[1]; Paul Kowalski[2]; Bradley Davis[3]; Madison Turner[3]; Siavash Vahidi[3]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Waters Corporation, Milford, MA; [3]University of Guelph, Guelph, ON*

ThP 139 **Tetraalkylammonium Ions Unfold on Collisional Activation and Refold as They Cool: Experimental and Computational Results**; Sanaz Mohammadzadeh Koumleh[1]; David V Dearden[1]; *[1]Brigham Young University, Provo, UT*

ThP 140 **Practical Quadrupole Theory: Surface Induced Dissociation (SID) Energetics Characterization**; Luke Metzler[1]; Randall E Pedder[1]; *[1]Ardara Technologies, Ardara, PA*

ThP 141 **Negative electron transfer dissociation on an Orbitrap Tribrid mass spectrometer to characterize glycosaminoglycans, peptides, and glycopeptides**; Haley M. Schramm[1]; Christopher Mullen[2]; Joshua D. Hinkle[2]; John E. P. Syka[2]; Nicholas M. Riley[1]; *[1]University of Washington, Seattle, WA; [2]Thermo Fisher Scientific, San Jose, California*

ThP 142 **SimIonSPA: Collision Heating and Cooling in Mass Spectrometry Collision Cells with Simion**; Ken Newton[1]; Austin W Green[1]; James S. Prell[1]; *[1]University of Oregon, Eugene, OR*

ThP 143 **Charge reduction of guests in gas phase fragmentation of host-guest complexes**; Hugo Y. Samayoa-Oviedo[1]; Daniel M. Hristov[1]; Bethany A. Phillips[1]; Julia Laskin[1]; *[1]Purdue Univeristy, West Lafayette, IN*

ThP 144 **Unfolding of super stable proteins during nano-ESI – lessons for structural mass spectrometry**; Thomas D Hoare[1]; Xudong Wang[1]; Hanan Messiha[1]; Kathleen Cain[1]; Xamuel Lund[2]; Pau Bernadó[2]; Perdita E Barran[1]; *[1]Manchester Institute of Biotechnology, University of Manchester, Manchester, United Kingdom; [2]INSERM, Montpellier, France*

ThP 145 **CAD Mechanisms of Protonated Aromatic Compounds Relevant to Polystyrene Fast Pyrolysis**; Tuong V Nguyen[1]; Tanya Sharma[1]; Annika M Little[1]; Kumari Anshu[2]; John J. Nash[1]; Hilkka I. Kenttämaa[1]; *[1]Purdue Univeristy, West Lafayette, IN; [2]Indian Institute of Technology Roorkee, Roorkee, India*

ThP 146 **Exploring the ‘negative’ side of the proteomic landscape using top-down mass spectrometry**; Cynthia N. Nagy[1]; Joshua D. Hinkle[2]; John E. P. Syka[2]; Ryan T. Fellers[3]; Joseph B. Greer[3]; Kenneth R. Durbin[3]; Luca Fornelli[1, 4]; *[1]School of Biological Sciences, Norman, Oklahoma; [2]ThermoFisher Scientific, San Jose, CA; [3]Proteinaceous, Evanston, IL; [4]Department of Chemistry and Biochemistry, University of Oklahoma, Norman, Oklahoma*

ThP 147 **Charge transfer dissociation mass spectrometry (CTD-MS) for the structural characterization of synthetic polymers**; Emily A. Ruiz[1]; Inès Aloui[2]; William Buchmann[2]; Jean-Yves Salpin[2]; Glen Paul Jackson[1, 3]; *[1]C. Eugene Bennett Department of Chemistry, West Virginia University, Morgantown, WV; [2]Université Paris-Saclay, Univ Évry, CY Cergy Paris Université, CNRS, LAMBE, Évry-Courcouronnes, France; [3]Department of Forensic and Investigative Science, West Virginia University, Morgantown, WV*

ThP 148 **Charge transfer dissociation mass spectrometry (CTD-MS) for the structural characterization of monomeric and dimeric phospholipids**; Courtney E. LaPointe[1]; Glen Paul Jackson[1]; *[1]West Virginia University, Morgantown, WV*

ThP 149 **UV Photofragments of native-like proteins maintain a ‘memory’ of the precursor protein conformation**; Christian Bleiholder[1]; Jusung Lee[1]; Kaira Mayberry[1]; Mark Ridgeway[2]; Christopher A Wootton[3]; Alina Theisen[3]; Erin M Panczyk[2]; Benjamin J Jones[2]; Fanny C Liu[1]; Melvin A Park[4]; *[1]Florida State University, Tallahassee, FL; [2]Bruker Daltonics, Billerica, MA; [3]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [4]Bruker Switzerland AG, Fällanden, Switzerland*

ThP 150 **Assigning internal energies to nucleic acid fragmentation patterns through calibration of effective temperatures in a quadrupole ion trap**; Flaela Kalemi[1]; Emilie Bertrand[1]; Frédéric Rosu[1]; Valerie Gabelica[1]; *[1]University of Geneva, Geneva, Switzerland*

ThP 151 **New combinations of activation methods applied in tandem on the new timsOmni platform for enhanced top-down sequencing of oligonucleotides**; Frederic Rosu[1]; Rim Chiba[1]; Arjun Mallika[1]; Jean-François Greisch[2]; Eduardo Carrascosa[3]; Ioannis Orfanopoulos[4]; Athanasios Smyrnakis[4]; Dimitris Papanastasiou[4]; Valerie Gabelica[1]; *[1]University of Geneva, Geneva, Switzerland; [2]Bruker Switzerland AG, Fällanden, Switzerland; [3]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [4]Fasmatech Science & Technology, Athens, 15233, Greece*

ThP 152 **Leveraging the unique fragmentation of sodiated species involving covalent-bond cleavages to expedite small molecule characterization**; Annelaure DAMONT[1]; Imma FONTENELLE[1]; Clément CHALET[1]; Chenqin CAO[1]; Anaïs LEGRAND[1]; Jean-Claude TABET[1, 2]; François FENAILLE[1]; *[1]Université Paris-Saclay, CEA, INRAE, Département Médicaments et Technologies pour la Santé (DMTS), MetaboHUB, Gif sur Yvette, France; [2]Sorbonne Université, Faculté des sciences et de l'ingénierie, Institut Parisien de Chimie Moléculaire, Paris, France*

ThP 153 **Enhanced LC-MS/MS Workflow Integrating CID, EAD, and UVPD Activation Methods for Metabolite Identification and Characterization in Biofluids**; Romain Giraud[1]; Mircea Guna[2]; Yves Le Blanc[2]; Gerard Hopfgartner[1]; *[1]University of Geneva, LSMS, Geneva, Switzerland; [2]SCIEX, Concord, ON*

ThP 154 **Towards instrument-independent non-resonant tandem mass spectrometry**; Amandine Hueber[1]; Sophie Liuu[1]; Chenqin Cao[2]; Ekaterina Darii[3]; Annelaure Damont[2]; Olivier Firmesse[1]; François Fenaille[2]; Jean-Claude Tabet[2, 4]; *[1]ANSES, Maisons-Alfort, France; [2]CEA, Saclay, France; [3]Genoscope-CEA, Evry, France; [4]Sorbonne-University, Paris, France*

ThP 155 **Optimization of Electron Transfer Dissociation (ETD) MS/MS spectral generation rates on a Tribrid mass spectrometer for peptide-based workflows**; Christopher Mullen[1]; Graeme C. McAlister[1]; Joshua D. Hinkle[1]; Rafael D. Melani[1]; John E. P. Syka[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

FUNDAMENTALS: UNCONVENTIONAL APPROACHES IN MS
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ThP 156 **Development of a Cryogenic Digital Mass Spectrometer for Multiplexed IR Action Spectroscopy**; Grace O Capek[1]; Etienne Garand[1]; *[1]University of Wisconsin - Madison, Madison, WI*

ThP 157 **Investigation and Profiling of the Aroma Components by GC-SICRIT-QTOF**; Nan Hu[1]; Jianzhong Li[1]; Yixuan Duan[1]; Xiaokun Duan[2]; Charles C. Liu[2]; *[1]Agilent Technologies, Beijing, China; [2]ASPEC Technologies, Beijing, China*

ThP 158 **Electron capture charge reduction enables recording long transients in Orbitrap-based CDMS for low mass analytes**; Manuel D. Peris Díaz[1]; Evolène Deslignière[1]; Arjan Barendregt[1]; Tobias P Wörner[2]; Kyle L. Fort[1, 2]; Alexander Makarov[1, 2]; Albert J.R. Heck[1]; *[1]Utrecht University, Utrecht, Netherlands; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

ThP 159 **Ionization Effects and δ^{13}C Precision in Naphthenic Acid Mixtures: Insights from ESI Orbitrap-MS**; Giovanni Bonatti Bevilaqua[1]; Gabriel Franco Dos Santos[1]; Hugo Gontijo Machado[1]; Júlio César Oliveira Ribeiro[1]; Alexandre A. Ferreira[2]; Ygor dos Santos Rocha[2]; Boniek Gontijo Vaz[1]; *[1]Federal University of Goiás, Goiânia, Brazil; [2]PETROBRAS, Rio de Janeiro, Brazil*

ThP 160 **Integration of Spray-Based Ionization Techniques with Acoustic Ion Manipulation (AIM) at Atmospheric Pressure**; Julia L Danischewski[1]; Yi You[2]; Josefin Hufgard[2]; Lauren Bauer[1]; Jens Riedel[2]; Jacob T. Shelley[1]; *[1]Rensselaer Polytechnic Institute, Troy, NY; [2]Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, Germany*

ThP 161 **Distinguishing peptide b- and y-ions using Kendrick mass defect (KMD) analysis**; Mario Cindric[1]; David R. Goodlett[2]; Abanoub Mikhael[2]; *[1]Rudjer Boskovic Institute, Zagreb, Croatia; [2]University of Victoria GBC Proteomics Centre, Victoria, BC, BC*

ThP 162 **How to Quantitate a Drug Glucuronide without Reference Standard? - The APCI In-Source Decay Story**; Uwe Thuss; *Bayer AG, Wuppertal, Germany*

ThP 163 **Selective Partitioning of Ion Populations in a Linear Quadrupole Ion Trap via Axial Alternating Current Barriers**; Seth A Horn[1]; Nicolas J Pizzala[1]; Scott A. McLuckey[1]; *[1]Purdue Univeristy, West Lafayette, IN*

ThP 164 **Traveling Wave Acoustic Ion Manipulation (AIM) for Ion Trajectory Alteration**; Josefin Hufgard[1]; Julia L Danischewski[2]; Jacob T. Shelley[2]; Jens Riedel[1]; Yi You[1]; *[1]German Federal Institute for Materials Research and Testing, Berlin, Germany; [2]Rensselaer Polytechnic Institute, Troy, NY*

ThP 165 **Exploration of Acoustic Ion Manipulation (AIM) for Differential Ion Mobility Spectrometry**; Yi You[1]; Josefin Hufgard[1]; Julia L. Danischewski[2]; Jacob T. Shelley[2]; Jens Riedel[1]; *[1]German Federal Institute for Materials Research and Testing, Berlin, Germany; [2]Rensselaer Polytechnic Institute, Troy, NY*

ThP 166 **Catalyst-free Accelerated Synthesis of Pyrazoles in Water Microdroplets**; Manish Jana[1]; Keerthana Unni[1, 2]; Thalappil Pradeep[2]; R. Graham Cooks[1]; *[1]Department of Chemistry, Purdue University, West Lafayette, IN; [2]DST unit of Nanoscience (DST UNS) and Thematic unit of Excellence (TUE), Department of Chemistry, Indian Institute of Chemistry Madras, Chennai, India*

ThP 167 **Using the Agilent 7250 GC-QTOF for Quantitation of 12C and 13C Methane Enables a New Capability for Methanogen Research**; Karl K Weitz[1]; Jared Ellenbogen[2]; Rosalie K Chu[1]; Kelly Wrighton[2]; Mary S. Lipton[1]; *[1]Battelle Pacific Northwest National Laboratories, Richland, WA; [2]Colorado State University, Fort Collins, CO*

ThP 168 **Developing instrumentation for spontaneous ionization in vacuum and what it tells us about the ionization mechanism**; Charles N McEwen[1]; Jessalyn Aquilino[1, 2]; Adetoun Adeniji-Adele[3]; John Tomsho[3]; Milan Pophristic[2, 3]; Ellen Inutan[2, 4]; I-Chung Lu[5]; Sarah Trimpin[2, 6]; *[1]Saint Joseph Univ.University, Philadelphia, PA; [2]MSTM, Newark, DE; [3]Saint Joseph's University, PHILADELPHIA, PA; [4]Mindanao State University - Iligan Institute of Technology, Illigan City, Philippines; [5]National Chung Hsing University, Taichung, Taiwan; [6]Wayne State University, Detroit, MI*

H/D EXCHANGE: HARDWARE, SOFTWARE AND METHODOLOGY
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ThP 169 **An automated HDX-MS strategy for probing the structural dynamics of integral membrane proteins under physiological conditions**; Damon Griffiths[1]; Juan Pablo Rincon Pabon[1]; Charlotte Guffick[1]; Satomi Inaba-Inoue[2]; Konstantinos Beis[3]; Argyris Politis[1]; *[1]The University of Manchester, Manchester, United Kingdom; [2]Hokkaido University, Sapporo, Japan; [3]Imperial College London, London, United Kingdom*

ThP 170 **Evaluation of H/D Scrambling Propensities of various proteins and peptides**; Charles Mundorff[1]; Sarah Hadley[1]; Yuqi Shi[2]; Graeme McAlister[2]; Rosa Viner[2]; Miklos Guttman[1]; *[1]University of Washington, Seattle, WA; [2]Thermo Fisher Scientific, San Jose, CA*

ThP 171 **Advancing HDX-MS for Structural Insights into Large Viral Protein Complex**; Chunyang Guo[1]; Alison E. Varghese[1]; Shijie Zheng[1]; Seungil Han[1]; Graham M. West[1]; *[1]Pfizer, Groton, CT*

ThP 172 **PFNet: a machine learning method for high-accuracy HX/MS data analysis at single-site resolution**; Chenlin Lu[1]; Kyle C. Weber[1]; Anum Glasgow[1]; *[1]Columbia University, NEW YORK, NY*

ThP 173 **Rapid Removal of IgG1 Carryover on Protease Column Using Protease-Safe Wash Solutions Delivered with LC Pump for HDX-MS Systems**; Sandeep Kumar[1]; Kyle W. Anderson[1, 2]; *[1]Institute for Bioscience and Biotechnology Research, National Institute of Standards and Technology* *and the University of Maryland, College Park, Rockville, MD; [2]National Institute of Standards and Technology, Bioprocess Measurements Group, Biomolecular Measurement Division, Gaithersburg, MD*

ThP 174 **Developing HX-MS2 into a Higher Throughput Screening Tool for Drug Discovery**; Morgan Hepburn[1]; D. Alex Crowder[1]; Frantisek Filandr[1]; Vladimir Sarpe[2]; Wesley A. Mosimann[3]; Liam Worrall[3]; Natalie C.J. Strynadka[3]; David C. Schriemer[1]; *[1]University of Calgary, Calgary, AB; [2]Trajan Scientific and Medical, Ringwood, Australia; [3]University of British Columbia, Vancouver, BC*

ThP 175 **Expanding support for flexible DIA collection strategies in automated HDX analysis**; Vladimir Sarpe[1]; Morgan Hepburn[2]; Natalie C.J. Strynadka[3]; Wesley A. Mosimann[3]; Liam Worrall[3]; David C. Schriemer[2]; *[1]Trajan Scientific and Medical, Ringwood, Australia; [2]University of Calgary, Calgary, AB; [3]University of British Columbia, Vancouver, BC*

ThP 176 **Optimization of ZrO2 use for efficient lipid removal in hydrogen exchange experiments for membrane proteins**; Juan P Rincon Pabon[1]; Charlotte Guffick[1]; Zulaikha Akbar[1]; Argyris Politis[1]; *[1]The University of Manchester, Manchester, United Kingdom*

ThP 177 **A Comprehensive Standardization Strategy for Hydrogen/Deuterium Exchange Mass Spectrometry**; Taylor A Murphree[1]; Clint Vorauer[1]; Mason Saunders[1]; Miklos Guttman[2]; *[1]University of Washington, Seattle, WA; [2]University of Washington, Seattle, WA*

ThP 178 **Observing Single Amino Acid Millisecond HDX Kinetics on a QTOF Mass Spectrometer with Electron Activated Dissociation (EAD)**; Joseph Anacleto[1]; Madeline Blanco[2]; Ebadullah Kabir[2]; Yves Le Blanc[3]; Cristina Lento[2]; Derek J Wilson[2]; *[1]Emeritus, Brampton, ON; [2]York University, Toronto, ON; [3]SCIEX, Concord, ontario*

ThP 179 **SpyCatcher-SpyTag for Hydrogen Deuterium Exchange Mass Spectrometry in Complex Protein Matrices**; Daniele Peterle[1]; Bindu Y Srinivasu[1]; Zachary A Cohen[1]; John R Engen[1]; Thomas E Wales[1]; *[1]Northeastern University, Boston, MA*

ThP 180 **Inferring single-residue resolution from peptide-level HDX-MS data: Different ways to square the circle**; Michele Stofella[1]; Antonio Grimaldi[2]; Emanuele Paci[2]; Frank Sobott[1]; *[1]University of Leeds, Leeds, United Kingdom; [2]University of Bologna, Bologna, Italy*

ThP 181 **Water Vapor: An Overlooked Influencer in Hydrogen Deuterium Exchange**; Alesi R Escobedo[1]; Taylor A Murphree[1]; Miklos Guttman[1]; *[1]University of Washington, Seattle, WA*

ThP 182 **Quantifying Hydrogen Deuterium Reaction Orders and Reaction Rates Using Traveling Wave Structures for Lossless Ion Manipulation**; Daniel Wu[1]; Brian H. Clowers[1]; *[1]Washington State University, Pullman, WA*

ThP 183 **Sarlacc: Predicting Non-Specific Protein Digestion**; Kiran S. Bhat[1]; Nolan K. McLaughlin[1]; Michael L. Gross[1]; *[1]Washington University in St. Louis, University City, MO*

ThP 184 **Assessment of amide H/D scrambling with UVPD**; Sarah N Hadley[1]; Yuqi Shi[2]; Charles Mundorff[1]; Rosa Viner[2]; Miklos Guttman[1]; *[1]University of Washington, Seattle, WA; [2]Thermo Fisher Scientific, San Jose, CA*

HIGH THROUGHPUT MS II
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ThP 185 **Coupling a 3D-printed composable platform to mass spectrometry for high-throughput analysis**; Olanrewaju Adedayo Awoyemi[1]; Amanda Devor[1]; Herbi Yuliantoro[1]; Samuel Fisher[1]; Stephen J. Valentine[1]; Peng Li[1]; *[1]West Virginia University, Morgantown, WV*

ThP 186 **45-Plex tandem mass tag mass spectrometry enabling accurate quantification by interference correction**; Nan Zhang[1]; Zhen Wang[1]; Ya Huang[1]; Ju Wang[1]; Zuofei Yuan[1]; Xusheng Wang[2]; Junmin Peng[1]; *[1]St. Jude Children's Research Hospital, Memphis, TN; [2]University of Tennessee Health Science Center, Memphis, TN*

ThP 187 **Acoustic Ejection Differential Mobility-Multimodal Tandem Mass Spectrometryfor General Screening of Drugs of Abuse and Metabolites in Blood and Urine**; Patrick Mueller[1]; Lysi Ekmekciu[1]; Stefan Koenig[2]; Chang Liu[3]; Thomas R. Covey[3]; Yves Le Blanc[3]; Gerard Hopfgartner[1]; *[1]University of Geneva, Geneva, Switzerland; [2]University of Bern, Bern, Switzerland; [3]SCIEX, Concord, ON*

ThP 188 **Fast histone extraction and sample automation for high-throughput PTM analysis**; Francisca N De Luna Vitorino[1]; Renee Dean[1]; Xingyu Liu[1]; Shri Pinjarla[1]; Emily Zahn[1]; Benjamin A Garcia[1]; *[1]Washington University School of Medicine, St. Louis, MO*

ThP 189 **Accelerating lipidomic analysis with the acoustic ejection sampling technology**; Pradeep Narayanaswamy[1]; Eva Duchoslav[2]; Venkatesha Gaddemane Narasimha[1]; Hyungwon Choi[3]; *[1]SCIEX, Singapore, Singapore; [2]SCIEX, Concord, ontario; [3]National University of Singapore, Singapore, Singapore*

ThP 190 **Automated High-Throughput Sample Preparation workflow: Integrating Depletion, Desalting, and Glycopeptide Enrichment**; Jung Hoon Choi[1, 2]; Geul Bang[3]; Jin Young Kim[3]; *[1]Korea Basic Science Institute, Cheongjusi, South Korea; [2]Chungnam National University, Dajeon, South Korea; [3]Korea Basic Science Institute, Cheongju, South Korea*

ThP 191 **Multiplexed Online Ion Exchange SPE combined with LC/MS/MS for the Simultaneous Analysis of Common Drugs in Human Plasma**; Eishi IMOTO[1]; Vikki JOHNSON[2]; Logan Miller[1]; Daiki Fujimura[3]; Toshiya Matsubara[1]; *[1]Shimadzu Scientific Instruments, Columbia, MD; [2]Shimadzu Scientific Instruments, Carlsbad, CA; [3]Shimadzu, Kyoto, Japan*

ThP 192 **Automating Proteomics Data Quality Control: A metadata-informed report integrating sample type-specific QC metrics**; Jana Zecha[1]; Benjamin Pullman[2]; Stewart MacArthur[3]; Matthew Glover[1]; Sonja Hess[1]; *[1]Dynamic Omics, Centre for Genomics Research (CGR), Discovery Sciences, BioPharmaceuticals R&D, AstraZeneca, Gaithersburg, MD; [2]Bioinformatics, Centre for Genomics Research (CGR), Discovery Sciences, BioPharmaceuticals R&D, AstraZeneca, Gaithersburg, Maryland; [3]Bioinformatics, Centre for Genomics Research (CGR), Discovery Sciences, BioPharmaceuticals R&D, AstraZeneca, Cambridge, United Kingdom*

ThP 193 **Efficient Tandem Capillary Flow LC-MS with Short µPAC Columns and a Single Ionization Source**; Paul Jacobs[1]; Natalie Van Landuyt[1]; Jeff Op De Beeck[1]; *[1]Thermo Fisher Scientific, Ghent, Belgium*

ThP 194 **Label-free analysis and printing of cells from droplets as individual colonies from water-in-oil emulsions**; Emmanouil Mavrakis[1]; G. Thomas Knecht[1]; Maxwell J. Unger[1, 2]; Alison R.H. Narayan[1, 2, 3]; Robert T Kennedy[1]; *[1]Department of Chemistry, University of Michigan, Ann Arbor, MI; [2]Life Sciences Institute, University of Michigan, Ann Arbor, Michigan, United States, Ann Arbor, MI; [3]Program in Chemical Biology, University of Michigan, Ann Arbor, Michigan, United States, Ann Arbor, MI*

ThP 195 **A robust, cost-efficient and scalable plasma proteomics pipeline utilizing the Evotip Pure subjected to more than 1,100 patient samples**; Pia H. Jensen[1]; Camilla O. Kyhl[1]; Frederik Tolberg[1]; Joel Vej-Nielsen[1]; Stoyan Stoychev[1]; Nicolai Bache[1]; Dorte B. Bekker-Jensen[1]; Michael L. Nielsen[1]; *[1]Evosep, Odense, Denmark*

ThP 196 **Application of a targeted PFAS quantitation method within a high-throughput untargeted LC-HRMS workflow**; Catherine Mullins[1]; Douglas I Walker[1]; *[1]Emory University, Atlanta, GA*

ThP 197 **MRM switching on-the-fly enables ultra-high throughput bioanalysis for in vito microsomal stability assay**; Craig B Gutierrez[1]; Chang Lu[2]; Neal Liddle[1]; Hui Zhang[1]; *[1]Iambic Therapeutics, San Diego, CA; [2]SCIEX, Concord, ontario*

ThP 198 **High-Throughput Reaction Screening For Energetic Relevant Compounds Using a Liquid Handling Robot Coupled to Desorption Electrospray Ionization Mass**

Spectrometry; Matthew J Carlo[1]; Patrick W. Fedick[1]; *[1]Naval Air Warfare Center Weapons Division, China Lake, CA*

ThP 199 **Optimization of Sample Preparation Methods to Enable Ultra-High Throughput PK Analysis using Acoustic Ejection Mass Spectrometry**; Michelle Robinson[1]; Kenneth Anderson[1]; Lisa O'Callaghan[1]; *[1]Merck, West Point, PA*

ThP 200 **Unlocking next-generation insights in LC-MS based proteomics with a scalable and sustainable workflow strategy**; Magnus Huusfeldt[1]; Stoyan Stoychev[1]; Camilla Olson Kyhl[1]; Nicolai Bache[1]; Dorte Bekker-Jensen[1]; *[1]Evosep, Odense, Denmark*

ThP 201 **High throughput quantification of 13 amino acids in 10 seconds per sample**; Francis Brière[1, 2]; Serge Auger[3]; Pierre Picard[3]; Claudia Carpentier[2]; Jacques Corbeil[1, 2]; *[1]CRCHU de Quebec - Université Laval, Quebec, QC; [2]Linearis Labs, Québec, QC; [3]Phytronix Technologies, Quebec, QC*

ThP 202 **Ultra high throughput chemoproteomics screening on the Stellar Mass Spectrometer**; Lilian Randolph Heil[1]; Brett Larsen[1]; Kevin Yang[1]; Ariana E. Shannon[2]; Philip Remes[3]; Cristina Jacob[3]; Lindsay K Pino[4]; Brian C. Searle[2]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Ohio State University, Columbus, OH; [3]Thermo Fisher Scientific, San Jose, California; [4]Talus Bioscience, Seattle, WA*

ThP 203 **Microfluidic Reaction Assembly and Fast Analysis Platform for High-Throughput Screening in-Flow**; Yue Xin[1]; Alan K Wortman[2]; Ryan T Snyder[1]; Kaid C Harper[3]; Anna V Bay[3]; Nick Cowper[3]; Corey R.J. Stephenson[4]; Robert T Kennedy[1]; *[1]University of Michigan-Ann Arbor, Ann Arbor, MI; [2]University of Oxford, Oxford, United Kingdom; [3]AbbVie Inc, North Chicago, IL; [4]University of British Columbia, Vancouver, BC*

ThP 204 **Characterization of the Redox Regulation of S-Adenosylhomocysteine Hydrolase Using High-Throughput Desorption Electrospray Ionization Mass Spectrometry**; Yunfei Feng[1]; Sarah C Stanhope[2]; Nicolas M Morato[2]; Vikki M Weake[2]; Robert Graham Cooks[2]; *[1]Purdue University, West Lafayette, IN; [2]Purdue Univeristy, West Lafayette, IN*

ThP 205 **Peptides Stability Studies and Compound Purity Assessment Using High Throughput UPLC-MS and Echo-MS**; Wilfredo Pinto[1]; Foster Tenkorang[2]; *[1]Merck, Rahway, NJ; [2]Merck & Co., Rahway, NJ*

ThP 206 **Analytical Procedure Development and Validation of High-throughput ZipChip CZE-MS Method for Quantitative Oligonucleotide Analysis**; Nadia Tasnim Ahmed[1]; Joshua Shipman[1]; Md Rabiul Islam[1]; Cynthia Sommers[1]; Jason Rodriguez[1]; Kui Yang[1]; *[1]Food and Drug Administration, Saint Louis, MO*

IMAGING MS: PHARMACEUTICALS, METABOLITES, LIPIDS, AND GLYCANS II

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ThP 207 **Fatty acid and lipid analysis of pediatric low-grade gliomas using MALDI mass spectrometry imaging**; Julia R Bonney[1]; Rishov Goswami[2, 3]; Pruthvi Gowda[2, 3]; Magdalena Bachmann[2, 3]; Kaitlyn E Bootz[1]; Nika N Danial[2, 3]; Nathalie Y.R. Agar[1]; *[1]Department of Neurosurgery, Brigham and Women's Hospital, Harvard Medical School, Boston, MA; [2]Department of Cancer Biology, Dana-Farber Cancer Institute, Harvard Medical School, Boston, MA; [3]Department of Medicine, Harvard Medical School, Boston, MA*

ThP 208 **Quantification of N-Linked Glycans in Brain Using IR-MALDESI Mass Spectrometry Imaging**; Adeleke A Adepoju[1]; Tana V. Palomino[2]; David C Muddiman[2]; *[1]Biological Imaging Laboratory for Disease and Exposure Research, Department of Chemistry, North Carolina State University, Raleigh, North Carolina; [2]Biological Imaging Laboratory for Disease and Exposure Research, Department of Chemistry, North Carolina State University,, Raleigh, North Carolina*

ThP 209 **MALDI Mass Spectrometry Imaging of Metabolites and Lipids in Neurological Disease Development**; Arya I Lall[1]; Siyu Lin[2]; Weidi Zhang[2]; Yongheng Wang[3]; Aijun Wang[2]; Elizabeth K Neumann[2]; *[1]University of California, Davis, Davis, CA; [2]University of California Davis, Davis, CA; [3]Massachusetts Institute of Technology, Cambridge, MA*

ThP 210 **Imaging Mass Spectrometry Reveals Triterpenoid Localization in Soybean Secondary Aerenchyma**; Yushiro Fuji[1]; Tetsuya Mori[1]; Noriko Kamiya Takeda[1]; Mana Jitsui[2]; Kiminori Toyooka[1]; Hikaru Seki[3]; Hirokazu Takahashi[2]; Masami Yokota Hirai[1, 2]; *[1]RIKEN CSRS, Yokohama, Japan; [2]Department of Applied Biosciences, Graduate School of Bioagricultural Sciences and School of Agricultural Sciences, Nagoya University, Nagoya, Japan; [3]Department of Biotechnology, Graduate School of Engineering, Osaka University, Osaka, Japan*

ThP 211 **Rapid spatial molecular insights into human brain tumors by axial MALDI TOF mass spectrometry imaging**; Jasmine Reese[1]; Janina Oetjen[2]; Michele Genangeli[2]; Olaf Ansorge[1]; *[1]Nuffield Department of Clinical Neurosciences, University of Oxford, Oxford, United Kingdom; [2]Bruker Daltonics GmbH & Co. KG, Bremen, Germany*

ThP 212 **Targeting neurotransmitter alterations following drug treatment using mass spectrometry imaging and cloud-based data analysis using Weave**; Nathan Heath Patterson[1]; Rabindranath Andujar[1]; Sarah Diez[2]; Alice Ly[1]; Marc Claesen[1]; Nico Verbeeck[1]; Zoi Balla[2]; Eliza Koros[2]; Michael Becker[2]; *[1]Aspect Analytics, Genk, Belgium; [2]Boehringer Ingelheim, Biberach, Germany*

ThP 213 **Quantitative Spatial Profiling of Gangliosides Across Human and Murine Brain Tissues**; Maria José Q Mantas[1]; Shadrack M Mutuku[2]; Nicolas Tomasiello[2]; Greg Sutherland[3]; Caine Smith[3]; Nathan Heath Patterson[1]; Marc Claesen[1]; Alice Ly[1]; Nathan G. Hatcher[4]; Nico Verbeeck[1]; Kim Ekroos[5]; Shane R. Ellis[2]; *[1]Aspect Analytics, Genk, Belgium; [2]Molecular Horizons and School of Chemistry and Molecular Bioscience, University of Wollongong, Wollongong, Australia; [3]New South Wales Brain Tissue Research Centre, Charles Perkins Centre and School of Medical Sciences, Faculty of Medicine and Health, The University of Sydney, Sydney, Australia; [4]Merck & Co., Inc., West Point, PA; [5]Lipidomics Consulting Ltd, Esbo, Finland*

ThP 214 **Mass Spectrometry Imaging of Pimonidazole as a Hypoxia Marker in 3D Cell Cultures**; Andrew T. Freeman[1]; Arbil Lopez[1]; Amanda B. Hummon[1, 2]; *[1]Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH; [2]Comprehensive Cancer Center, The Ohio State University, Columbus, Ohio*

ThP 215 **High-resolution imaging of metabolites and lipids in frozen hydrated and freeze dried Zebrafish retina using Water Cluster SIMS**; Naoko Sano[1]; Elkan Lau[2]; Johanna Von Gerichten[2]; Kate McHardy[1]; Paul Blenkinsopp[1]; Maya Al Sid Cheikh[3]; Melanie Bailey[2, 4]; *[1]Ionoptika Ltd, Eastleigh, United Kingdom; [2]University of Surrey, Guildford, United Kingdom; [3]University of Edinburgh, Edinburgh, United Kingdom; [4]King's College London, London, United Kingdom*

ThP 216 **Multiomic Drug and Metabolite Imaging Combined with Targeted Protein and mRNA Imaging on the Same Tissue using Mass-Tagged Probes**; Gargey B. Yagnik[1]; Zhi Wan[2]; Jonathan Bell[2]; Leonardo G. Dettori[2]; Philip Carvalho[2]; Kenneth J. Rothschild[2, 3]; Mark J. Lim[2]; *[1]AmberGen, Inc., Billerica, MA; [2]AmberGen Inc., Billerica, MA; [3]Boston University, Boston, MA*

ThP 217 **Mapping Physiologically Relevant Concentrations of Antibiotics Ceftriaxone and Levofloxacin in the Murine Liver by IR-MALDESI MSI**; Yury Desyaterik[1]; Sarah E. Rowe[1]; Michelle Angeles-Solano[1]; Angela D. M. Kashuba[1]; Elias P. Rosen[1]; *[1]UNC, Chapel Hill, NC*

ThP 218 **Negative Ion Mode MALDI-Mass Spectrometric Imaging of Orthotopic Mouse Glioma**; Hay-Yan J Wang[1]; Chiung-Yin Huang[2, 3]; Kuo-Chen Wei[2, 3, 4, 5]; Kuo-Chen Hung[6]; *[1]Nat'l Sun Yat-Sen University, Kaohsiung City, Taiwan; [2]Neuroscience Research Center, Chang Gung Memorial Hospital, Taoyuan City, Taiwan; [3]Department of Neurosurgery, New Taipei Municipal TuCheng Hospital, New Taipei City, Taiwan; [4]Department of Neurosurgery, Chang*

Gung Memorial Hospital, Taoyuan City, Taiwan; [5]School of Medicine, Chang Gung University, Taoyuan City, Taiwan; [6]Division of General and Digestive Surgery, Kaohsiung Medical University Chung-Ho Memorial Hospital, Kaohsiung City, Taiwan

ThP 219 **Improving sensitivity and resolving the complexity of spatial lipidomics with MALDI-TIMS MSI**; Georgia Charkoftaki[1]; Reza Aalizadeh[1]; Varvara Nikolopoulou[1]; Alvaro Santos-Neto[2]; Athina Lisgara[1]; Jordan Hartig[3]; Scott Pennino[3]; Vladimir V. Papov, Jr. [3]; Vasilis Vasiliou[1]; *[1]Yale University, New Haven, CT; [2]University of São Paulo, São Carlos, Brazil; [3]Boehringer Ingelheim Pharmaceuticals, Inc., Ridgefield, CT*

ThP 220 **Desorption electrospray ionization multiple reaction monitoring mass spectrometry imaging of tryptophan and TCA cycle metabolites separated by thin layer chromatography**; Istvan Pap[1]; Virág Sági-Kiss[2]; Gabriel Stefan Horkovics-Kováts[1]; Daniel Simon[1]; Katja Dettmer-Wilde[3]; Peter Oefner[3]; Chotima Böttcher[4]; Zoltan Takats[1]; *[1]University of Regensburg, Department of Immune Medicine Multimodal Imaging of Intracellular Communication, Regensburg, Germany; [2]Imperial College London, Division of Systems Medicine, London, United Kingdom; [3]University of Regensburg, Department of Functional Genomics, Regensburg, Germany; [4]Charité University Medicine, Berlin, Germany*

ThP 221 **A mass spectrometry-based immunology panel for the investigation of N-glycans in biofluids**; Ariana E Stratton[1]; Hassan Moussa[2]; Carl Atkinson[2]; Boone M Prentice[1]; *[1]Department of Chemistry, University of Florida, Gainesville, FL; [2]Northwestern University Feinberg School of Medicine, Chicago, IL*

ThP 222 **RARγ isoform selective agonist CD437 as a dual treatment to abate inflammation in a MRSA infection mouse model**; Temple Andrews[1]; Samuel Krug[1]; Ravineel Singh[2]; Jianshi Yu[1]; Mehari M. Weldemariam[1]; Nageswara Pilli[1]; Keven Robinson[2]; Maureen A Kane[1]; *[1]University of Maryland School of Pharmacy, Baltimore, MD; [2]University of Pittsburgh, School of Medicine, Department of Medicine, Pittsburgh, PA*

ThP 223 **Spatial lipid profiling of human brain tissue with alpha-synuclein-related pathology using DESI Imaging Mass Spectrometry**; Artur Lazarian[1]; David Pisapia[1]; Krista Wartchow[1]; William Dartora[1]; Carmen Barrios Castellanos[1]; Laura Beth McIntire[1]; *[1]Weill Cornell Medicine, New York, NY*

ThP 224 **MALDI Mass Spectrometry Imaging Reveals Distinct Nucleotidase Localizations Throughout Mouse Organs**; Maisa A Khan[1]; Nav Raj Phulara[1]; Herana Kamal Seneviratne[1]; *[1]University of Maryland, Baltimore County, Baltimore, MD*

ThP 225 **Spatially Resolved Metabolomics and Transcriptomics Uncovers Tissue-Specific Renal Alterations Following Cisplatin Exposure**; Jephte Akakpo[1]; Erika Abbott[2]; Benjamin L. Woolbright[3]; Anup Ramachandran[1]; Rick G. Schnellmann[4]; John A. Taylor[3, 5]; *[1]Department of Pharmacology, Toxicology and Therapeutics, University of Kansas Medical Center, Kansas City, Kansas; [2]Department of Urology, University of Kansas Medical Center, Kansas City, Kansas; [3]Department of Cancer Biology, University of Kansas Medical Center, Kansas City, Kansas; [4]Department of Pharmacology and Toxicology, University of Arizona,, Tucson, Arizona; [5]Department of Urology, University of Kansas Medical Center,, Kansas City, Kansas*

ThP 226 **Single-Cell MALDI-MS Imaging of Trichomes with Isotope Labeling**; Sumin Na[1]; Young Jin Lee[1]; *[1]Iowa State University, Ames, IA*

ThP 227 **Mapping Metabolites in Human Eye: Integrating High Spatial Resolution Imaging Mass Spectrometry and Histology for a Human Atlas Reference**; Ali Zahraei[1, 2]; Lukasz G Migas[3]; Martin Dufresne[2, 4]; David M.G. Anderson[2, 4]; Madeline E. Colley[1, 2]; Angela R. S. Kruse[1, 2]; Thai Pham[1, 2]; Jeffrey D. Messinger[5]; Christine A. Curcio[5]; Raf Van De Plas[2, 3, 4]; Kevin L. Schey[2, 4]; Jeffrey M. Spraggins[1, 2, 4, 6]; *[1]Department of Cell and Developmental Biology, Vanderbilt University School of Medicine, Nashville, TN; [2]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [3]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [4]Department of Biochemistry, Vanderbilt University School of Medicine, Nashville, TN; [5]Department of Ophthalmology and Visual Sciences, Heersink School of Medicine, University of Alabama, Birmingham, Alabama; [6]Department of Chemistry, Vanderbilt University, Nashville, TN*

ThP 228 **Investigating the Influence of NIST Particulate Matter on Human Bronchial Epithelial Cells Using Confocal Raman Microscopy and TOF-SIMS Imaging**; Manale Noun[1]; Razane El Annan[1, 2]; Sandrine Villette[2]; Jean-Paul Salvetat[3]; Imane Abbas[1]; Anthony Verdin[4]; Ghida Badran[5]; Mohamad Roumie[1]; Sophie Lecomte[2]; *[1]Lebanese Atomic Energy Commission-National Council for Scientific Research CNRSL, Beirut, Lebanon; [2]Univ. Bordeaux, CNRS, Bordeaux INP, CBMN, UMR 5248, Pessac, France; [3]Placamat, UAR 3626, CNRS, Université de Bordeaux, Pessac, France; [4]Univ.* Littoral Côte d'Opale, Unité de *Chimie Environnementale et Interactions sur le Vivant, UCEIV, Dunkerque, France; [5]Universite Paris-Saclay, Inserm, Inflammation microbiome immunosurveillance, Orsay, France*

ThP 229 **Comprehensive spatial metabolomics of developmental mouse brain**; Lele Xu[1]; Shu Zhang[1]; Jiazhang Chen[1]; Areej Niaz[1]; Ye He[1]; *[1]CUNY Advanced Science Research Center, New York, NY*

ThP 230 **Site-Specific Retinal Pharmacology of a Photoreceptor-Protective Small Molecule Revealed by MALDI-MSI**; Dheeraj K. Agrohia[1]; Kaori Ueda[1]; Anand Swaroop[1]; *[1]Neurobiology, Neurodegeneration and Repair Laboratory, National Eye Institute, National Institutes of Health, Bethesda, Maryland*

ThP 231 **Comparing MALDI Imaging Platforms: A Systematic Evaluation of Lipid Imaging Performance**; Megan Ward[1, 2]; Madeline E Colley[1, 3]; Martin Dufresne[1, 3]; Ali Zahraei[1, 3]; Lukasz G Migas[1, 4]; Melissa Farrow[1, 3]; Raf Van De Plas[1, 4, 5]; Jeffrey M Spraggins[1, 2, 3, 5, 6, 7]; *[1]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [2]Chemical and Physical Biology Program, Vanderbilt University School of Medicine, Nashville, TN; [3]Department of Cell and Developmental Biology, Vanderbilt University School of Medicine, Nashville, TN; [4]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [5]Department of Biochemistry, Vanderbilt University School of Medicine, Nashville, TN; [6]Department of Chemistry, Vanderbilt University, Nashville, TN; [7]Department of Pathology, Microbiology, and Immunology, Vanderbilt University Medical Center, Nashville, TN*

ThP 232 **Advanced Neutral Lipid Imaging with Salt-Enhanced MALDI TIMS IMS**; Kameron Molloy[1, 2]; Martin Dufresne[2, 3]; Madeline Colley[2, 3]; Lukasz G Migas[2, 4]; Raf Van De Plas[2, 4, 5]; Jeffrey M Spraggins[1, 2, 3, 5, 6]; *[1]Department of Chemistry, Vanderbilt University, Nashville, TN; [2]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [3]Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; [4]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [5]Department of Biochemistry, Vanderbilt University, Nashville, TN; [6]Department of Pathology, Microbiology, and Immunology, Vanderbilt University Medical Center, Nashville, TN*

IMAGING: SPATIALLY-RESOLVED OMICS II
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ThP 233 **Spatially-Resolved Proteoform Signatures in Kidney Diseases**; Pei Su[1]; Michael Hollas[1]; Indira Pla[1]; Ryan Fellers[1]; Amanda Knoten[2]; Joseph Gaut[2]; Sanjay Jain[2]; Michael Caldwell[1]; Jared Kafader[1]; Neil Kelleher[1]; *[1]Northwestern University, Evanston, IL; [2]Washington University School of Medicine, St. Louis, MO*

ThP 234 **Organophosphate Exposure in Mouse Models: Using LC-MS/MS and MALDI IMS to Identify Off-Target Effects of Chlorpyrifos**; Kes A. Luchini[1]; Jamie L. Inman[2]; Madison Grace Thornhill[1]; Jessica A. Salguero[1]; Philip M. Mach[1]; Brett R. Blackwell[1]; Antoine M. Snijders[2, 3]; Trevor G. Glaros[1]; Emilio S. Rivera[1]; [1]*Biochemistry and Biotechnology Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM;* [2]*Biological Systems & Engineering Division, Lawrence Berkeley National Laboratory, Berkeley, CA;* [3]*Current Address: Biosciences and Biotechnology Division, Physical & Life Sciences Directorate, Lawrence Livermore National Laboratory, Livermore, CA*

ThP 235 **Mass Spectrometric Visualization of Glycolytic-TCA cycle flux interactions in the Tumor Microenvironment (TEM) of mutant Kras p53 pancreatic adenocarcinoma models**; Sanjay Pandey[1]; Yunping Qiu[1]; Bindesh Shrestha[2]; Hardik Shah[3]; Kevin Zematis[4]; Christopher Jurtschenko[2]; Chandan Guha[1]; Irwin J Kurland[5]; [1]*Albert Einstein College of Medicine, Bronx, New York;* [2]*Waters Corp., Milford, MA;* [3]*University of Chicago, Chicago, IL;* [4]*Pacific Northwest National Laboratory (PNNL), Richland, WA;* [5]*Stable Isotope and Metabolomics Core Facility, Albert EInstein, Bronx, NY*

ThP 236 **Secondary Photocleavable Mass-tagged Probes for Highly Multiplexed Tandem MALDI-IHC Imaging of Difficult to Detect Proteins in Tissues**; Ziying Liu[1]; Zhi Wan[1]; Gargey B. Yagnik[1]; Philip Carvalho[1]; Andrew Yatsuhashi[1]; Kenneth J. Rothschild[1, 2]; Mark Lim[1]; [1]*AmberGen, Billerica, MA;* [2]*Department of Physics and Photonics Center, Boston University, Boston, MA*

ThP 237 **Characterizing molecular heterogeneity of Staphylococcus aureus colonies in response to varied cellular microenvironments**; Jacqueline M Van Ardenne[1, 2]; Lukasz G Migas[2, 3]; Thai H Pham[2, 4]; Anna J Smith[2, 4]; Martin Dufresne[2, 4]; Jeffrey A Freiberg[5, 6]; Kyle T Enriquez[5, 6]; Rachel Finegan[2]; Melissa A Farrow[2, 4]; Raf Van De Plas[2, 3, 7]; Eric P Skaar[5, 6, 8]; Jeffrey M Spraggins[1, 2, 4, 5, 6, 7]; [1]*Department of Chemistry, Vanderbilt University, Nashville, TN;* [2]*Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN;* [3]*Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands;* [4]*Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN;* [5]*Department of Pathology, Microbiology, and Immunology, Vanderbilt University Medical Center, Nashville, TN;* [6]*Vanderbilt Institute for Infection, Immunology, and Inflammation, Vanderbilt University Medical Center, Nashville, TN;* [7]*Department of Biochemistry, Vanderbilt University, Nashville, TN;* [8]*Vanderbilt Institute for Chemical Biology, Vanderbilt University, Nashville, TN*

ThP 238 **Impact of Aging and Alzheimer's Disease on Vascular Biomechanics and Brain Biochemistry**; Allison R. Jones[1]; Amin Jarrahi[1]; Kylee Karpowich[1]; Lindsay Brown[1]; Anna Colleen Crouch[1]; [1]*University of Tennessee, Knoxville, TN*

ThP 239 **Capturing the complex molecular composition of human lungs by spatial multi-omic analysis and integration**; Brittney L Gorman[1]; Dusan Velickovic[1]; Jamie Verheyden[2]; Gail Deutsch[3]; Naina A Beishembieva[1]; Heidie Huyck[4]; Gloria Pryhuber[4]; Geremy C Clair[1]; Christopher Anderton[1]; [1]*Pacific Northwest National Lab, Richland, WA;* [2]*Department of Pediatrics, School of Medicine, University of California San Diego, San Diego, CA;* [3]*Department of Laboratory Medicine and Pathology, University of Washington School of Medicine, Seattle, WA;* [4]*Department of Pediatrics, University of Rochester Medical Center, Rochester, NY*

ThP 240 **Detection and identification of oxidatively-truncated PE during Ferroptosis in vitro and in vivo**; L.J. Sparvero[1]; Yulia Y. Tyurina[1]; Vladimir A. Tyurin[1]; Svetlana N. Samovich[2]; Haider H. Dar[1]; Alexander Kapralov[1]; Yuri L. Bunimovich[1]; Hülya Bayir[2]; Valerian E. Kagan[1]; [1]*University of Pittsburgh, Pittsburgh, PA;* [2]*Columbia University, New York, NY*

ThP 241 **Advancing Spatial Omics in Cancer Research: Image-Guided Laser Ablation System for Single-Cell Resolution in 3D Tissue, Translational Models, and Organisms**; Jan Hahn[1, 2, 3]; Manuela Moritz[1]; Ayham Moustafa[1, 2, 3, 4]; Wael Y. Mansour[2, 3, 4, 5]; Cedric Heuermann[6]; Manfred Jücker[6]; Matthias Dottermusch[7]; Julia Neumann[7, 8]; Hartmut Schlüter[1, 3]; [1]*Section Mass Spectrometry and Proteomics, Center for Diagnostics, University Medical Center Hamburg-Eppendorf, Hamburg, Germany;* [2]*Mildred Scheel Cancer Career Center Hamburg HaTriCS4, University Medical Center Hamburg-Eppendorf, Hamburg, Germany;* [3]*University Cancer Center Hamburg (UCCH), University Medical Center Hamburg-Eppendorf, Hamburg, Germany;* [4]*Department of Radiotherapy and Radiation Oncology, Center for Oncology, Hamburg, Germany;* [5]*II. Medical Oncology Clinic and Polyclinic, University Medical Center Hamburg-Eppendorf, Hamburg, Germany;* [6]*Institute of Biochemistry and Signal Transduction, Center for Experimental Medicine, University Medical Center Hamburg-Eppendorf, Hamburg, Germany;* [7]*Institute of Neuropathology, University Medical Center Hamburg-Eppendorf, Hamburg, Germany;* [8]*Research Group Molecular Pathology in Neurooncology, Center for Molecular Neurobiology (ZMNH), University Medical Center Hamburg-Eppendorf, Hamburg, Germany*

ThP 242 **Multimodal mass spectrometry imaging of postmortem formalin-fixed paraffin-embedded and fresh frozen human brain in Alzheimer's disease**; Tassia Venga Mendes[1]; Patrick R. Hof[2]; Dan Meyer[3]; Merina Varghese[4]; Livia S. Eberlin[1]; [1]*Baylor College of Medicine, Houston, TX;* [2]*Icahn School of Medicine at Mount Sinai, New York City, NY;* [3]*GE HealthCare, Niskayuna, NY;* [4]*University of Rhode Island, Kingston, RI*

ThP 243 **Spatial Characterization of Altered Metabolic and Lipidomic Signatures in Normal Tissue Adjacent to Lung Adenocarcinoma Tumor**; Faith E. Jackobs[1]; Yasmin Shanneik[1]; R. Taylor Ripley[1]; Livia S. Eberlin[1]; [1]*Baylor College of Medicine, Houston, TX*

ThP 244 **Establishing a multi-omic spatial ECM proteome and N-glycome of pancreatic ductal adenocarcinoma tissues**; Caroline Kittrell[1]; Jade K Macdonald[1]; Blake Sells[2]; Lyndsay Young[1]; David DeNardo[2]; Peggi M Angel[1]; Richard R Drake[1]; [1]*Medical University of South Carolina, Pharmacology & Immunology, Charleston, South Carolina;* [2]*Washington University in St. Louis, St. Louis, Missouri*

ThP 245 **Characterization of molecular markers for discernment of Oxaliplatin treatment-resistant pancreatic ductal adenocarcinoma (PDAC) using Desorption Electrospray-Mass Spectrometry Imaging (DESI-MSI)**; Raul Villacob[1]; Harinarayanan Janakiraman[1]; Michael Tuck[1]; Yasmin Shanneik[1]; Faith E. Jackobs[1]; E. Ramsay Camp[1]; Livia S. Eberlin[1]; [1]*Baylor College of Medicine, Houston, TX*

ThP 246 **Automated Spatial Barcoding with SPOTTER for Spatially Resolved Proteomic Mapping**; Yuanwei Xu[1, 2]; Yuehan Liu[1, 2]; Cheng-Yu Lee[1, 2]; Tung-Shing M Lih[3]; Xingde Li[2, 4]; Hui Zhang[3, 4]; [1]*Johns Hopkins University, Baltimore, MD;* [2]*Johns Hopkins University School of Medicine, Baltimore, Maryland;* [3]*Johns Hopkins School of Medicine, Baltimore, MD;* [4]*Johns Hopkin University, Baltimore, MD*

ThP 247 **Spatial omics to understand atherogenesis in hyperlipidemic male and female mice**; ROBIN JOSHI[1]; Soon Yew Tang[1]; Ujjalkumar Subhash Das[1]; Dan Boehmler[1]; E. James Petersson[1]; Aalim Weljie[1]; Garret A FitzGerald[1]; [1]*University of Pennsylvania, Perelman School of Medicine, Philadelphia, PA*

ThP 248 **Sequential Imaging and Collagenase Digest Peptide Identification from a Multi-Organ Tissue Microarray**; Erin H Seeley[1]; Aarti Bashyal[1]; Maria D. Person[1]; Christopher D Pacheco[2]; Christopher P Ly[2]; Taghi Manshouri[2]; C. Cameron Yin[2]; Ivo Veletic[2]; [1]*University of Texas at Austin, Austin, TX;* [2]*MD Anderson Cancer Center, Houston, TX*

ThP 249 **Molecular mapping of amyloid pathology across organs: integration of imaging mass spectrometry, single cell spatial transcriptomics, and microscopy**; Angela R. S. Kruse[1]; Lukasz G Migas[2]; Roy Lardenoije[3]; Claire F Scott[4, 5]; Cody R Marshall[4, 5]; Morad C Malek[4, 5]; Adel Eskaros[6]; Thai

H Pham[4, 5]; Madeline Colley[4, 5]; Kristie I Aamodt[7]; Melissa A. Farrow[4, 5]; Raf Van De Plas[2, 4, 8]; Joana P. Gonçalves[3]; Matthew S Schrag[9]; Alvin C Powers[6, 10, 11]; Jeffrey M Spraggins[4, 5, 8, 12]; *[1]Vanderbilt University, Nashville, TN; [2]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [3]Department of Intelligent Systems, Delft University of Technology, Delft, Netherlands; [4]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [5]Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; [6]Department of Molecular Physiology and Biophysics, Vanderbilt University School of Medicine, Nashville, TN; [7]Division of Pediatric Endocrinology, Department of Pediatrics, Vanderbilt University Medical Center, Nashville, TN; [8]Department of Biochemistry, Vanderbilt University, Nashville, TN; [9]Department of Neurology, Vanderbilt University, Nashville, TN; [10]Division of Diabetes, Endocrinology and Metabolism, Department of Medicine, Vanderbilt University Medical Center, Nashville, TN; [11]Veteran Affairs Tennessee Valley Healthcare System, Nashville, TN; [12]Department of Chemistry, Vanderbilt University, Nashville, TN*

ThP 250 **Next-generation Micro-scaffold Assisted Spatial Proteomics (MASP-II) for Whole-tissue Mapping and Application in Measuring the Intra-brain Distribution of Monoclonal Antibodies**; Shihan Huo[1]; Min Ma[1]; Shuo Qian[1]; Ming Zhang[1]; Jun Qu[1]; *[1]University at Buffalo, Buffalo, NY*

ThP 251 **A Novel Phos-MASP Technique for Whole-Tissue Mapping of >30,000 Phosphosites, Revealing Novel Distribution of Phosphorylation Sites in Alzheimer's Disease**; Min Ma[1]; Maosheng Wei[1]; Shihan Huo[1]; Ming Zhang[1]; Jun Qu[1]; *[1]University at Buffalo, Buffalo, NY*

ThP 252 **Spatial multi-omics study for dilated cardiomyopathy delineates possible link between macrophage driven inflammation and copper dyshomeostasis**; Maiko Okamura[1]; Koji Okuda[2]; Shuji Yamashita[1]; Shinichi Yamaguchi[2]; Takushi Yamamoto[2]; Hidetoshi Masumoto[3]; Satoru Noguchi[4]; Kenji Minatoya[3]; Ichizo Nishino[4]; Takashi Nirasawa[5]; Hatsue Ishibashi Ueda[6, 7]; Masaya Ikegawa[1]; *[1]Doshisha University, Kyotanabe-city, Japan; [2]Shimadzu Co., Kyoto, Japan; [3]Department of Cardiovascular Surgery, Graduate School of Medicine, Kyoto, Japan; [4]Department of Neuromuscular Research, National Center of Neurology and Psychiatry, Kodaira, Japan; [5]Bruker Japan, Yokohama, Japan; [6]Department of Pathology, National Cerebral and Cardiovascular Center, Suita, Japan; [7]Department of Diagnostic Pathology, Hokusetsu General Hospital, Takatsuki, Japan*

ThP 253 **Multimodal molecular imaging of human colorectal cancer biopsies combining matrix-assisted laser desorption/ionization imaging mass spectrometry, CODEX, and spatial transcriptomics**; Martin Dufresne[1]; A Joey Simmons[1]; Lukasz G Migas[2]; Thai H Pham[1]; Monica E Brown[1]; Seug Woo Kang[1]; Harsimran Kaur[1]; Jamie L Allen[1]; Audra M Judd[1]; Anna J Smith[1]; Melissa A Farrow[1]; Raf Van De Plas[2]; Ken S Lau[1]; Jeffrey M Spraggins[1]; *[1]Vanderbilt University, Nashville, TN; [2]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands*

ThP 254 **Imaging Human Retinal Tissue: 3-D Molecular Mapping Lipids and Protein Species in the Multiple Cell Types in the Human Retina**; David M.G. Anderson[1]; Angela R. S. Kruse[2]; Martin Dufresne[2]; Lukasz G Migas[3]; Thai H Pham[2]; Jeffrey D Messinger[4]; Melissa A. Farrow[2]; Christine A Curcio[4]; Raf Van De Plas[3]; Kevin L. Schey[5]; Jeffrey M Spraggins[2]; *[1]Vanderbilt University, Nashville, TN; [2]Department of Cell and Developmental Biology, Vanderbilt University School of Medicine, Nashville, TN; [3]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [4]3. Department of Ophthalmology, University of Alabama, Birmingham, Alabama; [5]Department of Biochemistry, Vanderbilt University, Nashville, TN*

INFORMATICS: PROTEIN ID AND QUANTIFICATION

255-270

ThP 255 **DIA-based proteomics of Legionella pneumophila clinical strains integrating allelic variability**; Agnès Dupas[1]; Marine Ibranosyan[2, 3]; Christophe Ginevra[2, 3]; Sophie Jarraud[2, 3]; Jérôme Lemoine[1]; *[1]Institut des Sciences Analytiques - Université Claude Bernard Lyon 1, Villeurbanne, France; [2]Centre National de Référence des Légionelles, Hospices Civils de Lyon, Lyon, France; [3]Legiopath, Centre International de Recherche en Infectiologie, Lyon, France*

ThP 256 **Correcting Bias in Quantitative Label-free Proteomics: A Shared-Protein Normalization Approach for Samples with Largely Differential Numbers of Identifications**; Li Wang[1]; Jana Zecha[1]; Matthew Glover[1]; Erik L. Allman[1]; Kristin Hicks[1]; Dmitry Gabrilovich[1]; Sonja Hess[1]; *[1]AstraZeneca, Gaithersburg, MD*

ThP 257 **Mining Tandem Mass Spectra for Chimeras Yields Massive Gains in Peptide and Proteoform Identifications**; Nicholas Bollis[1]; Michael R. Shortreed[1]; Lloyd M. Smith[1]; *[1]University of Wisconsin Madison, Madison, WI*

ThP 258 **Advancements in Multi-Protein Quantitation Software for Chinese Hamster Ovary Proteomics**; Alex Zhai[1]; Joshua L Justice[2]; Gihoon Lee[2]; K Ilker Sen[1]; Harsha P Gunawardena[2]; *[1]Protein Metrics, LLC, Boston, Massachusetts; [2]JOHNSON AND JOHNSON, Spring House, PA*

ThP 259 **Improving de novo sequencing methods and post translational modification screening tools for the analysis of complex protein mass spectra**; Mariangela Kosmopoulou[1]; George Alevizos[1]; Georgia Orfanoudaki[1]; Dimitris Papanastasiou[2]; Detlev Suckau[3]; Boris Krichel[4, 5, 6, 7]; Hsin-Ju Chan[8]; Charlotte Uetrecht[9, 10]; Ying Ge[4, 5, 8]; *[1]Fasmatech Science & Technology, Chalandri, Greece; [2]Fasmatech, Athens, Greece; [3]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [4]Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI; [5]Human Proteomics Program, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI; [6]CSSB Centre for Structural Systems Biology, Deutsches Elektronen-Synchrotron DESY & Leibniz Institute of Virology (LIV) & University of Lübeck, Hamburg, Germany; [7]Institute of Chemistry and Metabolomics, University of Lübeck, Lübeck, Germany; [8]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [9]CSSB Centre for Structural Systems Biology, Deutsches Elektronen-Synchrotron DESY & Leibniz Institute of Virology (LIV) & University of Lübeck, Notkestraße, Hamburg, Germany; [10]Institute of Chemistry and Metabolomics, University of Lübeck, Hamburg, Germany*

ThP 260 **Dedicated methods for feature detection and quantification in large molecule mass spectrometry analyses**; Gary Wilson[1]; Ignat Shilov[1]; *[1]Protein Metrics, LLC, Boston, Massachusetts*

ThP 261 **JUMPlib: Integrative Search Tool Combining Fragment Ion Indexing with Comprehensive TMT Spectral Libraries**; Suresh Poudel[1]; Zuo-Fei Yuan[1]; Yingxue Fu[1]; Long Wu[1]; Him Shrestha[1]; Anthony A. High[1]; Junmin Peng[1]; Xusheng Wang[2]; *[1]St. Jude Children's Research Hospital, Memphis, TN; [2]University of Tennessee Health Science Center, Memphis, TN*

ThP 262 **ProteomicsDB Reloaded: cross-species insights, drug-response data, and enhanced identification accuracy with Oktoberfest rescoring**; Armin Soleymaniniya[1]; Mario Picciani[1]; Miriam Abele[2, 3]; Amirhossein Sakhteman[2, 3]; Matthew The[3]; Christina Ludwig[2]; Bernhard Kuster[2, 3, 4]; Mathias Wilhelm[1, 4]; *[1]Computational Mass Spectrometry, School of Life Sciences, Technical University of Munich, Freising, Germany; [2]Bavarian Center for Biomolecular Mass Spectrometry (BayBioMS), Freising, Germany; [3]Chair of Proteomics and Bioanalytics, School of Life Sciences, Technical University of Munich, Freising, Germany; [4]Munich*

Data Science Institute (MDSI), Technical University of Munich, Garching b. München, Germany

ThP 263 **Implementation of automated intelligent data acquisition and analysis for top-down proteomics**; Amy Carfagno[1]; Linda B. Lieu[1]; Jake T Kline[1]; Ken Durbin[2]; Luca Fornelli[1]; *[1]University of Oklahoma, Norman, OK; [2]Proteinaceous, Evanston, IL*

ThP 264 **Benchmarking SILAC Proteomics Workflows and Data Analysis Platforms**; Ashley M. Frankenfield[1]; Kevin Yang[2]; Wan Nur Atiqah Binti Mazli[3]; Jamison Shih[1]; Fengchao Yu[2]; Edwin Lo[4]; Alexey I. Nesvizhskii[2]; Ling Hao[3]; *[1]George Washington University, Washington, DC; [2]University of Michigan, Ann Arbor, MI; [3]University of Maryland, College Park, MD; [4]University of Chicago, Chicago, IL*

ThP 265 **Machine learning-enabled Mascot Server API improves LFQ in client software like Thermo Proteome Discoverer**; Ville Koskinen[1]; Patrick Emery[1]; *[1]Matrix Science, London, United Kingdom*

ThP 266 **Proteoform Identification in Top-Down Proteomics Using In-Source Dissociation**; Zhuoxin Shi[1]; Austin V. Carr[1]; Claire E. Boos[1]; Mark Scalf[1]; Nicholas Bollis[1]; Michael R. Shortreed[1]; Lloyd M. Smith[1]; *[1]University of Wisconsin - Madison, Madison, WI*

ThP 267 **Ultra-fast spectral searching with deep learning based vector embedding algorithms**; Liyanage Tharanga Darshani[1]; Anshan Lahiru Kavinda[1]; Janith Sanjula Kumarasinghe[1]; Lalin Theverapperuma[2]; Thanuja D. Ambegoda[1]; *[1]University of Moratuwa, Moratuwa, Sri Lanka; [2]Expert Intelligence, Santa Clara, CA*

ThP 268 **Updates in FragPipe Computational Proteomics Platform: Improved DDA, DIA, and TMT Capabilities**; Fengchao Yu[1]; Daniel Polasky[1]; Ruohong Li[1]; Kevin L Yang[1]; Kai Li[1]; Yi Hsiao[1]; Carolina Rojas Ramirez[1]; Yamei Deng[1]; Jiechen Shen[1]; Guo Ci Teo[1]; Alexey Nesvizhskii[1]; *[1]University of Michigan, Ann Arbor, Michigan*

ThP 269 **Improved detection of differentially abundant proteins through FDR-control of peptide-identity-propagation**; Alexander Solivais[1]; Hannah Boekweg[2]; Lloyd M Smith[1]; William S. Noble[3]; Michael R Shortreed[1]; Samuel H. Payne[4]; Uri Keich[5]; *[1]University of Wisconsin-Madison, Chemistry, Madison; [2]Brigham Young University, Provo; [3]University of Washington - Genome Sciences, Seattle, WA; [4]Brigham Young University, Provo, UT; [5]University of Sydney, Sydney, Australia*

ThP 270 **Evaluating the benefits of real-time optimization of data acquisition based on protein differential expression in tandem mass tag mass spectrometry**; Aarthie Senathirajah[1]; Daniel Figey[1]; Theodore Perkins[1,2]; Mathieu Lavallée-Adam[1]; *[1]University of Ottawa, Ottawa, ON; [2]Ottawa Hospital Research Institute, Ottawa, ON*

INFORMATICS: WORKFLOW AND DATA MANAGEMENT
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ThP 271 **Advancements in Multi-Protein Quantitation for Host Cell Protein Discovery**; Antony Harvey[1]; Lawrie Veale[1]; Krisztina Radi[1]; Lukas Tvrdy[2]; Michael Georgoulopoulos[2]; *[1]Protein Metrics, LLC, Boston, Massachusetts; [2]Milo Solutions, Warszawa, Poland*

ThP 272 **Virtual MS for the Development of Real-Time Data Analysis and Instrument Control Applications**; Michael R Hoopmann[1]; Chris McGann[2]; Devin Schweppe[1]; *[1]University of Washington, Seattle, WA; [2]University of Washington, Seattle, WA*

ThP 273 **Spectronaut-nf: A Nextflow binding for Spectronaut search tool for parallel processing of DIA rawfiles in high-performance clusters**; Chinmaya Narayana Kotimoole[1]; Mohammad Arefian[2]; Sandeep Kasaragod[3]; Ben C. Collins[2]; *[1]Queens University Belfast, Belfast, United Kingdom; [2]Queens University Belfast, belfast, United Kingdom; [3]School of Biodiversity, One Health & Veterinary Medicine, University of Glasgow, Glasgow, UK, Glasgow, United Kingdom*

ThP 274 **OpenMS WebApps: A Streamlit-based framework for user-friendly mass spectrometry data analysis**; Arslan Siraj[1,2]; Tom David Müller[1,3]; Axel Walter[1,2]; Samuel Wein[1,2]; Ayesha Feroz[1,2]; Matteo Pilz[1,2]; Kyowon Jeong[1,2]; Justin Cyril Sing[4,5]; Joshua Charkow[4,5]; Hannes Luc Röst[4,5]; Oliver Kohlbacher[1,2,6]; Timo Sachsenberg[1,2]; *[1]Applied bioinformatics group, University of Tübingen, Tuebingen, Germany; [2]Institute of Bioinformatics and Medical Informatics, University of Tübingen, Tübingen, Germany; [3]Institute of Bioinformatics and Medical Informatics, University of Tübingen, Tuebingen, Germany; [4]Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, Ontario M5S 3E1; [5]Department of Molecular Genetics, University of Toronto, Toronto, Ontario M5G 1A8; [6]Institute for Translational Bioinformatics, University Hospital Tübingen, Tübingen, Germany*

ThP 275 **Accelerating the data-driven development of deep learning models for MS proteomics with automated and scalable MLOps**; Ignacio Jauregui Novo[1]; Alexandros Pachos[2]; An-phi Nguyen[2]; George Rosenberger[3]; Tejas Gandhi[2]; Dennis Trede[4]; Lukas Reiter[2]; *[1]Mestrelab Research S.L., Santiago de Compostela, Spain; [2]Biognosys AG, Schlieren, Switzerland; [3]Bruker Switzerland AG, Fällanden, Switzerland; [4]Bruker Daltonics GmbH & Co. KG, Bremen, Germany*

ThP 276 **PFAS IMplementor for Mass Spectrometry (PIMMS): Non-Targeted Analysis Software for Data with Liquid Chromatography, Ion Mobility, and Mass Spectrometry Separations**; Gregory Kudzin[1]; James N. Dodds[1]; Anna K. Boatman[1]; Kaylie I. Kirkwood-Donelson[2]; Jessie R. Chappel[1]; Dylan Johnson[3]; Adam Schiffenbauer[4]; Kakali Sarkar[4]; Payam Noroozi Farhadi[4]; Frederick W. Miller[4]; Alan K Jarmusch[2]; Lisa G. Rider[4]; Erin S. Baker[1]; *[1]University of North Carolina at Chapel Hill, Chapel Hill, NC; [2]Immunity, Inflammation, and Disease Laboratory, Division of Intramural Research, NIEHS, NIH, Research Triangle Park, NC; [3]Integrative Bioinformatics Support Group, Division of Intramural Research, NIEHS, NIH, Research Triangle Park, NC; [4]Environmental Autoimmunity Group, Clinical Research Branch, NIEHS, NIH, Bethesda, MD*

ThP 277 **pyOpenMS-viz: Mass Spectrometry Data Visualization with pandas**; Timo Sachsenberg[1,2]; Justin Cyril Sing[3,4]; Joshua Charkow[5,6]; Tom David Müller[1]; Mingxuan Gao[5]; Wout Bittremieux[7]; Axel Walter[1,2]; Hannes Luc Röst[5,6,8]; *[1]Applied Bioinformatics, Dept. of Computer Science, University of Tübingen, Tübingen, Germany; [2]Institute for Bioinformatics and Medical Informatics, University of Tubingen, Tubingen, Germany; [3]Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, ON; [4]Department of Molecular Genetics, University of Toronto, Toronto, ON; [5]Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, Ontario M5S 3E1; [6]Department of Molecular Genetics, University of Toronto, Toronto, Ontario M5G 1A8; [7]Department of Computer Science, Antwerp, Belgium; [8]Department of Computer Science, University of Toronto, Toronto, ON*

ThP 278 **An Easy Workflow for the Characterisation and Relative Quantification of Recombinant Adeno-Associated Viruses (rAAVs) using Charge Detection Mass Spectrometry**; Anisha Haris[1]; David Eatough[1]; Rebecca J D'Esposito[2]; David Bruton[1]; Keith Richardson[1]; Jakub Ujma[1]; Chris Wheeldon[1]; Alistair Schofield[1]; Michael Danby[1]; Kevin Giles[1]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Waters Corporation, Milford, MA*

ThP 279 **Mass Spectrometric Detected Protein Database as Proteomic Resources: Advancements and Insights**; Yuanyu Huang[1]; Yingwei Hu[1]; Liyuan Jiao[2]; Yuefan Wang[1]; Zhenyu Sun[1]; Hongyi Liu[1]; Jongmin Woo[1]; Mamie Lih[1]; Lijun Chen[1]; Hui Zhang[1]; *[1]Johns Hopkin University, Baltimore, MD; [2]Johns Hopkins University, Baltimore, MD*

ThP 280 **Enabling secure controlled-access MassIVE datasets for sharing of highly sensitive proteomics data**; Jeremy Carver[1]; Nuno Bandeira[1]; *[1]UCSD, La Jolla, CA*

ThP 281 **Use of real-time data for analytical quality control**; Jesse D. Canterbury[1]; Philip Remes[1]; William Barshop[1]; David Bergen[1]; Graeme C. McAlister[1]; Jay Shah[1]; Peter Mowlds[1]; Rafael Melani[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

ThP 282 **MSConnect: Open-source, end-to-end platform for automated mass spectrometry data management, analysis and visualization**; Xiaofeng Xie[1]; Parker Stone Reyes[2]; Hsien-Jung Lin[2]; Alex Mannewitz[2]; Thy Truong[2]; Kei G. I. Webber[2]; Samuel H. Payne[2]; Ryan Kelly[2]; *[1]MicrOmics Technologies, LLC, Spanish Fork, UT; [2]Brigham Young University, Provo, UT*

ThP 283 **A Graph Knowledge Base for Multi-Omics Entity Mapping and Integration: Bridging Experimental and External Knowledge Layers**; Andrew I. Webb[1]; Anna Quaglieri[1]; Mansi Aggarwal[1]; Mark R. Condina[1, 2]; Aaron Triantafyllidis[1]; Paula Burton Ngov[1]; Giuseppe Infusini[1]; *[1]Mass Dynamics, Melbourne, Australia; [2]Clinical & Health Sciences, University of South Australia, Adelaide 5095, Australia*

ThP 284 **KPOP: Establishing an open access repository for proteomics data sharing**; Seungjin Na[1]; Jingi Bae[2]; Hokeun Kim[2]; Heeyoun Hwang[1]; Shinyeong Ju[3]; Cheolju Lee[3]; Jin Young Kim[1]; Sang-Won Lee[2]; Eunok Paek[4]; *[1]Korea Basic Science Institute, Cheongju, South Korea; [2]Korea University, Seoul, South Korea; [3]Korea Institute of Science and Technology, Seoul, South Korea; [4]Hanyang University, Seoul, South Korea*

ThP 285 **No One is Left Behind: Empowering Bioinformaticians with MD 3.0's Custom Workflow Capability**; Anna Quaglieri[1]; Brendan Spinks[1]; Andrew I. Webb[1]; Giuseppe Infusini[1]; Aaron Triantafyllidis[1]; *[1]Mass Dynamics, Melbourne, Australia*

ThP 286 **Spectronaut in the Cloud: Scalable Solutions for Large-Scale Proteomics**; Patrick Van Zalm[1]; Jan Muntel[1]; Eduardo Yago Vicent[1]; Damiano Robbiani[1]; Grzegorz Skoraczyński[1]; Haley Oller[1]; Nicole Barlow[1]; Lucas Habegger[1]; Tejas Gandhi[1]; Jakob Vowinckel[1]; *[1]Biognosys, Zurich, Switzerland*

ThP 287 **IsoQuaC: A Web Tool for Quality Control and Differential Abundance Analysis in Isobaric Labelled Proteomics**; Frédérique Vilenne[1]; Roel Sprimont[1]; Dirk Valkenborg[2]; *[1]Hasselt University, Diepenbeek, Belgium; [2]Hasselt University, Hasselt, Belgium*

ThP 288 **PyC2MC: A Workflow-Driven Framework for FTMS Data Processing and Molecular Attribution**; Maxime SUEUR[1, 2, 3]; Germain Salvato Vallverdu[2, 4]; Julien Maillard[2, 3]; Christopher Rüger[2, 5]; Alvaro J. Tello-Rodríguez[2, 6]; Martha L. Chacón-Patiño[2, 6]; Brice Bouyssiere[2, 4]; Ryan P Rodgers[2, 4, 6]; Pierre Giusti[2, 3, 4]; Carlos Afonso[2, 7]; *[1]Normandie Univ, UNIROUEN, INSA Rouen, CNRS, CARMeN, Mont Saint Aignan, France; [2]International Joint Laboratory, iC2MC: Complex Matrices Molecular Characterization, Harfleur, France; [3]TotalEnergies Research and Technology Gonfreville, Harfleur, France; [4]Université de Pau et des Pays de l'Adour, IPREM UMR-CNRS, Pau, France; [5]University of Rostock, Chair of Analytical Chemistry and Dept. of Life, Light and Matter, Rostock, Germany; [6]Florida State University, Tallahassee, FL; [7]Normandie Univ, UNIROUEN, INSA Rouen, CNRS, CARMeN, 76000 Rouen, France., Mont Saint Aignan, France*

ThP 289 **Enhancing an AI-Driven Proteomics Drug Discovery Engine with Scalable Metadata Collection**; Anastasiya Prymolenna[1]; Sebastian J. Paez[1]; Kyle Siebenthall[1]; Lindsay K Pino[1]; Alexander J. Federation[1]; William E. Fondrie[1]; *[1]Talus Bioscience, Seattle, WA*

ThP 290 **Mass Difference Analysis Combined with Graph Theory for Confident Molecular Formula Assignment in Complex Mixtures Analyzed by FT-ICR Mass Spectrometry**; Teja Potu[1, 2]; Ryan P Rodgers[2, 3, 4]; Martha Liliana Chacón-Patiño[2, 3]; Christopher Paul Rüger[3, 5]; Pierre Giusti[3, 6]; Germain S. Vallverdu[3, 7]; *[1]Florida State University, Tallahassee, FL; [2]National High Magnetic Field Laboratory, Tallahassee, FL; [3]International Joint Laboratory - iC2MC: Complex Matrices Molecular Characterization, TRTG, BP 27, 76700 Harfleur, France., Harfleur, France; [4]Université de Pau et des Pays de l'Adour, Pau, France; [5]University of Rostock, Chair of Analytical Chemistry and Dept. of Life, Light and Matter, Rostock, Germany; [6]TotalEnergies OneTech R&D, Total Research & Technology Gonfreville, BP 27, 76700 Harfleur, France, Harfleur, France; [7]Université de Pau et des Pays de l'Adour, Pau, France*

ThP 291 **Utilizing a Novel Software Application for the Analysis of Synthetic Peptides and Oligonucleotides**; Lee Bertram[1]; Tristan Chutka[1]; *[1]Agilent Technologies, Santa Clara, CA*

ThP 292 **Cloud scale directDIA processing pipeline using AWS and Spectronaut yields decreased runtime, improved scalability and robustness for large-scale studies**; Simon Perkins[1]; Andrew Chambers[2]; Yeoun Jin Kim[2]; Shichen Shen[2]; Kathy Ushakov[3]; Snow Naing[3]; *[1]AstraZeneca, Cambridge, United Kingdom; [2]AstraZeneca, Gaithersburg, Maryland; [3]AstraZeneca, Waltham, MA*

ThP 293 **The MS-DAP 2.0 data pipeline enables downstream analysis of large datasets**; Frank Koopmans; *VU university, Amsterdam, Netherlands*

ThP 294 **MBI SDK: Cross-language access to full-profile MOBIE LC-IM-MS data, enabling bioinformatic analysis and fast preprocessing**; Bennett Kalafut[1]; Ding Zhang[1]; Lauren Royer[1]; Daniel DeBord[1]; *[1]Mobilion Systems Inc., Chadds Ford, PA*

ThP 295 **Skyline and msconvert in Docker: broadening access to powerful MS data processing tools beyond Windows environments**; Matthew C Chambers[1]; Brendan X. MacLean[1]; Michael J MacCoss[1]; *[1]University of Washington - Genome Sciences, Seattle, WA*

ThP 296 **Limelight – a generalized web app for analyzing, visualizing, and sharing DDA proteomics data and results**; Michael Riffle[1]; Alex Zelter[1]; Daniel Jaschob[1]; Michael R Hoopmann[1, 2]; Danielle A Faivre[1]; Robert L Moritz[2]; Trisha N Davis[1]; Michael J MacCoss[1]; Nina Isoherranen[1]; *[1]University of Washington, Seattle, WA; [2]Institute for Systems Biology, Seattle, WA*

ThP 297 **MiCId: Multiplexing the Identification of Microorganisms via Tandem Mass Tag Labeling Augmented by Interference Removal**; Gelio Alves[1]; Aleksey Y Ogurtsov[1]; Yi-Kuo Yu[1]; *[1]NLM NIH, Bethesda, MD*

ThP 298 **Chaparral SaaS platform: Rapid and Scalable Proteomics Data Analysis Using a SaaS Cloud Platform**; Robin Park; *Chapparal Labs, San Diego, CA*

ThP 299 **A seamless pipeline for global mapping and quantification of protein modifications detected by open search in any proteome**; Joshua W Smith[1, 2]; Sean M Burke[3]; Michael Considine[2]; Leslie Cope[2]; John D Groopman[3]; Robert N Cole[2]; *[1]Johns Hopkins University, Baltimore, MD; [2]Johns Hopkins School of Medicine, Baltimore, MD; [3]Johns Hopkins Bloomberg School of Public Health, Baltimore, MD*

ThP 300 **ADAP informatics for untargeted mass spectrometry-based metabolomics and exposomics big data**; Aleksandr Smirnov[1]; Toan Nguyen[1]; Radha Krishna Balaji Ponnuru[1]; Wimal Pathmasiri[2]; Blake Rushing[2]; Susan McRitchie[2]; Timothy Fennell[3]; Rodney Snyder[3]; Susan Sumner[2]; Xiuxia Du[1]; *[1]University of North Carolina at Charlotte, Charlotte, NC; [2]University of North Carolina at Chapel Hill, Chapel Hill, NC; [3]RTI International, Research Trinagle Park, NC*

INSTRUMENTATION: MINI/PORTABLE/FIELDABLE MS
301-318

ThP 301 **A miniature LA-MIP-MS for in situ compositional analyses of planetary surfaces**; Mazdak Taghioskoui[1]; Benjamin J Farcy[2, 3]; Jacob D Graham[2]; Madeline Raith[3]; Ricardo Arevalo[3]; Sierra Budinoff[2, 4]; Amy McAdam[2]; Jane Lee[2]; Ryan M Danell[2, 5]; Desmond A Kaplan[2, 6]; Cindy Gundersen[2, 4]; William F McDonough[3]; *[1]Trace Matters Scientific LLC, North Bethesda, MD; [2]NASA Goddard Space Flight Center, Greenbelt, MD; [3]University of Maryland, College Park, MD; [4]AMU Engineering, Inc, Miami, Florida;*

[5]Danell Consulting, Inc., Winterville, North Carolina; [6]KapScience, Tewksbury, Massachusetts

ThP 302 **Portable Aerosol Mass Spectrometer with Enhanced Resolution**; Vadym Berkout[1]; Stuart Collymore[1]; Scott Ecelberger[1]; Max Cetta[1]; Lara Moore[1]; Mike McLoughlin[1]; Wayne Bryden[1]; *[1]Zeteo Tech, Inc., Sykesville, MD*

ThP 303 **Direct determination of histamine in fish products using a miniature, portable/field deployable, mass spectrometer**; Tommaso Gatti[1]; Francesco Saliu[1]; Alice Passoni[2]; Enrico Davoli[2]; *[1]University of Milano Bicocca, Milano, Italy; [2]Istituto di Ricerche Farmacologiche Mario Negri IRCCS, Milano, Italy*

ThP 304 **A Proton Transfer Reaction Residual Gas Analyzer for VOC Analysis and Instrument Development**; Steven J Kregel[1]; Kevin Wokosin[2]; Matthew C Zoerb[3]; Timothy H. Bertram[2]; *[1]Bradley University, Peoria, IL; [2]University of Wisconsin - Madison, Madison, WI; [3]California Polytechnic State University, San Luis Obispo, CA*

ThP 305 **Small Footprint Analysis: Advancing Peptide Characterization with a Miniature Portable Mass Spectrometer and HPLC system**; Caleigh R O'Connor[1]; Vladimir Doroshenko[1]; Oscar Cabrices[1]; Matthew Morse[2]; Venkateswarlu Panchagnula[1]; *[1]MassTech Inc., Columbia, MD; [2]Axcend, Lehi, UT*

ThP 306 **Multimodal DBDI-APCI-APPI Ionization Source for Expanded Threat Detection in Miniature Field Mass Spectrometry**; Nathan Grimes[1]; Krisztian Gabor Torma[1]; Mike Chai[1]; William Terziyan[1]; *[1]BaySpec, San Jose, CA*

ThP 307 **A Field-Portable High Resolution Ion Mobility Spectrometer for Trace Detection of Illicit Drugs in Complex Matrices**; Jack A. Syage[1, 2]; Sean Mathisen[1]; Naomi Hernandez[1]; Andrey Vilkov[1]; *[1]Analytical Detection, LLC, Lake Forest, California; [2]ImmunogenX, Newport Beach, CA*

ThP 308 **Development of Extraterrestrial Molecular Indicators of Life Investigation (EMILI): A Gas Chromatography and Capillary Electrophoresis Electrospray Ionization Mass Spectrometer**; Jacob D. Graham[1]; Desmond A. Kaplan[1, 2]; Fernanda Mora[3]; Tomas Drevinskas[4]; Marco E. Castillo[1, 5]; Ryan M. Danell[1, 6]; Friso Van Amerom[7]; Xiang Li[1]; Andrej Grubisic[1]; Bethany P. Theiling[1]; Noell C. Aaron[4]; Antonio J. Ricco[8]; Joseph M. Pasterski[1]; Maeva Millan[9]; Vivien Tranier[9]; Vincent Guerrini[9]; Malak Bigourd[9]; Cyril Szopa[9]; Arnaud Buch[10]; Caroline Freissinet[9]; Peter A. Willis[4]; William B. Brinckerhoff[1]; *[1]NASA Goddard Space Flight Center, Greenbelt, MD; [2]KapScience, Tewksbury, MA; [3]Jet Propulsion Laboratory, Pasadena, CA; [4]Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA; [5]Aerodyne, Cape Canaveral, FL; [6]Danell Consulting, Inc., Winterville, NC; [7]Mini-Mass Consulting, Inc., Hyattsville, MD; [8]NASA Ames Research Center, Mountain View, CA; [9]LATMOS, Guyancourt, France; [10]Centre national d'études spatiales, Paris, France*

ThP 309 **Development of MS/MS Calibration Routines for Autonomous Operations in a Miniature Linear Ion Trap for Space Flight Applications**; Desmond A. Kaplan[1, 2]; Victoria Dapoian[1]; Eric Lyness[1]; Ryan M. Danell[1, 3]; Xiang Li[1]; Marco E. Castillo[1, 4]; M. Joseph Pasterski[1]; Jacob D. Graham[1]; Friso Van Amerom[1, 5]; William B, Brinckerhoff[1]; Andrej Grubisic[1]; Melissa Trainer[1]; *[1]NASA Goddard Space Flight Center, Greenbelt, MD; [2]KapScience LLC, Tewksbury, MA; [3]Danell Consulting, Inc., Winterville, NC; [4]Aerodyne, Cape Canaveral, FL; [5]Mini-Mass Consulting, Inc., Hyattsville, MD*

ThP 310 **Laser Ablation Mass Analyzer (LAMA) for Lunar Surface Exploration**; Xiang Li[1]; William B Brinckerhoff[2]; Benjamin J Farcy[3]; Jacob D Graham[2]; Friso Van Amerom[4]; Jane Lee[2]; Anthony Yu[2]; Molly Fahey[2]; *[1]Goddard Space Flight Center, Greenbelt, MD; [2]NASA Goddard Space Flight Center, Greenbelt, MD; [3]University of Maryland, College Park, MD; [4]Mini-Mass Consulting, Inc., Hyattsville, MD*

ThP 311 **An Atmospheric Pressure Photoionization Source Coupled to a Miniature High Pressure Mass Spectrometer for Detection of Volatile Organic Compounds**; Alan Rowland[1]; Stephen E Smith[1]; Ella F Vandergriff[1]; Kevin P Schultze[2]; Mac Gilliland[1]; *[1]Furman University, Greenville, SC; [2]908 Devices Inc., Boston, MA*

ThP 312 **Point-of-need chemical analysis: From on-site illicit drug and explosive identification to point-of-care pharmaceutical manufacturing quality assurance**; Thomas P. Forbes[1]; Elizabeth L. Robinson[1]; Edward Sisco[1]; Greg Gillen[1]; *[1]National Institute of Standards and Technology, Gaithersburg, MD*

ThP 313 **Explosives Detection using Two-Dimensional Mass Spectrometry**; Paul S Demond[1]; Conor C Jenkins[2]; Dalton Snyder[3]; Elizabeth S Dhummakupt[2]; *[1]Excet A Precise Systems Company, Bel Air, MD; [2]DEVCOM Chemical Biological Center, Aberdeen Proving Ground, MD; [3]Teledyne FLIR, West Lafayette, IN*

ThP 314 **Rapid Detection and Mapping of PFAS Contamination in Soil Using 3D-Printed Cone Spray Ionization and Field-Portable Mass Spectrometry**; Jamie P Butalewicz[1]; Patrick W. Fedick[1]; *[1]Naval Air Warfare Center Weapons Division, China Lake, CA*

ThP 315 **MOMA Flight Spare Temperature and Vacuum Qualification**; Friso H.W. van Amerom[1]; Xiang Li[2]; Desmond A. Kaplan[2, 3]; Ryan M. Danell[2, 4]; Marco E. Castillo[2, 5]; Andrej Grubisic[2]; William B. Brinckerhoff[2]; Fabien Stalport[6]; Caroline Freissinet[7]; Arnaud Buch[8]; Noel Grand[9]; Cyril Szopa[9]; And The MOMA Team[10]; *[1]Mini-Mass Consulting, Inc, Hyattsville, MD; [2]Goddard Space Flight Center, Greenbelt, MD; [3]KapScience LLC, Tewksbury, MA; [4]Danell Consulting, Inc., Winterville, NC; [5]Aerodyne, Cape Canaveral, FL; [6]Laboratoire Interuniversitaire des Systèmes Atmosphériques (LISA), Université Paris-Est, Paris, France; [7]Laboratoire Atmosphères, Observations Spatiales, Paris, France; [8]centrale supelec, Laboratoire Lumière, Matière et Interfaces, Paris, France; [9]Faculté des Sciences et technologies - Laboratoire LISA, Paris, France; [10]Max Planck Institut für Sonnensystemforschung, Goettingen, Germany*

ThP 316 **Demonstration of tandem MS using a planetary science instrument prototype with a linear ion trap integrated to an OrbitrapTM analyzer**; Adrian Southard[1]; Lucas Taft Andrews[2]; Ryan M Danell[3]; Friso van Amerom[4]; Ryan Barnhart[5]; Ricardo Arevalo Jr[2]; *[1]CRESST-II Univ. of Maryland, CP, and NASA GSFC, Greenbelt, MD; [2]University of Maryland, College Park, Maryland; [3]Danell Consulting, Inc., Winterville, NC; [4]Mini-Mass Consulting, Inc, Hyattsville, MD; [5]University of Michigan-Ann Arbor, Ann Arbor, MI*

ThP 317 **Achieving and Verifying the Analytical Dynamic Range Requirements for a Linear-Ion-Trap Mass Spectrometer Destined to Analyze the Complexities of Titan**; Ryan M. Danell[1, 2]; Jacob D Graham[1]; Andrej Grubisic[1]; Desmond A. Kaplan[1, 3]; Friso H.w. Van Amerom[1, 4]; Marco E. Castillo[1, 5]; Joseph M. Pasterski[1]; William B Brinckerhoff[1]; Melissa G. Trainer[1]; *[1]NASA Goddard Space Flight Center, Greenbelt, MD; [2]Danell Consulting, Inc., Winterville, NC; [3]KapScience LLC, Tewksbury, MA; [4]Mini-Mass Consulting, Inc., Hyattsville, MD; [5]Aerodyne, Cape Canaveral, FL*

ThP 318 **Energy-Programmable Plasma Desorption Ionization Coupled with Portable Mass Spectrometer for Rapid Analysis In Situ**; Feng Liu[1]; Xiaofeng Dong[1, 2]; Xinglei Zhang[1]; Eric Handberg[1]; Jize Duan[1]; Shuibing Li[1]; Shuinan Yu[1]; Shuanglong Wang[1, 3]; *[1]East China University of Technology, Nanchang, China; [2]School of Mechanical and Electronic Engineering, East China University of Technology, Nanchang, China; [3]Evaluation and Research Center of Dao-di Herbs of Jiangxi Province, Nanchang, China*

INSTRUMENTATION: NEW DEVELOPMENTS IN MASS ANALYZERS AND ION DETECTION

319-333

ThP 319 **Implementation of the Charge Detection FTICR MS using STORI analysis of individual ions**; Daniil G Ivanov[1]; Elizaveta I Shestoperova[1]; Igor A Kaltashov[1]; *[1]University of Massachusetts Amherst, Amherst, MA*

ThP 320 **Next Generation Orbitrap Astral Mass Spectrometer Accelerates Discovery via Enhanced Speed, Sensitivity, Resolving Power and Dynamic Range**; Hamish Stewart[1]; Johannes Petzoldt[1]; Eduard Denisov[1]; Matthew James Garland[1]; Amelia Peterson[1]; Christopher Rathje[1]; Dmitry Grinfeld[1]; Eugen Damoc[1]; Martin Zeller[1]; Tabiwang Arrey[1]; Anna Pashkova[1]; Julia Kraegenbring[1]; Bernard Delanghe[1]; Arne Kreutzmann[1]; Bernd Hagedorn[1]; Immo Colonius[1]; Arne Stefes[1]; Ankit Dwivedi[1]; Daniel Mourad[1]; Max Hoek[1]; Yannick Mueller[1]; Till Zickmantel[1]; Philipp Cochems[1]; Robert Ostermann[1]; Maximilian Ochmann[1]; Marek Niemiec[1]; Peter Krueger[1]; Alexander Wagner[1]; Sebastian Kanngiesser[1]; Michael Wiedemeyer[1]; Carla Flosky[1]; Florian Bonn[1]; Anastassios Giannakopulos[1]; Daniel Hermanson[1]; Vlad Zabrouskov[1]; Alexander Makarov[1]; Christian Hock[1]; *[1]Thermo Fisher Scientific, Bremen, Germany*

ThP 321 **Enabling up to 270Hz Acquisition Speed on a Modified Orbitrap Astral MS**; Johannes Petzoldt[1]; Bernd Hagedorn[1]; Eduard Denisov[1]; Daniel Mourad[1]; Hamish Stewart[1]; Yannick Müller[1]; Christopher Rathje[1]; Arne Kreutzmann[1]; Matthew James Garland[1]; Arne Stefes[1]; Immo Colonius[1]; Adrian Schütz[1]; Amelia Corinne Peterson[1]; Max Hoek[1]; Marek Niemiec[1]; Philipp Cochems[1]; Maximilian Ochmann[1]; Eugen Damoc[1]; Christian Hock[1]; *[1]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

ThP 322 **CDMS of MDa ions with the Orbital Frequency Analyser**; Aleksandr Rusinov[1]; Jack Roberts[1]; Sergey Smirnov[1]; Gordon Kearney[1]; Patrick Knight[1]; Shigeyoushi Horiike[1]; Tiago Moreira[2]; Dinesh Chinthapalli[2]; Frank Sobott[2]; *[1]Shimadzu Research Laboratory (Europe) Ltd., Manchester, United Kingdom; [2]University of Leeds, Leeds, United Kingdom*

ThP 323 **Development of ion detection module with a preamplifier for time-of-flight mass spectrometry**; Hiroshi Kobayashi[1]; Tsuyoshi Hirao[1]; Hayato Inoue[1]; *[1]HAMAMATSU PHOTONICS K.K., Iwata, Japan*

ThP 324 **The universal Orbitrap instrument - from metabolomics over targeted proteomics to native analyses**; Jan-Peter Hauschild[1]; Christian Thöing[1]; Peter Krüger[1]; Erik Couzijn[1]; Andreas Kühn[1]; Hartmut Kuipers[1]; Matthias Lange[1]; Bastian Reitemeier[1]; Yovany Cordero Hernandez[1]; Adrian Schütz[1]; Amelia Peterson[1]; Jordi Bertran Vicente[1]; Nicole Zehethofer[1]; Siegrun Mohring[1]; Claire Dauly[1]; Heiner Koch[1]; *[1]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

ThP 325 **A dual conversion dynode ion detection system designed for ultimate polarity switching speed**; Oleg Silivra[1]; Darren Yu[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

ThP 326 **Fast and High Dynamic Range Detector for TOF-MS**; Amit Weingarten[1]; Semyon Shofman[1]; Dmitry Zakgeim[1]; Anatoly Verenchikov[2]; Aleksey Vorobyev[2]; *[1]El-Mul Technologies, Rehovot, Israel; [2]MSC - CG, Bar, Montenegro*

ThP 327 **Enhanced resolution multi-pass mode for a modified Astral analyzer**; Christopher Rathje[1]; Hamish Stewart[1]; Bernd Hagedorn[1]; Eduard Denisov[1]; Robert Ostermann[1]; Johannes Petzoldt[1]; Daniel Mourad[1]; Philipp Cochems[1]; Florian Bonn[1]; Martin Zeller[1]; Julia Kraegenbring[1]; Eugen Damoc[1]; Bernard Delanghe[1]; Michael Wiedemeyer[1]; Alexander Wagner[1]; Alexander Makarov[1]; Dmitry Grinfeld[1]; Christian Hock[1]; *[1]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

ThP 328 **Calibration of Charge Detection MS Instruments**; Keith Richardson[1]; Kevin Giles[1]; Anisha Haris[1]; Benjamin E Draper[2]; Martin Jarrold[2]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Megadalton Solutions, Bloomington, Indiana*

ThP 329 **Improving Tribrid MS reliability through a new ion trap electron multiplier with a longer lifetime**; Graeme C McAlister[1]; Daen Ekers[2]; Liangxuan Fu[1]; Antony Jones[2]; Raman Mathur[1]; Mike Senko[1]; Aditya Wakhle[2]; *[1]Thermo Fisher Scientific, San Jose, California; [2]IMI Adaptas, Sydney, Australia*

ThP 330 **TMT HR Mode On a Modified Orbitrap-Astral Mass Spectrometer Enables TMTproD 35plex Analysis**; Steven Shuken[1]; Martin Zeller[2]; Julia Kraegenbring[2]; Hamish Stewart[3]; Joao A. Paulo[4]; Vlad Zabrouskov[5]; Johannes Petzoldt[2]; Steven P Gygi[4]; *[1]Harvard Medical School, Boston, MA; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [3]Thermo Fisher Scientific, Bremen, Germany; [4]Department of Cell Biology, Harvard Medical School, Boston, MA; [5]Thermo Fisher Scientific, San Jose, California*

ThP 331 **The Need for SPEeD: Rapid Characterization of Ultra-High Mass Analytes Using Charge Detection Mass Spectrometry**; Matthew S. McPartlan[1]; Conner C. Harper[1]; Evan R. Williams[1]; *[1]University of California, Berkeley, Berkeley, CA*

ThP 332 **Sensitivity Improvement on Mega-Dalton Protein Measurement**; Feng Zhong[1]; Igor Chernushevich[1]; Bill Loyd[1]; Hassan Javaheri[1]; Doug Simmons[1]; Mircea Guna[1]; *[1]SCIEX, Concord, ON*

ThP 333 **Demonstration of a 'Trap-in-a-Trap' Dual Electrostatic Linear Ion Trap (ELIT) for Flexibility in the Trade-off Between Resolution and Mass Range**; Jordan M Fritz[1]; Ian J Carrick[1]; Nicholas R Ellin[1]; Eric T Dziekonski[1]; Scott A McLuckey[1]; *[1]Purdue Univeristy, West Lafayette, IN*

ION MOBILITY: APPLICATIONS II
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ThP 334 **Ion Mobility-Mass Spectrometry for Untargeted Molecular Profiling of Pediatric Gastritis Biopsies**; Breland M Jones[1]; Michael J Dougherty[2]; Christopher D Chouinard[1]; *[1]Department of Chemistry, Clemson University, Clemson, SC; [2]Department of Pediatric Gastroenterology, Prisma Health, Greenville, SC*

ThP 335 **Utilizing in-source fragmentation for substructure analysis of small molecules by ion mobility spectrometry mass spectrometry**; Chris J Brown[1]; Ruwan Kurulugama[2]; Jeffrey R Gilbert[3]; *[1]Corteva Agrisciences, Indianapolis, IN; [2]Agilent Technologies, Santa Clara, CA; [3]Corteva Agriscience, Indianapolis, IN*

ThP 336 **Development of a cyclic ion mobility-mass spectrometry method for the rapid characterization of N-linked glycans in mAbs**; Nicole A Rivera-Fuentes[1]; Addison E. Bergman[1]; Matthew A Vallano[1]; Youngseo Na[2]; Anna Schwendeman[2]; Brandon T. Ruotolo[1]; *[1]Department of Chemistry, University of Michigan, Ann Arbor, MI; [2]Department of Medicinal Chemistry, University of Michigan, Ann Arbor, MI*

ThP 337 **Assessing the detectability of oxidative induced changes on mAb stability and structure using ion mobility-mass spectrometry and collision induced unfolding**; Nicole A Rivera-Fuentes[1]; Michael R. Armbruster[1]; Brandon T. Ruotolo[1]; *[1]Department of Chemistry, University of Michigan, Ann Arbor, MI*

ThP 338 **DISSECTING DISSOLVED ORGANIC MATTER COMPLEXITY WITH LC-TIMS-MS/MS**; Andrew R Forero[1]; Pablo Batista Oliveira[1]; Lilian Valadares Tose[1]; Kevin Jeanne Dit Fouque[1]; Francisco Fernandez-Lima[1, 2]; *[1]Department of Chemistry and Biochemistry, Florida International University, Miami, FL; [2]Biomolecular Sciences Institute, Florida International University, Miami, FL*

ThP 339 **Enhanced detection of targeted phospholipids by native ion mobility–mass spectrometry with selective lipid binding and collisional ligand ejection**; Michael R Armbruster[1]; Brandon T. Ruotolo[1]; *[1]University of Michigan, Ann Arbor, Michigan*

ThP 340 **Isomer Separation in Environmental Monitoring and Food & Flavor Chemistry Using PTR-SLIM-TOF-MS**; Jacob Jordan[1, 2]; Christian Lindinger[2]; Gernot Hanel[2]; Martin K. Beyer[1]; Philipp Sulzer[2]; Alfons Jordan[2]; *[1]Depart-ment of Ion Physics and Applied Physics, University of Innsbruck, Innsbruck, Austria; [2]IONICON Analytik GmbH., Innsbruck, Austria*

ThP 341 **Unveiling the PFAS fingerprint in biota leveraging the technique LC-VIP HESI(-)-TIMS-HRMS and novel chemometric tools supporting untargeted workflows**;

Georgios Gkotsis[1]; Dimitrios E. Damalas[1]; Reza Aalizadeh[1]; Ilona Nordhorn[2]; Birgit Schneider[2]; Samuel Putnam[3]; Carsten Baessmann[2]; Nikolaos S. Thomaidis[1]; *[1]National and Kapodistrian University of Athens, Athens, Greece; [2]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [3]Bruker Scientific, Billerica, MA*

ThP 342 **Exploring the effect of trapped IMS in LC-HRMS untargeted workflows for identifying xenobiotics by utilizing its data-dependent acquisition scheme (PASEF)**; Konstantina S. Diamanti[1]; Dimitrios E. Damalas[1]; Carsten Baessmann[2]; Ilona Nordhorn[2]; Birgit Schneider[2]; John Brann[3]; Nikolaos S. Thomaidis[1]; *[1]National and Kapodistrian University of Athens, Athens, Greece; [2]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [3]Bruker Scientific, Billerica, MA*

ThP 343 **Influence of cyclic ion mobility parameters on ion fragmentation and arrival time distribution profiles characteristic of isomers**; Štěpán Dostál[1]; Marianna Nytka[1]; Karel Lemr[1]; *[1]Dept. of Analytical Chemistry, Faculty of Science, Palacky University, Olomouc, Czech Republic*

ThP 344 **Separation of pyrrolizidine alkaloid isomers using a SLIM-based IMS-QToF approach**; Maria Del Mar Aparicio Muriana[1]; Michela Pacchione[2]; Miriam Fico[3]; Kelly Wormwood Moser[3]; Christopher Elliott[2, 4]; Nick Birse[1]; *[1]Queens University Belfast, Belfast, United Kingdom; [2]Queen's University Belfast, Belfast, United Kingdom; [3]MOBILion Systems, Inc., Chadds Ford, PA; [4]Thammasat University, Rangsit, Thailand*

ThP 345 **Characterization of phosphorothioate (PS) diastereomers in a phosphorothioated antisense oligonucleotide using ion mobility mass spectrometry**; Jonathan E Fox[1]; Jo-Anne Riley[2]; Heidi Gastall[3]; Jorge Smith[4]; Dale A Cooper-Shepherd[3]; *[1]Waters, Wilmslow, United Kingdom; [2]Waters Corportaion, Cheshire, United Kingdom; [3]Waters Corporation, Wilmslow, United Kingdom; [4]Waters Corporation, Milford, MA*

ThP 346 **Towards attribution of smokeless powders by Trapped Ion Mobility Spectrometry-Mass Spectrometry (TIMS-MS)**; Salvator J. Palmisano[1]; Emilio S. Rivera[1]; Christopher E. Freye[2]; Colleen L. Ray[2]; Austin R. Anderson[2]; Trevor G. Glaros[1]; Zachary J. Sasiene[1]; *[1]Biochemistry and Biotechnology Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; [2]High Explosives Science and Technology Group, Los Alamos National Laboratory, Los Alamos, NM*

ThP 347 **Comparative analysis of electronic materials by LC-MS, MALDI and Ion Mobility Spectrometry-Mass Spectrometry (IMS-MS)**; Adway O. Zacharias[1]; Timothy J. Eugster[1]; Jinhee Lim[1]; *[1]DuPont, Marlborough, MA*

ThP 348 **Investigation of RF/DC voltages and gases for high-mass transmission of antibody drug conjugates in a SLIM ion mobility-qTOF system**; Justin Mak[1]; Amin Famili[1]; Christopher M Crittenden[1]; *[1]Genentech, South San Francisco, CA*

ThP 349 **Forever chemical, perfluorooctanoic acid, impacts hemoglobin structure and activity at low nanomolar concentrations**; Monika Tokmina-Lukaszewska[1]; Rhys C Trousdale[1]; Robert A Walker[1]; Brian Bothner[1]; *[1]MSU; BOZEMAN, MT, Bozeman, MT*

ThP 350 **Stochiometric and Conformational Changes of CvFAP revealed with Photo-IM-MS experiments and statistical evaluation of salient features**; Liuwei Meng[1]; Jason Kalapothakis[1]; Ana Bath Alen[1]; Junfeng Ma[1]; Harry Spacey[1]; Derren Heyes[1]; Nigel Scrutton[1]; Perdita Barran[1]; *[1]The manchester of university, Manchester, United Kingdom*

ThP 351 **Characterization of Phosphorothioate Diastereomers in Synthetic Oligonucleotides Using High-Resolution Ion Mobility-Mass Spectrometry (HRIM-MS)**; Leonard Yoon[1]; Nadia Tasnim Ahmed[1]; Md Rabiul Islam[1]; Nnenna Dieke[1]; Cynthia Sommers[1]; Jason Rodriguez[1]; Deyi Zhang[2]; Yan Wang[2]; Kui Yang[1]; *[1]Food and Drug Administration, St. Louis, MO; [2]Food and Drug Administration, Silver Spring, MD*

ThP 352 **AI enabled metabolomics with annotation and absolution quantitation - implementation on an ion mobility time-of-flight mass spectrometer**; Ana S. H. Costa[1]; Xuejun Peng[2]; Devesh Shah[1]; Erica Forsberg[3]; Jennifer M Campbell[1]; Jack Geremia[1]; *[1]Matterworks, Somerville, MA; [2]Bruker Scientific LLC, Billerica, MA; [3]Bruker Daltonics Inc, 101 Daggett Dr., San Jose, CA*

ThP 353 **Human anencephaly associated gangliosidome is high complex as revealed by ion mobility tandem mass spectrometry**; Roxana Biricioiu[1, 2]; Mirela Sarbu[1]; Raluca Ica[1]; David E. Clemmer[3]; Željka Vukelić[4]; Alina D. Zamfir[1, 5]; *[1]National Inst for R&D in Electrochemistry and Condensed Matter, Timisoara, Romania; [2]West University of Timisoara, Timisoara, Romania; [3]Department of Chemistry, The College of Arts & Science, Indiana University, Bloomington, IN; [4]Department of Chemistry and Biochemistry, Faculty of Medicine, University of Zagreb, Zagreb, Croatia; [5]Department of Technical and Natural Sciences, “Aurel Vlaicu” University of Arad, Arad, Romania*

ThP 354 **Exploring molecular self-association to separate budesonide epimers**; Sudam S Mane[1]; David V Dearden[1]; Kenneth W Lee[1]; *[1]Brigham Young University, Provo, UT*

ThP 355 **Accurate Direct Identification within Bile Arisaema by REIMS and Separation of the Marker Bile Acid Isomers by Cyclic Ion Mobility**; Yisheng Xu[1]; Peng peng Liu[2]; *[1]Waters cooperation, Beijing, China; [2]Key Laboratory of Ministry of Education for TCM Viscera-State Theory and Applications, Liaoning University of Traditional Chinese Medicine, Dalian, China*

ThP 356 **Comparison of Drift Tube and SLIM IMS in Intact Multi-Attribute Monitoring (iMAM) for Protein Characterization**; JAHZIEL CHASE[1]; Md Amin Hossain[1, 2]; Jeffrey Agar[1]; Jared Auclair[1]; *[1]Northeastern University, Boston, MA; [2]Harvard Medical School, Boston, Massachusetts*

ION MOBILITY: FAIMS/DMS
357-362

ThP 357 **Separations of Lipid Head Group Regioisomers using Ion Mobility Spectrometry with Orbitrap MS**; Hayden A. Thurman[1]; Vasily Grebennikov[2]; Alexandre A. Shvartsburg[1]; Davide Bleiner[2]; *[1]Wichita State University, Wichita, KS; [2]Swiss Federal Laboratories for Materials Science and Technology, Zurich, Switzerland*

ThP 358 **Macromolecular Separations Based on the Ion Focusing in Divergent Asymmetric Electric Fields of Switchable Polarity**; Adetayo S Afolayan[1]; Hayden A Thurman[1]; Atena Tajaddodi[1]; Alexandre A Shvartsburg[1]; *[1]Wichita State University, Wichita, KS*

ThP 359 **Optimizing FAIMS-DIA Mass Spectrometry for Comprehensive Phosphoproteome Analysis on the Orbitrap Astral**; Kento T Abe[1]; Charlotte Peijie Zuo[1]; Ugo Dionne[1]; Brendon Seale[1]; Cassandra Wong[1]; Anne-Claude Gingras[1]; *[1]Lunenfeld-Tanenbaum Research Institute, Toronto, ON*

ThP 360 **Development of a Chiral LC-MS/MS Method for the Analysis of Tramadol and O-Desmethylvenlafaxine in Fish Tissue** ; Rashne Vakharia[1, 2]; A. Dawson McLachlan[1, 2]; Emir Nazdrajić[1]; Diana M. Cardenas-Soraca[2]; Leslie M. Bragg[2]; W. Scott Hopkins[1]; Mark R. Servos[2]; *[1]Department of Chemistry, University of Waterloo, Waterloo, ON; [2]Department of Biology, University of Waterloo, Waterloo, ON*

ThP 361 **The benefit of ethylacate modifier in differential mobility separation (DMS) for peptide analysis**; Yves Le Blanc[1]; Harikrishnan Sukumar[2]; Bradley Schneider[2]; *[1]SCIEX, Concord, On, ON; [2]SCIEX, Concord, ontario*

ThP 362 **Unraveling FAIMS Variability: Effects on DIA Proteomics and the Need for Device-Specific Optimization**; JEAN-CLAUDE CHARTRAND[1]; Kevin Ly[1]; Simon Perrin[1]; Hugo Gagnon[1]; *[1]Allumiqs, Sherbrooke, QC*

ION MOBILITY: GENERAL
363-371

ThP 363 **Variable Traveling Wave Profiles in the MOBILion MOBIE Platform: Implications Towards Collision Cross Section Reproducibility and Mobility Filtering**; James Dodds[1]; Amie M. Solosky[1]; Erin S. Baker[1]; [1]*University of North Carolina at Chapel Hill, Chapel Hill, NC*

ThP 364 **Multipass CCS Refiner: A Web Application for Fine Collisional Cross Section Calibration in Cyclic Ion Mobility**; Eric Gier[1]; Dmitry Leontyev[1]; Facundo M Fernández[1]; [1]*Georgia Institute of Technology, Atlanta, GA*

ThP 365 **Revealing Anisotropic Growth of Liraglutide Oligomers by Native Ion Mobility Mass Spectrometry and Molecular Dynamics Simulation**; Zhenyu Xi[1]; Syuan-Ting Kuo[1]; Xiao Cong[2]; Yan Xin[1]; David H. Russell[1]; [1]*Texas A&M University, College Station, TX;* [2]*Boehringer Ingelheim Pharmaceuticals, Inc., Ridgefield, CT*

ThP 366 **Development of a PTR-SLIM-TOF-MS Instrument: Selective Trace Gas Analysis with High-Resolution Ion Mobility and High-Resolution TOF Mass Spectrometry**; Christian Lindinger[1]; Jacob Jordan[1, 2]; Gernot Hanel[1]; Tobias Fügenschuh[1]; Philipp Sulzer[1]; Alfons Jordan[1]; [1]*IONICON Analytik GmbH., Innsbruck, Austria;* [2]*Depart-ment of Ion Physics and Applied Physics, University of Innsbruck, Innsbruck, Austria*

ThP 367 **Evaluating Data Analysis Techniques for LC-IM-MS Data: Preprocessing, Untargeted Feature Finding, and DIA Fragmentation Alignment**; Sarah M. Stow[1]; Andrea Harrison[2]; Bryson Gibbons[2]; Olivier Chevallier[1]; David A Weil[1]; Ruwan T. Kurulugama[1]; Aivett Bilbao[2]; [1]*Agilent Technologies, Santa Clara, CA;* [2]*Pacific Northwest National Laboratory, Richland, Washington*

ThP 368 **Ion Mobility Mass Spectrometry into the Gigadalton Regime: Coupling Drift Tube Ion Mobility with Charge Detection Mass Spectrometry (IM-CD-MS)**; David Reitenbach[1]; Raj Parikh[1]; David E. Clemmer[1]; Martin Jarrold[1]; [1]*Indiana University Bloomington, Bloomington, IN*

ThP 369 **Enhancing Cyclic Ion Mobility Separation of Stereoisomers via Gas-Phase Complexation with Crown Ether Derivatives**; Aunika E DelHoyo[1]; Chao Pang[2]; Kenneth W Lee[2]; [1]*Brigham Young University, Provo, UT;* [2]*Brigham Young University, Provo*

ThP 370 **Improving Ion Transmission, Mobility Resolution and CCS Measurement Precision of Small Molecules in Trapped Ion Mobility Spectrometry**; Siya Deng[1]; Kimberly C. Fabijanczuk[1]; Jody C May[1]; Karly B Serrano[1]; Erica Marie Forsberg[2]; Matthew R. Lewis[3]; John A McLean[1]; [1]*Vanderbilt University, Nashville, TN;* [2]*Bruker Scientific, Billerica, MA;* [3]*Bruker Daltonics GmbH & Co.KG, Bremen, Germany*

ThP 371 **Design and Optimization of a Structures for Lossless Ion Manipulations (SLIM)-based Ion Mobility Spectrometer for Environmental and Clinical Applications**; Viraj D Gandhi[1]; Kimberly Youandi Kartowikromo[1]; Gordon A. Anderson[2]; Aneesh Prabhakaran[3]; Ahmed M Hamid[1]; [1]*AUBURN UNIVERSITY, Auburn, AL;* [2]*GAA Custom Electronics, LLC, Kennewick, WA;* [3]*Bruker Daltonics GmbH & Co. KG, Bremen, Germany*

LC/MS: CHROMATOGRAPHY AND SOFTWARE

372-386

ThP 372 **Streamlining System Suitability Testing Data Analysis with Automation**; Nicola Tonge[1]; Alvaro Taboada[2]; Gary Sharman[1]; Gavin Shear[1]; Rafael Cela[3]; [1]*Mestrelab Research S.L., Santiago de Compostela, Spain;* [2]*Centro de Investigación Mestrelab (CIM), Santiago de Compostela, Spain;* [3]*Centro de Investigación Mestrelab (CIM), Santiago de Compostela, Spain*

ThP 373 **LC-MS Computer System Validation and Data Life Cycle in a GLP Laboratory**; Oleg Chepelin; *Charles River Laboratories, Edinburgh, United Kingdom*

ThP 374 **Evaluation of Retention Indexing in Reversed-Phase LC-MS Applications**; Katherine Sanders[1]; Pei Liu[1]; Kevin Ray[1]; [1]*Millipore Sigma, St. Louis, MO*

ThP 375 **Streamlining Chromatographic Method Evaluation and Ensuring Data Quality through Advanced Tools**; Kristie Adams[1]; Mitcheell Maestre[1]; Agustin Barba[1]; Nicola Tonge[1]; Gary Sharman[1]; Gavin Shear[1]; [1]*Mestrelab Research S.L., Santiago de Compostela, Spain*

ThP 376 **A novel nano UHPLC system for high robustness and reproducible proteomics analysis**; Irina Märki[1]; Florian Busch[1]; Emmanouil Methymakis[1]; Claudia Martelli[1]; Goran Mitulovic[2]; Manuel Bauer[1]; Mario Francesco Mirabelli[1]; [1]*Bruker Switzerland AG, Fällanden, Switzerland;* [2]*Bruker Austria GmbH, Vienna, Austria*

ThP 377 **Automatic detection and grouping of MS1 fragmentation in LC-MS data**; Tim Stratton[1]; Vilmantas Pedišius[2]; [1]*Thermo Fisher Scientific, San Jose, CA;* [2]*Thermo Fisher Scientific, Vilnius, Lithuania*

ThP 378 **Improved sensitivity and throughput for low-input phosphoproteomics using short monolithic columns**; Felix Rudolf Schneidmadel[1]; Yue Yang[1]; Goran Mitulovic[2]; Mario Mirabelli[3]; Petra Martinovic[4]; Florian Busch[3]; Florian Meier-Rosar[1]; [1]*Uniklinikum Jena, Functional Proteomics, Friedrich-Schiller-Universität, Jena, Germany;* [2]*Bruker Austria GmbH, Vienna, Austria;* [3]*Bruker Switzerland AG, Fällanden, Switzerland;* [4]*Bruker Daltonics GmbH & Co. KG, Bremen, Germany*

ThP 379 **Using a vacuum jacketed column with a multi reflecting time-of-flight MS to increase extractables analysis throughput whilst maintaining identification confidence**; Rachel J Sanig[1]; Bindesh Shrestha[2]; Matthew Daly[1]; Lee Gethings[1]; [1]*Waters Corporation, Wilmslow, United Kingdom;* [2]*Waters Corp., Milford, MA*

ThP 380 **A Novel Cation-Exchange Chromatography-MS/MS Method for the Analysis of Basic Metabolites and Metal Ions in Biological Samples**; Rachel Williams[1]; Ingvild Comfort Hvinden[2]; John Walsby-Tickle[1]; Isabelle Legge[1]; Judith B Ngere[3]; Susan Bird[4]; James S. O. McCullagh[1]; [1]*University of Oxford, Oxford, United Kingdom;* [2]*Norwegian Defence Research Establishment (FFI), Oslo, Norway;* [3]*Thermo Fisher Scientific, Hemel Hempstead, United Kingdom;* [4]*Thermo Fisher Scientific, Boston, MA*

ThP 381 **Pharmacokinetics Analysis of DSPE-MPEG2000 in Rat plasma using a QTOF mass spectrometer**; Min Lei; *SCIEX, Application specilist, Guangzhou, China*

ThP 382 **Enhanced MRM Quantification with Physics Inspired Neural Network(PINN) model for PFAS analysis**; Mihira K Vithanage[1]; Rukshan Wijesinghe[1]; Pulasthi Ekanayake[1]; Sanoj Silva[1]; Lalin Theverapperuma[1]; [1]*Expert Intelligence, Santa Clara, CA*

ThP 383 **The Best Of Both Worlds - Tailored Analysis Of Affinity Selection MS Data With A Generic Automation Engine**; Gary Sharman[1]; Agustin Barba[1]; Marcel Lachenmann[1]; [1]*Mestrelab Research S.L., Santiago de Compostela, Spain*

ThP 384 **System Performance Check (SPC): The Essential Partner for Multi-Attribute Method (MAM)**; JAHZIEL CHASE[1]; Melissa Sato[2]; Jared Auclair[1]; Mike Knierman[2]; [1]*Northeastern University, Boston, MA;* [2]*Agilent Technologies, Santa Clara, CA*

ThP 385 **Evaluation of HALO® 2.0µm positively charged Superficially Porous Particle silica (PCS-C18) for Complex Peptide Separations in LC/MS Workflows**; Joshua McBee[1]; Barry E Boyes[1]; [1]*Advanced Materials Technology, Wilmington, DE*

ThP 386 **At the intersection between chromatographic performance, ESI efficiency and instrument productivity: nano to capillary flow LC/MS on long µPAC columns**; Riccardo Stucci[1]; Jeff Op De Beeck[2]; Dominic Hoch[1]; Natalie Van Landuyt[2]; Paul Jacobs[2]; [1]*Thermo Fisher Scientific, Reinach, Switzerland;* [2]*Thermo Fisher Scientific, Ghent, Belgium*

LC/MS: SAMPLE PREPARATION II

387-407

ThP 387 **Development and evaluation of new Empore TiO2 membrane for phosphopeptide enrichment in phosphoproteomic studies**; Gregory A Davidson[1]; Cheng Tse Huang[1]; Guotao Lu[1]; Xiaohui Zhang[1]; [1]*CDS Analytical LLC, Oxford, PA*

ThP 388 **Evaluation of a new CDS Empore automated machine for high-throughput proteomics sample preparation**; Gregory A Davidson[1]; Cheng Tse Huang[1]; Guotao Lu[1]; Xiaohui Zhang[1]; [1]*CDS Analytical LLC, Oxford, PA*

ThP 389 **Evaluating Sample Normalization Methods for MS-based Multi-Omics and the Application to a Neurodegenerative Mouse Model**; Gwangbin Lee[1]; Cha Yang[2]; Fenghua Hu[2]; Ling Hao[1]; [1]*University of Maryland, College Park, MD;* [2]*Cornell University, Ithaca, NY*

ThP 390 **Automated extraction method for oligonucleotides using magnetic solid phase extraction for measurement with LC-MS/MS**; Michael Johnson[1]; Jenny Zhang[2]; Jingran Zhang[3]; Vincent Wen[2]; [1]*BioQual Solutions Inc, San Diego, CA;* [2]*Unified Separation Technologies Inc., Newark, DE;* [3]*Agile Bio, Suzhou, China*

ThP 391 **Automatable One-Step 5-minute Sample Preparation with Novel Hyperthermoacidic Proteases Generates Novel Protein ID's and Sequence**; Steven M Yannone; *CinderBio, San Leandro, CA*

ThP 392 **Optimizing Testing Capacity for a Clinical Proteomics MRM Assay: Expanding HPLC and Plate-Based Depletion Methods**; Sarah Phillips[1]; Dylan Flohrschutz[1]; Gary A Pestano[2]; Laura J Peek[1]; [1]*Biodesix, De Soto, KS;* [2]*Biodesix, Louisville, CO*

ThP 393 **Developing a flexible pipeline for the automation of proteomics sample quantitation and processing with an Opentrons FlexTM liquid-handling robot**; Nico To[1]; Laura C McGary[1]; Sasha Morozova[1]; Brendon Seale[1]; Cassandra Wong[1]; Anne-Claude Gingras[1, 2]; [1]*Lunenfeld-Tanenbaum Research Institute, Toronto, ON;* [2]*Department of Molecular Genetics, University of Toronto, Toronto, ON*

ThP 394 **Automated Sample Extraction Technique for LC-MS\MS Analysis of the Pharmaceutical Drug Zolmitriptan in Human Plasma**; Amber Cain[1]; Yuan Li[1]; Kyle Dukes[1]; Sohel Rana[1]; Lee Williams[2]; Esraa AboJasser[1]; [1]*Biotage, Charlotte, NC;* [2]*Biotage GB Limited, Cardiff, United Kingdom*

ThP 395 **Evaluating the effects of sample matrix to develop an endogenous opioid MRM method**; Thomas Lubinsky[1]; David Foreman[2]; Mayuri N Patil[2]; Gaurav Chopra[2]; [1]*Purdue University, West Lafayette, IN;* [2]*Purdue Univeristy, West Lafayette, IN*

ThP 396 **High-throughput automated sample preparation and validation for untargeted exposomics**; Maria E Cardelino[1]; Catherine E. Mullins[1]; Douglas I. Walker[1]; [1]*Emory University, Atlanta, GA*

ThP 397 **High-Throughput Extraction of Proteins from Single FFPE sections using the BeatBox**; Dragana Noe[1]; Jessica Moore[1]; Kyra Richardson[1]; Jaison Arivalagan[1]; Tiffany Louie[1]; Don Skifter[1]; Danielle Gutierrez[1]; [1]*Discovery Life Sciences, Huntsville, AL*

ThP 398 **Solid Phase Extraction of 40 Per- and Polyfluoroalkyl Substances (PFAS) Compounds**; Dongmei Alvi[1]; Jody Smiley[1]; Joan Wirt[1]; [1]*Occoquan Watershed Monitoring Laboratory, Manassas, VA*

ThP 399 **An AFA assisted workflow for mass-spectrometry based proteomics analysis of low input FFPE samples**; Anu Jain[1]; Hiroshi Nishida[1]; Amy J French[2]; Dong-Gi Mun[2]; Sameer Vasantgadkar[3]; Debadeep Bhattacharyya[3]; Akhilesh Pandey[2]; [1]*Mayo Clinic, Rochester, MN;* [2]*Mayo Clinic, Rochester;* [3]*Covaris, Woburn, MA*

ThP 400 **Digital microfluidic sample preparation for trace analysis in LC-MS proteomics**; Stephen Vanderburgt[1]; R. J. Dwayne Miller[1]; Aaron Wheeler[1]; Khaled Madhoun[1]; N. Sathishkumar[1]; [1]*University of Toronto, Toronto, ON*

ThP 401 **Electromembrane Extraction: A novel and green sample preparation method used for the analysis of antidepressants in human serum**; Fabian Simon[1, 2]; Michal Rackiewicz[2]; Max Diesner[2]; Maria Kristina Parr[1]; Franz Paul Armbruster[2]; [1]*Institute of Pharmacy, Freie Universität Berlin, Berlin, Germany;* [2]*Immundiagnostik AG, Bensheim, Germany*

ThP 402 **Size Matters in Sample Preparation for LC/MS Analysis**; William Brewer; *DPX Technologies, Inc., Columbia, SC*

ThP 403 **Rapid purification and LC-MS/MS analysis of large molecules using monolithic silica spin columns**; Yuko Yui[1]; Konno Yukinori[1]; Shigenori Ota[1]; Takumi Kunieda[1]; Ken Kanno[1]; Kousuke Kabe[1]; [1]*GL Sciences Inc., Iruma-shi, Japan*

ThP 404 **Optimized FFPE Tissue Processing: Enhancing Flexibility and Scalability with BeatBox Tissue Kit 24x for in-depth proteome analysis**; Cameron Ellis[1]; Silvia Wuertenberger[2]; Jasmin Johansson[2]; Katrin Hartinger[2]; Nils Kulak[2]; [1]*PreOmics, Billerica, MA;* [2]*PreOmics GmbH, Martinsried, Germany*

ThP 405 **Streamlining Plasma Proteomics with a Rapid, High-Throughput, and Standardized Automation**; Fabian Wendt[1]; Zehan Hu[2]; Claudia Martelli[3]; Katrin Hartinger[2]; [1]*Tecan, Männedorf, Switzerland;* [2]*PreOmics, Planegg/Martinsried, Germany;* [3]*Bruker Switzerland AG, Fällanden, Switzerland*

ThP 406 **ENRICHplus enables quantitative and precise plasma proteome analysis along with enhanced proteome coverage**; Katharina Limm[1]; Zehan Hu[2]; Xaver Wurzenberger[2]; Godfred Boateng[2]; Nils Kulak[2]; [1]*PreOmics, Planegg/Martinsried, Germany;* [2]*PreOmics GmbH, Martinsried, Germany*

ThP 407 **Deciphering biology with innovative in-cell processing and single-shot LC-DIA MS/MS**; Yanbao Yu; *University of Delaware, Newark, DE*

LIPIDS: GENERAL
408-436

ThP 408 **Comparing Heavy-labeled Internal Standards for Lipidomic Identifications and Quantification in Platforms Coupling Liquid Chromatography, Ion Mobility and Mass Spectrometry**; Quentin M DuVal-Smith[1]; Amie M. Solosky[1]; James N. Dodds[1]; Erin S. Baker[1]; [1]*University of North Carolina at Chapel Hill Chemistry Department, Chapel Hill, NC*

ThP 409 **Rapid Analysis of Lipid Components in Biological Samples using the Echo® MS+ system**; Mengqing Xiao[1]; Chenchun Zhong[1]; Zhimin Long[1]; Bingjie Liu[2]; [1]*SCIEX, Shanghai, China;* [2]*SCIEX, Beijing, China*

ThP 410 **Lipidomics and Machine Learning for Rare Dementia Diagnosis: Insights from PSI-MS and LC-MS/MS**; Jean Carlos Pereira Sousa[1]; Hugo Gontijo Machado[2]; Gesiane da Silva Lima[2]; Iron Dangoni Filho[3]; Leonardo Ferreira Caixeta[3]; Boniek Gontijo Vaz[1, 2]; [1]*Faculty of Pharmacy, Federal University of Goiás, Goiânia, Brazil;* [2]*Institute of Chemistry, Federal University of Goiás, Goiânia, Brazil;* [3]*Faculty of Medicine, Federal University of Goiás, Goiânia, Brazil*

ThP 411 **Assessing Bile Acid Changes in Liver Tissue with Liquid Chromatography, Ion Mobility Spectrometry and Mass Spectrometry Measurements**; Sadie Disselkoen[1]; Guozhi Zhang[1]; James N. Dodds[1]; Erin S. Baker[1]; [1]*University of North Carolina at Chapel Hill, Chapel Hill, NC*

ThP 412 **Noninvasive Lipid Analysis of Children and Adults: ESI-MS and Machine Learning on Skin Surface Residues**; Madeline Isom[1]; Aleesa E Chua[1]; Disni Dedunupitiya[1]; Eden P Go[1]; Heather Desaire[1]; [1]*University of Kansas, Lawrence, KS*

ThP 413 **Development of a Multi-Sorbent SPE Cartridge for Online Mass Spectrometry Analysis of Complex Mixtures**; Octavion Spears[1]; Dmytro Kulyk[1]; Abraham K. Badu-Tawiah[1]; [1]*Ohio State University, Columbus, OH*

ThP 414 **Lipid Mapping: Using micro-LC-ESI-MS/MS for Untargeted Spatial Analysis of Tissue**; Caley Campkin[1]; Vi Thanh Tran[1]; Liang Li[1, 2]; [1]*University of Alberta, Edmonton, AB;* [2]*The Metabolomics Innovation Centre (TMIC), University of Alberta, Edmonton, AB*

ThP 415 **Lipidomics Analysis Reveals the Role of Diacyl-Phosphatidylcholine in Ferroptosis**; Fereshteh Zandkarimi[1]; Baiyu Qiu[1]; Brent R. Stockwell[1]; [1]*Columbia University, New York, NY*

ThP 416 **Organic modifier in Fluoroalcohol-Induced Aqueous-based Multiphase Extraction and Fractionation systems**

in Lipidomics; Md Al Amin[1]; Morteza Gholi Khaledi[1]; *[1]The University of Texas at Arlington, ARLINGTON, TX*

ThP 417 **Site-specific characterization of oxygen exchange in phosphatidylserine using MS and MS/MS**; Evgenii B. Serebriakov[1]; Daniil G. Ivanov[1]; Igor A. Kaltashov[1]; *[1]University of Massachusetts Amherst, Amherst, MA*

ThP 418 **Exploring the Lipidomic Impact of Cisplatin and Rapamycin in A549 Monolayer and Spheroid Models Using Micro-LC-MS**; Fernanda Sousa Monteiro[1]; Cyrene Catenza[1]; Liang Li[1, 2]; *[1]University of Alberta, Edmonton, AB; [2]The Metabolomics Innovation Centre (TMIC), Edmonton, AB*

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ThP 486 **Prediction of Staphylococcus aureus resistance or susceptibility to methicillin using machine learning and MALDI-TOF spectrum: it's not that easy!**; Louise Ruyer[1]; Frederic Jauffrit[1]; Nadine Perrot[2]; Olivier Dauwalder[3]; Elizabeth Keskinen-Allen[4]; Laurent Boulet[1]; Remi-Vinh Coudert[1, 5]; Celine Blangy[1]; Geraldine Durand[2]; Daniel D. Rhoads[4, 6, 7]; Jean-Philippe Rasigade[3, 8]; Jean-Philippe Charrier[1]; [1]*bioMerieux, Marcy l'Etoile, France;* [2]*bioMerieux, La Balme Les-Grottes, France;* [3]*Hospices Civils de Lyon, Institut des Agents Infectieux, Lyon, France;* [4]*Department of Pathology and Laboratory Medicine, Cleveland Clinic, Cleveland, OH;* [5]*Université Claude Bernard Lyon 1, LYON, France;* [6]*Department of Pathology, Cleveland Clinic Lerner College of Medicine, Case Western Reserve University, Cleveland, OH;* [7]*Infection Biology Program, Lerner Research Institute, Cleveland Clinic, Cleveland, OH;* [8]*CIRI - Centre International de Recherche en Infectiologie, Ecole Normale Supérieure de Lyon, Université Claude Bernard Lyon-1, Inserm U1111, CNRS UMR5308, LYON, France*

ThP 487 **DETECTION AND IDENTIFICATION OF MICROORGANISMS BY VOC ANALYSIS**; Sarah Kingsley[1]; Ana Duran-Viseras[1]; Thomas Orlando[1]; Kostas Konstantinidis[1]; [1]*Georgia Institute of Technology, Atlanta, GA*

ThP 488 **Investigating systemic consequences following the depletion of native murine intestinal flora**; Douglas V. Guzior[1]; Ethan Stancliffe[1]; Joe L. Rowles III[2]; Monil Gandhi[1]; Kevin Cho[2]; Ashima Mehta[1]; Adam Richardson[1]; Tom Cohen[1]; Gary Patti[2]; [1]*Panome Bio, Saint Louis, MO;* [2]*Washington University in St. Louis, University City, MO*

ThP 489 **Spatial proteomics reveals lipid droplet reorganization in symbiotic Paramecium bursaria cells**; Yan-Jun Chen[1]; Kamal Md Mostafa[1]; Chuan-Chih Hsu[1]; Jun-Yi Leu[1]; [1]*Academia Sinica, Taipei, Taiwan*

ThP 490 **Improving Metaproteomics Data Analysis with the Ghent Metaproteomics Tools Suite**; Tim Van Den Bossche[1, 2]; Pieter Verschaffelt[1, 2, 3]; Tanja Holstein[1, 2]; Tibo Vande Moortele[3]; Simon Van De Vyver[3]; Lennart Martens[1, 2]; Bart Mesuere[3]; [1]*VIB - UGent Center for Medical Biotechnology, VIB, Ghent, Belgium;* [2]*Department of Biomolecular Medicine, Faculty of Medicine and Health Sciences, Ghent University, Ghent, Belgium;* [3]*Department of Mathematics, Computer Science and Statistics, Ghent University, Ghent, Belgium*

ThP 491 **Towards revealing metabolic and lipidomic differences between living individual yeast cells from a clonal population**; Ting Zeng[1]; Erin Bredeweg[1]; Christopher R Anderton[1]; Andreas Vasdekis[2]; Dusan Velickovic[1]; [1]*PNNL, Richland, WA;* [2]*University of Idaho, Moscow, IA*

ThP 492 **Improving spatial and temporal proteome mapping of fungal infection dynamics to reveal novel druggable targets**; Jennifer Geddes-McAlister[1]; Michael Woods[2]; Benjamin Muselius[2]; Lauren Segeren[2]; Jared Deyarmin[3]; Amirmansoor Hakimi[3]; Daniel Hermanson[3]; Jana Richter[4]; Stephanie Samra[3]; [1]*University of Guelph, GUELPH, ON;* [2]*University of Guelph, Guelph, ON;* [3]*Thermo Fisher Scientific, San Jose, CA;* [4]*Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

ThP 493 **Advancing temporal resolution of fungal proteome modulation for personalized signature detection**; Jennifer Geddes-McAlister[1]; Michael J P Woods[2]; Jason McAlister[2]; Lauren Segeren[2]; Jared Deyarmin[3]; Amirmansoor Hakimi[3]; Daniel Hermanson[3]; Jana Richter[4]; Stephanie Samra[3]; [1]*University of Guelph, GUELPH, ON;* [2]*University of Guelph, Guelph, ON;* [3]*Thermo Fisher Scientific, San Jose, CA;* [4]*Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

ThP 494 **Untargeted lipidomics and proteomics of mleNcompensatory mutation and penA41 resistance mutation in Neisseria gonorrhoeae**; Julia W Adug[1]; Stephanie L Bishop[2]; Ian Lewis[1]; Adriana Zardini Buzatto[1]; [1]*University of Calgary, Calgary, AB;* [2]*Western University, London, Ontario*

ThP 495 **Achieving High-Throughput and Quantitative Accuracy in Metaproteomics: A Benchmark of Short LC Gradients Over 1,000 Human Gut Samples**; Ravi Kumar RK[1]; Feng Xian[1]; Mario Mirabelli[2]; Florian Busch[2]; Torsten Mueller[3]; Goran Mitulovic[4]; David Gómez-Varela[1]; [1]*Department of Pharmaceutial Sciences, Faculty of Life Sciences,University of Vienna, Vienna, Austria, Vienna, Austria;* [2]*Bruker Switzerland AG, Fällanden, Switzerland;* [3]*Bruker Daltonik GmbH, Bremen, Germany;* [4]*Bruker Austria GmbH, Vienna, Austria*

ThP 496 **Comparison of surface-adsorbed microbial metabolites across polymer films using mass spectrometry imaging**; Emily A Kurfman[1]; Vilmos Kertesz[1]; Charini Maladeniya[1]; Zhefei Yang[1]; Spenser R Brown[1]; Jennifer L Morrell-Falvey[1]; John F Cahill[1]; [1]*Oak Ridge National Laboratory, Oak Ridge, TN*

ThP 497 **Metaproteomics Initiative CAMPI-3: Assessing the impact of Bioinformatic Decision Points on Taxonomic and Functional Annotations in a Simplified Microbial Community**; Benoit Kunath[1]; Lucia Grenga[2]; Zhibin Ning[3]; Samantha Peters[4]; Gelio Alves[5]; Hamid Hachemi[2]; Tim Van Den Bossche[6]; Bart Measure[6]; Robert Hettich[4]; Pratik Dilip Jagtap[7]; [1]*University of Luxembourg, Luxembourg City, Luxembourg;* [2]*Atomic Energy and Alternative Energies Commission, Paris, France;* [3]*University of Ottawa, Ottawa, Canada;* [4]*Oak Ridge National Laboratory, Oak Ridge, TN;* [5]*National Institute of Health, Bethesda, MD;* [6]*Ghent University, Gent, Belgium;* [7]*University of Minnesota, Twin Cities, Minneapolis, MN*

ThP 498 **Uncovering small proteins in the gut-microbiome to investigate their possible functions and differentiation in**

healthy vs dysbiosis-associated diseases; Megan E. Davin[1, 2]; Júlia Ortis-Sunyer[3]; Oskar Hickl[3]; Tuesday Lowndes[3]; Cedric Christian Laczny[3]; Patrick May[3]; Steven L. Tavis[1, 2]; Rémy Villette[3]; Samantha L. Peters[2]; Paul Wilmes[3]; Robert L. Hettich[2]; *[1]University of Tennessee, Knoxville, TN; [2]Oak Ridge National Laboratory, Oak Ridge, TN; [3]University of Luxembourg, Esch-sur-Alzette, Luxembourg*

ThP 499 **From Dormancy to Growth: Proteomic Insights into Spore Germination in the Global Pathogen Cryptococcus neoformans**; Benjamin Chadwick[1]; Megan C McKeon[2]; Katherine A. Overmyer[1, 2]; Christina M Hull[2]; Joshua J. Coon[1, 2]; *[1]Morgridge Institute for Research, Madison, WI; [2]University of Wisconsin-Madison, Madison, WI*

ThP 500 **Deep profiling of complex marine metaproteomes in DIA and DDA with timsTOF technology and iterative database reduction**; Noelle Held[1]; Ruben Shrestha[2]; Matthew Willetts[3]; Matthew McIlvin[4]; Mak Saito[4]; *[1]University of Southern California, Los Angeles, CA; [2]Bruker Scientific LLC, San Jose, California; [3]Bruker Scientific LLC, Billerica, MA; [4]Woods Hole Oceanographic Institution (WHOI), Falmouth, MA 02543*

ThP 501 **Metaproteomic insights into canine bladder stone formation**; Andrew Rajczewski[1]; Emily Coffey[1]; Subina Mehta[1]; Pratik Dilip Jagtap[1]; Timothy J. Griffin[1]; *[1]University of Minnesota, Minneapolis, MN*

ThP 502 **Improve metaproteomic data analysis with a two-pass search workflow in FragPipe**; Yamei Deng[1]; Fengchao Yu[1]; Alexey I. Nesvizhskii[1]; *[1]University of Michigan, US*

ThP 503 **The commensal bacterium Limosilactobacillus reuteri generates novel microbial-conjugated bile acids in in vitro culture**; Selene Shore[1]; Melinda A Engevik[1]; Ben Ahiadu[2]; Alexey V Melnik[2]; James Versalovic[3, 4]; Thomas D Horvath[3, 4]; *[1]Medical University of South Carolina, Medicine, Charleston, SC; [2]BileOmix Inc., Farmington, Connecticut; [3]Texas Children's Hospital - Microbiome Center, Houston, TX; [4]Baylor College of Medicine, Houston, TX*

ThP 504 **Optimization of a rapid multi-omic extraction method for the identification of bacteria with ion mobility-mass spectrometry**; Alexis V Torrence[1]; Kelly M Hines[1]; *[1]University of Georgia, Athens, GA*

ThP 505 **Elucidating membrane changes in E.coli with mutations disrupting plasmid transfer ability using secondary ion mass spectrometry (SIMS)**; Alfred Fransson[1]; Anne Farewell[1]; John Fletcher[1]; *[1]University of Gothenburg, Gothenburg, Sweden*

ThP 506 **Alterations in Staphylococcus aureus Abscess Structure in Murine Bone Infection Visualized via MALDI Imaging Mass Spectrometry**; Lauren N. Emmerson[1, 2]; Madeline E Colley[1, 3]; Lukasz G Migas[1, 4]; Raf Van De Plas[1, 4, 5]; James E. Cassat[6, 7, 8, 9]; Jeffrey M Spraggins[1, 2, 3, 5, 6, 9, 10]; *[1]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [2]Chemical and Physical Biology Program, Vanderbilt University School of Medicine, Nashville, TN; [3]Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; [4]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [5]Department of Biochemistry, Vanderbilt University, Nashville, TN; [6]Department of Pathology, Microbiology, and Immunology, Vanderbilt University Medical Center, Nashville, TN; [7]Department of Pediatrics, Vanderbilt University Medical Center, Nashville, TN; [8]Department of Biomedical Engineering, Vanderbilt University, Nashville, TN; [9]Vanderbilt Institute for Infection, Immunology, and Inflammation, Vanderbilt University Medical Center, Nashville, TN; [10]Department of Chemistry, Vanderbilt University, Nashville, TN*

ThP 507 **Advanced Proteomic Analysis of Iron Homeostasis and MAP Kinase Signaling in Aspergillus nidulans Using DIA-PASEF**; JungHun Lee[1]; Olivia West[1]; Steven D Harris[2]; Michael Betenbaugh[3]; Mark R Marten[1]; *[1]Department of Chemical, Biochemical, and Environmental Engineering, University of Maryland, Baltimore County, Baltimore, Maryland; [2]Department of Plant Pathology, Entomology, and Microbiology, Iowa State University, Ames, Iowa; [3]Department of Chemical and Biomolecular Engineering, Johns Hopkins University, Baltimore, Maryland*

ThP 508 **Quantification of tryptophan and tyrosine metabolites to assess the role of the gut microbiome in HIV infection**; Charlotte R Hemmila[1, 2]; Sophia L Lebakken[2]; Christopher M Basting[2]; Ashma Chakrawarti[2]; Ty A Schroeder[2]; Timothy J Griffin[1, 3]; Nichole R Klatt[2]; Candace R Guerrero[1, 2]; *[1]University of Minnesota, Center for Metabolomics and Proteomics, Minneapolis, MN; [2]University of Minnesota, Department of Surgery, Division of Surgical Outcomes and Precision Medicine Research, Minneapolis, MN; [3]University of Minnesota, Department of Biochemistry, Molecular Biology, and Biophysics, Minneapolis, MN*

ThP 509 **Rapid identification of infections directly from isolates and clinical specimens with the MSPen Technology**; Manoj Kumar[1]; Coreen L. Johnson[2]; Faith Jackobs[1]; Jacob Mardick[1]; Micheal Keating[1]; Sarah Bench[1]; James J. Dunn[2]; Racheal D. Downey[3]; Lindsey M. Kirkpatrick[4]; Livia S. Eberlin[1]; *[1]Baylor College of Medicine, Dept. of Surgery, Houston, TX; [2]Texas Children's Hospital - Dept. of Surgery, Houston, TX; [3]Dell Children's Medical Center, Austin, TX; [4]Riley Hospital for Children, Dept. of Pediatric Infectious Diseases, Indianapolis, Indiana*

ThP 510 **The impact of arachidonic acid on the metabolic and proteomic changes and killing of MRSA**; Rutan Zhang[1]; Ismael Barreras Beltran[1]; Quynh Do[1]; Brian J. Werth[1]; Libin Xu[1]; *[1]University of Washington, Seattle, WA*

ThP 511 **Exploring Bacterial Fungal Interactions Through Multi-omic Spatial Characterization**; Mary S. Lipton[1]; Erin Bredeweg[2]; Arunima Bhattacharjee[2]; Trinidad D Alfaro[2]; Scott E Baker[2]; *[1]PNNL, Richland, WA; [2]Pacific Northwest National Laboratory (PNNL), Richland, WA*

ThP 512 **Elucidating the impact of nutrient metals on molecular profiles at the microbe-microbe interface**; Alexis P Pope[1, 2]; Jeffrey A Freiberg[3, 4]; Lukasz G Migas[5]; Raf Van De Plas[1, 5]; Eric P Skaar[3, 6]; Jeffrey M Spraggins[1, 6, 7, 8, 9, 10]; *[1]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [2]Chemical and Physical Biology Program, Vanderbilt University School of Medicine, Nashville, TN; [3]Vanderbilt Institute for Infection, Immunology, and Inflammation, Vanderbilt University Medical Center, Nashville, TN; [4]Division of Infectious Diseases, Department of Medicine, Vanderbilt University Medical Center,, Nashville, TN; [5]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [6]Department of Pathology, Microbiology, and Immunology, Vanderbilt University Medical Center, Nashville, TN; [7]Chemical and Physical Biology Program, Vanderbilt University, Nashville, TN, United States 2. Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [8]Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; [9]Department of Chemistry, Vanderbilt University, Nashville, TN; [10]Department of Biochemistry, Vanderbilt University, Nashville, TN*

ThP 513 **AI-Driven Bacterial Fingerprinting Using Vacuum Matrix-Assisted Ionization (vMAI) Mass Spectrometry and Ion Mobility Spectrometry**; Dushan Kovacevic[1]; Frank S Yenchick[1]; Charles N McEwen[2, 3]; Sarah Trimpin[1, 2]; *[1]Wayne State University, Detroit, MI; [2]MSTM, Newark, DE; [3]Saint Joseph's University, PHILADELPHIA, PA*

ThP 514 **Quantitative bile acid profiles elucidate Peptacetobacter hiranonis metabolism in vitro**; Amanda Blake[1]; Bruna C Lopes[1]; Luis Medina[1]; Christi M Shirley[1]; Rachel Pilla[2]; Jan S Suchodolski[1]; *[1]Gastrointestinal Lab, Texas A&M University, College Station, TX; [2]Department of Veterinary Pathology, Hygiene and Public Health, University of Milan, Milan, Italy*

ThP 515 **Old metabolite, new function: discovery of novel links between 2,3-dihydroxypropane-1-sulfonate (DHPS), metabolic dysregulation, and gut health**; Courtney J Christopher[1]; Shawn R Campagna[2, 3]; *[1]University of Tennessee, Knoxville, Knoxville, TN; [2]University of*

Tennessee, Knoxville, TN; [3]Biological and Small Molecule Mass Spectrometry Core, Knoxville, Tennessee

ThP 516 **Proteomic analyses of marine bacterium Vibrio natriegens during domestication for biotechnology**; Jaimee R Compton[1]; Dagmar Leary[1]; William Judson Hervey IV[1]; Tanya Tschirhart[1]; Grant A Rybnicky[1]; Scott N. Dean[1]; Sophie M. Colston[1]; Christopher J. Katilie[1]; Eric S Vanarsdale[1]; *[1]Naval Research Laboratory, Washington, DC*

ThP 517 **LC-MS/MS analysis of differences in melanin production in E.coli grown under microgravity conditions**; Dagmar Leary[1]; Christopher J. Katilie[1]; Jaimee R Compton[1]; William Judson Hervey IV[1]; Tiffany Hennessa[1]; Gaurav J. Vora[1]; Zheng Wang[1]; *[1]Naval Research Laboratory, Washington, DC*

NEUROSCIENCE AND NEURODEGENERATIVE DISEASE RESEARCH II

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ThP 518 **Pan-neurodegeneration proteomics reveal disease subtypes and altered molecular signatures across seven major neurodegenerative disorders**; Him K Shrestha[1]; Huan Sun[1]; DongGeun Lee[1]; Jay M Yarbro[1]; Boer Xie[1]; Danting Liu[1]; Suresh Poudel[1]; Yuxin Li[1]; Zuo-fei Yuan[1]; Zhen Wang[1]; Masihuz Zaman[1]; Ju Wang[1]; Meghan McReynolds[1]; Zhiping Wu[1]; Anthony A High[1]; Julia F Llorens[2]; Michael DeTure[3]; Pamela J McLean[3]; Dennis W Dickson[1]; Rui Chang[4]; Geidy E Serrano[5]; Thomas G Beach[5]; Gang Yu[6]; Rosa Rademakers[2]; Xusheng Wang[7]; Bin Zhang[8]; Junmin Peng[1]; *[1]St Jude Children's Research Hospital, Memphis, TN; [2]University of Antwerp, Antwerpen, Belgium; [3]Mayo Clinic, Jacksonville, FL; [4]University of Arizona, Tucson, AZ; [5]Banner Sun Health Research Institute, Sun City, AZ; [6]University of Texas Southwestern Medical Center, Dallas, TX; [7]University of Tennessee Health Science Center, Memphis, TN; [8]Icahn School of Medicine at Mount Sinai, New York City, NY*

ThP 519 **Multi-antibody immunoprecipitation with high-resolution FAIMS-PRM mass spectrometry effectively quantifies AAV-mediated human GBA1 expression in brain tissues, aiding GBA-PD drug development**; Mahmud Hossain[1]; Dhiman Ghosh[1]; Jae Ryu[1]; Bradford Elmer[1]; Swathi Ayloo[1]; Shyam Ramachandran[1]; Bailin Zhang[1]; *[1]Sanofi, Cambridge, MA*

ThP 520 **Exploring the mechanism of N-terminal germline H3.3 mutations in neurodevelopmental disorders**; Carolina Brás Costa[1]; Francisca NDL Vitorino[1]; Elizabeth G. Porter[1]; Joanna Lempiainen[1]; Benjamin A Garcia[1]; *[1]Washington University School of Medicine, St. Louis, MO*

ThP 521 **Unveiling Tau Pathogenesis in Alzheimer's Disease: A Label-Free Mass Spectrometry Study of Autopsy-Confirmed Brain Tissues**; Xuemei Zeng[1]; Yijun Chen[1]; Anuradha Sehrawat[1]; Eric E Abrahamson[1, 2]; Julia Kofler[1]; William R Paljug[1, 2]; Milos D Ikonomovic[1, 2]; Thomas K Karikari[1]; *[1]University of Pittsburgh, Pittsburgh, PA; [2]VA Pittsburgh HS, Pittsburgh, PA*

ThP 522 **Characterization of brain metabolic homeostasis in Alzheimer’s Disease by untargeted metabolomics and lipidomics analyses**; Cheuk Woon Lui[1]; Xuewei Ye[1, 2]; Elizabeth T. Anderson[1]; Qin Fu[1]; Gary E. Gibson[3]; Sheng Zhang[1]; *[1]Cornell University, Ithaca, NY; [2]Key Laboratory of Artificial Organs and Computational Medicine of Zhejiang Province, Shulan International Medical College, Zhejiang Shuren University, Hangzhou, China; [3]Brain and Mind Research Institute, Weill Cornell Medicine, Burke Neurological Institute, Whiteplain, NY*

ThP 523 **Probe-dependent Proximity Profiling (ProPPr) Uncovers Similarities and Differences in Phospho-Tau-Associated Proteomes Between Tauopathies**; Dmytro Morderer[1]; Melissa C Wren[1]; Feilin Liu[1]; Naomi Kouri[1]; Anastasiia Maistrenko[1]; Bilal Khalil[1]; Nora Pobitzer[1]; Michelle R. Salemi[2]; Brett S. Phinney[2]; Guojun Bu[3]; Na Zhao[1]; Dennis W Dickson[1]; Melissa E. Murray[1]; Wilfried Rossoll[1]; *[1]Mayo Clinic, Jacksonville, FL; [2]UC Davis, Davis, CA; [3]The Hong Kong University of Science and Technology, Hong Kong, China*

ThP 524 **Characterization of lipid droplet population dynamics in normal aging and Alzheimer's disease mouse models**; Manita Shakya[1]; Tialfi Bergamin De Castro[1]; Matthew Bonnet[1]; Matthew Briggs[2]; Shane R. Ellis[2]; Nathan Heath Patterson[3]; Alison J. Scott[1]; *[1]Department of Microbial Pathogenesis, University of Maryland School of Dentistry, Baltimore, Maryland; [2]University of Wollongong, Wollongong, Australia; [3]Aspect Analytics, Genk, Belgium*

ThP 525 **Defining the impact of pathological mutations of the O-GlcNAc Transferase in the murine brain**; Akanksha Aggarwal[1]; Fiddia Zahra[1]; Robert O’Meally[2]; Brian D. Foster[1]; Robert N. Cole[2]; Michael J. Wolfgang[1]; Natasha E. Zachara[1]; *[1]Johns Hopkins University School of Medicine, Baltimore, Maryland; [2]Johns Hopkins Applied Imaging Mass Spectrometry Core, Johns Hopkins University School of Medicine, Baltimore city, MD*

ThP 526 **Development and Evaluation of Senescence Signatures in Healthy and Diseased Neurons**; Alexandra W Montesinos; *National Institute on Aging, Baltimore, MD*

ThP 527 **Investigation of In Vitro Aggregation of Amyloid Beta 1-42 Utilizing Mass Spec-based Footprinting and the ThT Assay**; Cole Hediger[1]; Wesley Wagner[1, 2]; Kameswara Rao Mula[1]; Don Rempel[1]; Michael L Gross[1]; *[1]Washington University in St. Louis, University City, MO; [2]AbbVie, North Chicago, IL*

ThP 528 **Midkine Attenuates Aβ Fibril Assembly and Amyloid Plaque Formation**; Yanhong Hao[1]; Masihuz Zaman[1]; Shu Yang[1]; Ya Huang[1]; Jay Yarbo[1]; Zhen Wang[1]; Yun Jiao[1]; Zhiping Wu[1]; Ping-chung Chen[1]; Junmin Peng[1]; *[1]St.Jude Children's Research Hospital, Memphis, TN*

ThP 529 **Quantitative neuronal Cell-Type Proteomics workflow for neurodegenerative disease studies**; Pratigya Subba[1, 2]; Tanina Arab[3]; Juliana Salgado[3]; TuKiet T. Lam[1, 2, 4]; *[1]Department of Molecular Biophysics and Biochemistry, New Haven, CT; [2]Yale/NIDA Neuroproteomics Center, New Haven, CT; [3]Department of Neuroscience, Yale University School of Medicine, New Haven, CT; [4]Keck MS & Proteomics Resource, Yale School of Medicine, New Haven, CT*

ThP 530 **Temporal map of the serum proteome in multiple sclerosis relapse reveals the inflammatory process begins months before symptom onset**; Danielle M Caefer[1, 2]; Brenna Labarre[1, 2]; Devin King[1, 2]; Shrishti Saxena[1]; Anthilia Alchanat[1]; Alena Zhirova[1]; Kyle Downer[1]; Tanuja Chitnis[1, 2]; *[1]Brigham and Women's Hospital, Boston, MA; [2]Harvard Medical School, Boston, MA*

ThP 531 **Comparison of Proximity Proteomics Approaches and Biotinylation Reveals Distinct Biases in Local Proteomes**; Alexandria S. Battison[1]; Jeremy Balsbaugh[2]; Jeremy Borniger[1]; Neal Liddle[2]; *[1]Cold Spring Harbor Laboratory, Cold Spring Harbor, NY; [2]University of Connecticut, Storrs*

ThP 532 **Enhanced Brain Glycation-proteomics Profiling Reveals Increased Glycation of Key Proteins Associated with Alzheimer’s Disease**; Qin Fu[1]; Elizabeth T. Anderson[1]; Andy Lui[1]; Gary E. Gibson[2]; Sarah A. Flowers[3]; Sheng Zhang[1]; *[1]Proteomics and Metabolomics Facility, Cornell University, Ithaca, NY; [2]Brain and Mind Research Institute, Weill Cornell Medicine, Burke Neurological Institute, White Plains, NY; [3]Department of Neuroscience, University of Virginia, Charlottesville, VA*

ThP 533 **Single-neuron proteomics in Alzheimer’s disease to infer disease progression**; Corinna Friedrich[1]; Peyton Stewart[1]; Jason Derks[1]; Megan Elcheikhali[1]; Theresa Connors[2]; Alexandra Melloni[2]; Bradley T Hyman[2]; Mahlon Collins[1]; Nikolai Slavov[1]; *[1]Parallel Squared Technology Institute, Watertown, MA; [2]Department of Neurology, Massachusetts Alzheimer's Disease Research Center, Massachusetts General Hospital, Harvard Medical School, Boston, MA*

ThP 534 **Metabolomics identifies biotin as a protectant against the development of manganese-induced Parkinson’s disease-related neurotoxicity in Drosophila and human**

neurons; Yunjia Lai[1]; Pablo Reina-Gonzalez[2]; Gali Maor[3]; Gary W. Miller[1]; Souvarish Sarkar[2, 3]; *[1]Department of Environmental Health Sciences, Mailman School of Public Health, Columbia University, New York, NY; [2]Department of Environmental Medicine, University of Rochester School of Medicine and Dentistry, Rochester, NY; [3]Department of Pathology, Brigham and Women's Hospital, Harvard Medical School, Boston, MA*

ThP 535 **Label-free DIA-based single-cell proteomics of primary microglia from the human post-mortem brain using the Orbitrap Astral mass spectrometer**; Ashley Ives[1]; James M. Fulcher[1]; Pranav Dawar[1]; Sarai Williams[1]; Alex Bautista[2]; Phillip De Jager[2]; Vladislav Petyuk[1]; *[1]Pacific Northwest National Laboratory (PNNL), Richland, WA; [2]Columbia University, New York, NY*

ThP 536 **Ultra-Sensitive and Comprehensive Metabolomic Profiling of Dialyzed Blood for Rodent Behavior Studies at Temporal Resolution**; Nan Wang[1]; Michele Nardin[1]; Emily J. Dennis[1]; *[1]HHMI Janelia, Ashburn, VA*

ThP 537 **Peptide quantification in cerebrospinal fluid for the analysis of neurodegenerative diseases**; Gennifer E Merrihew[1]; Deanna L Plubell[1]; Michael Riffle[1]; Bo Wen[1]; Jessica Becker[2]; Julia E Robbins[1]; Brian C. Searle[3]; Christine Wu[1]; Kathleen Poston[4]; Thomas Montine[4]; Andrew N Hoofnagle[2]; Michael J MacCoss[1]; *[1]University of Washington - Genome Sciences, Seattle, WA; [2]University of Washington, Seattle, WA; [3]The Ohio State University, Columbus, OH; [4]Stanford University, Stanford, CA*

ThP 538 **Peptidomics and terminomics of human brain samples**; Hiroshi Nishida[1]; Firdous Bhat[1]; Anu Jain[1]; Dong-Gi Mun[1]; Amy J French[1]; Gunveen Sachdeva[1]; Richard K. Kandasamy[1, 2, 3, 4]; Akhilesh Pandey[1, 4]; *[1]Department of Laboratory Medicine and Pathology, Mayo Clinic, Rochester, MN; [2]Department of Quantitative Health Sciences, Mayo Clinic, Rochester, MN; [3]Department of Immunology, Mayo Clinic, Rochester, MN; [4]Center for Individualized Medicine, Mayo Clinic, Rochester, MN*

ThP 539 **An in-depth study of proteomic and phosphoproteomic dynamics in mouse models undergoing vaccination-guided prophylactic activity for Alzheimer's disease**; Maosheng Wei[1]; Min Ma[2, 3]; Ming Zhang[2, 3]; Yiting Song[4]; Chunling Dai[5]; Chengxin Gong[5]; Jonathan Lovell[4]; Jun Qu[2, 3]; *[1]Department of Chemical and Biological Engineering, State University of New York at Buffalo, Buffalo, NY; [2]Department of Pharmaceutical Sciences, State University of New York at Buffalo, Buffalo, NY; [3]New York State Center of Excellence in Bioinformatics & Life Sciences, Buffalo, NY; [4]Department of Biomedical Engineering, State University of New York at Buffalo, Buffalo, New York; [5]Department of Neurochemistry, Inge Grundke-Iqbal Research Floor, New York State Institute for Basic Research in Developmental Disabilities, Staten Island, NY*

ThP 540 **Profiling oxidized triacylglycerols isolated from a murine Alzheimer's Disease model using multiple reaction monitoring mass spectrometry**; Katherine A Walker[1]; Caitlin E Randolph[2]; Reagan N Fortwendel[2]; Gaurav Chopra[2, 3, 4, 5, 6, 7]; *[1]Purdue University, West Lafayette, IN; [2]Purdue Univeristy, West Lafayette, IN; [3]Purdue Institute for Drug Discovery, West Lafayette, IN; [4]Regenstrief Center for Healthcare Engineering, West Lafayette, IN; [5]Purdue Institute for Cancer Research, West Lafayette, IN; [6]Purdue Institute for Inflammation, Immunology, and Infectious Disease, West Lafayette, IN; [7]Purdue Institute for Integrative Neuroscience, West Lafayette, IN*

ThP 541 **Chemoproteomic Profiling of Neurosteroid Interacting Proteins in Live Hippocampal Neurons**; Zi-Wei Chen[1]; Ann Benz[1]; Steven Mennerick[1]; Douglas F Covey[1]; Alex S. Evers[1]; *[1]Washington University School of Medicine, St. Louis, MO*

NUCLEIC ACIDS AND OLIGONUCLEOTIDES III
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ThP 542 **Case Studies for Challenges and Solutions for Oligonucleotide Analysis by LC-MS/MS**; Shuming Yang[1]; Yanping Lin[1]; Tian-Sheng Lu[1]; Shuyu Hou[1]; *[1]Medpace, Cincinnati, OH*

ThP 543 **A novel mRNA capping efficiency assay by in situ stable isotope-labeled cap and LC-MRM**; Zhijun Cao[1]; Zhichun Wang[1]; Ying Zhang[1]; Jiang Qian[1]; *[1]CSL Seqirus, Holly Springs, NC*

ThP 544 **Manipulating Mobile Phases to Improve Sensitivity in Adductomic and Nucleic Acid-derived Molecule Analysis**; Michael C Sausen[1]; Michael A Terzidis[2]; Peter W Villalta[1]; Silvia Balbo[1, 3]; *[1]University of Minnesota, Twin Cities, Minneapolis, MN; [2]Department of Nutritional Sciences and Dietetics, International Hellenic University (IHU), Thermi, Greece; [3]Masonic Cancer Center, University of Minnesota, Minneapolis, MN*

ThP 545 **Characterization and Analysis of mRNA Poly(A) Tail by Liquid Chromatography – Mass Spectrometry (LC-MS)**; Jing Jiang[1]; Yun Zhang[1]; Mike Boggs[1]; *[1]MilliporeSigma, Rockville, MD*

ThP 546 **Key RNA-binding domains in the La protein establish tRNA modification levels in Trypanosoma brucei**; Lankani Gunarante[1]; Robert L Ross[2]; Juan Alfonzo[1]; *[1]Brown University, Providence, RI; [2]Thermo Fisher Scientific, Lexington, MA*

ThP 547 **Rapid identification of RNA modifications and isomers by UPLC-ion-mobility MS**; Cecilia Silva Sanchez[1]; Laura Bailey[1]; C. Eduardo Vallejos[1]; Kari B Basso[1]; *[1]University of Florida, Gainesville, FL*

ThP 548 **Fast Photochemical Oxidation of Nucleic Acids (FPONA) for High-Resolution Structural Characterization of Nucleic Acid Conformation**; Marek Polak[1, 2]; Evgeniya Biryukova[1, 2]; Jiří Černý[3]; Petr Novak[1, 2]; *[1]Institute of Microbiology, Prague, Czech Republic; [2]Faculty of Science, Charles University, Prague, Czech Republic; [3]Institute of Biotechnology, Vestec, Czech Republic*

ThP 549 **Improving Oligonucleotide MS Data Quality with Ion Source Conditions in a Single Quadrupole Mass Spectrometer**; Udara Jayasundara[1]; Vikki Johnson[1]; Toshiya Matsubara[1]; *[1]Shimadzu Scientific Instruments, Columbia, Maryland*

ThP 550 **Harnessing the power of DNA adductomics to study DNA mutations**; Foster C Jacobs[1]; Dylan Mckeon[1]; Yang Jiang[2]; Peter W Villalta[1]; Juan Garaycoechea[2]; Silvia Balbo[1]; *[1]Masonic Cancer Center - University of Minnesota, Minneapolis, MN; [2]Hubrecht Institute, Royal Netherlands Academy of Arts and Sciences (KNAW), Utrecht, Netherlands*

ThP 551 **A case study of aptamer-target complexes characterization by kinetic capillary electrophoresis and ion mobility mass spectrometry**; Zeina Hajjar[1]; Clara Davoine[1]; Johann Far[1]; Edwin De Pauw[1]; Marianne Fillet[1]; Gauthier Eppe[1]; *[1]University Liege, Liege, Belgium*

ThP 552 **Developing an Analytical Method for Oligonucleotide Incorporation Using Ion-Pair Reverse-Phase Liquid Chromatography with UV and Mass Spectrometric Detection (IP-RP-LC/UV/MS)**; Agbo-oma A. Uwakweh[1]; Rinky D. Parakra[1]; Juliet O. Obi[1]; Daniel J. Deredge[1]; *[1]University of Maryland School of Pharmacy, Baltimore, MD*

ThP 553 **Structural flexibility analysis of G-quadruplex DNA by droplet charge tuning with vibrating sharp-edge spray ionization – mass spectrometry**; Sultan Mahmud[1]; Vikum K. K. Dewasurendra[1]; Matthew B. Johnson[1]; Peng Li[1]; Stephen J Valentine[1]; *[1]West Virginia University, Morgantown, WV*

ThP 554 **Probing Nucleotide Methylation Dynamics altered by EZH2 Knockdown Using Ion Chromatography Coupled to Ultra-High-Resolution Mass Spectrometry**; Mohamed M. Y. Kaddah[1, 2, 3, 4]; Teresa W.-M. Fan[1, 2, 4]; Jahid M. M. Islam[1]; Andrew N. Lane[1, 2, 4]; Richard M. Higashi[1, 2, 4]; *[1]Center for Environmental and Systems Biochemistry (CESB), University of Kentucky, Lexington, KY 40536; [2]Markey Cancer Center, College of Medicine, University of Kentucky, Lexington, KY 40536; [3]Pharmaceutical and Fermentation Industries Development Center, City of Scientific Research* *and Technological Applications, New Borg El-Arab 21934, Egypt; [4]Department of Toxicology and Cancer Biology, University of Kentucky, Lexington, KY 40536*

ThP 555 **Photochemical Nitrile-Imine Cross-Linking in Ribonucleosides**; Chenyang Wei[1]; Frantisek Turecek[1]; *[1]University of Washington, Seattle, WA*

ThP 556 **A Software Workflow Using Wide Mass Range Single Quadrupole Mass Spectrometry Data Streams Applied to Oligonucleotide Confirmation**; Risa Suzuki[1, 2]; Kosuke Uchiyama[2]; Noriko Kato[2]; Yuka Fujito[2]; Jeff Dahl[1]; Simon Ashton[3]; Neil J Loftus[3]; Atsuhiko Toyama[2, 4]; *[1]Shimadzu Scientific Instruments, Columbia, MD; [2]Shimadzu Corporation, Kyoto, Japan; [3]Shimadzu Corporation, Manchester, United Kingdom; [4]Shimadzu Scientific Instruments, Boston, MA*

ThP 557 **Tandem LC-MS3 Qtrap enables improved sensitivity to quantify endogenous formaldehyde-DNA adducts in mammalian tissues**; Nicholas W Cheng[1]; Christopher Mellor[1]; Saeideh Azad[1]; Meng Wang[1]; *[1]Cornell University, Ithaca, NY*

ThP 558 **Improved Characterization of Heavily-Modified RNA Therapeutics through Activated-Ion Negative Electron Transfer Dissociation (AI-NETD)**; Daniel Jacob Nesbitt[1, 2]; Keaton L. Mertz[1, 2]; Trenton M. Peters-clarke[1, 2]; Mitchell D. Probasco[2, 3]; Scott T. Quarmby[1, 2]; Joshua J. Coon[1, 2, 3]; *[1]University of Wisconsin-Madison, Madison, WI; [2]National Center for Quantitative Biology of Complex Systems, Madison, WI; [3]Morgridge Institute for Research, Madison, WI*

ThP 559 **Utilizing a Novel Non-Ion Pairing Approach for Sequence Confirmation of Oligonucleotides**; Lee Bertram[1]; Jordy J Hsiao[1]; *[1]Agilent Technologies, Santa Clara, CA*

ThP 560 **Considerations for oligonucleotide analysis using microflow LC-MS**; Kyler Radmall[1]; Chris D Hardcastle[1]; Brandon Wilcock[1]; Troy Voelker[1]; *[1]Aliri Bioanalysis, Salt Lake City, UT*

ThP 561 **OligoFinder: A research software tool for automated Oligonucleotide MS/MS Spectral Annotation and LC-MS/MS Sequence Mapping**; Scott R. Kronewitter[1]; Alexander A. Gudzovskiy[2]; Ping F. Yip[1]; Joshua D. Hinkle[3]; Ismail Belmostefa[2]; William M. McGee[1]; Robert L. Ross[1]; Shweta Chhajed[1]; Gustavo J. Cavallero[1]; Ilkka J. Borg[2]; John E. P. Syka[3]; James L. Stephenson Jr. [1]; *[1]ThermoFisher Scientific, Lexington, MA; [2]Softability, Vantaa, Finland; [3]ThermoFisher Scientific, San Jose, CA*

ThP 562 **Development of an Optimized IP-RPLC-MS/MS mRNA Digested Oligonucleotide Sequencing, 5' Cap, and 3' PolyA Tail Characterization Workflow**; Steven Broome[1]; Maria Basanta-Sanchez[1]; Marshall Bern[1]; Roxana Eggleston-Rangel[2]; *[1]Protein Metrics, Boston, MA; [2]Phenomenex, Torrance, CA*

ThP 563 **Optimization of Isolation Q for Ultra-Sensitive Detection of Uridine and Thymidine Nucleosides**; Zheng Duan; *University of California Riverside, Riverside, CA*

ThP 564 **Diastereomer Characterization of Synthetic Phosphorothioate Oligonucleotides Utilizing Stereospecific Enzymatic Digestion**; Md Rabiul Islam[1]; Leonard Yoon[1]; Nnenna Dieke Afon[1]; Cynthia Sommers[1]; Jason Rodriguez[1]; Deyi Zhang[2]; Yan Wang[2]; Kui Yang[1]; *[1]U.S. Food and Drug Administration, St. louis, MO; [2]U.S. Food and Drug Administration, Silver Spring, MD*

ThP 565 **High-throughput Ion-Pairing Free Reversed Phase Analysis of Oligonucleotides using RapidFire Quadrupole Time-of-Flight Mass Spectrometry**; Guannan Li[1]; Lee Bertram[1]; *[1]Agilent Technologies, Santa Clara, CA*

ThP 566 **The physics of ion trap-type resonant collision induced dissociation enables maximization of the yield of sequence ions from oligonucleotide anions**; John E. P. Syka[1]; Joshua D. Hinkle[1]; Scott R. Kronewitter[2]; Ping Yip[2]; James L. Stephenson[2]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Lexington, MA*

ThP 567 **Identification of HELLS as a Novel G-quadruplex Helicase**; Zi Gao[1]; Xiaomei He[1]; Yie Woon Chong[1]; Jun Yuan[1]; Yinsheng Wang[1]; *[1]University of California Riverside, Riverside, CA*

ThP 568 **Mass spectrometry-based parallel analysis of protein expression levels from mRNA using peptide barcodes**; Shun Kumano[1]; Kazuki Tanaka[1]; Rena Akahori[2]; Akihiro Nojima[1]; *[1]Hitachi, Ltd., Kokubunji-Shi, Japan; [2]ARCALIS, Inc., Minami Soma, Japan*

ThP 569 **Mass spectrometry for illustrating the functions of HMGB3 in DNA damage recognition and repair**; Ting Zhao[1]; Xiaomei He[1]; Xiaochen Liang[1]; Yinsheng Wang[1]; *[1]UC Riverside, Riversdie, CA*

ThP 570 **Detection of dsDNA Extracted from Fossil Samples Using a DNA-Specific Fluorescent Dye**; Addison K. O'Brian[1]; J. Luke Sullivan[1]; Carissa Shipman[2]; Andrew J. Fabich[3]; Stephen Taylor[4]; Joseph E. Deweese[1, 5]; *[1]Freed-Hardeman University, Henderson, TN; [2]Huntington University, Huntington, IN; [3]Independent researcher, Gainesville, GA; [4]University of Liverpool, Liverpool, United Kingdom; [5]Vanderbilt University, Nashville, TN*

ThP 571 **Detection of dsRNA impurities in IVT synthesized mRNA using fluorescent PNA probes**; Kyle Jacob Tynan[1, 2]; Daniel Hunter[2]; Trina Mouchahoir[1, 2]; Mark S Lowenthal[1]; Karen Phinney[1]; *[1]National Institute of Standards and Technology (NIST), Gaithersburg, MD; [2]IBBR, Rockville, MD*

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ThP 572 **Evaluation and Optimization of Workflows to Translate DIA Proteomics Data to Develop Sensitive and Reproducible Targeted Proteomics Assays**; Omprakash Nacham; *AbbVie, North Chicago, IL*

ThP 573 **Comprehensive quantitation of the mitochondrial proteome with targeted mass spectrometry and real-time retention alignment on Eclipse and Stellar mass spectrometers**; Valerie Lynch[1]; Lilian Heil[2]; Christopher McGann[1]; Philip Remes[2]; Cristina Jacob[2]; Yasemin Sancak[1]; Devin Schweppe[1]; *[1]University of Washington, Seattle, WA; [2]Thermo Fisher Scientific, San Jose, CA*

ThP 574 **Enhanced HCP quantitation LC-MS/MS workflow solution using a magnetic MS sample prep method and heavy-peptide mixture**; Jae Choi[1]; Reiko Kiyonami[2]; Min Du[2]; Sarah Driscoll[3]; Km Shams Ud Doha[3]; Nikki Jarrett[1]; Kay Opperman[1]; Ryan Bomgarden[1]; Bhavin Patel[1]; *[1]Thermo Fisher Scientific, Rockford, IL; [2]Thermo Fisher Scientific, Lexington, MA; [3]Thermo Fisher Scientific, Grand Island, NY*

ThP 575 **Synchronous Precursor Selection of Light/Heavy Peptides on the MS-Level using the Stellar MS Platform**; Cristina C. Jacob[1]; Philip M Remes[1]; Linfan Li[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

ThP 576 **Detection and Quantification of GLP-1 Analogs in Human Plasma: A Comprehensive Analytical Approach**; Hao Yang[1]; Cristina Jacob[1]; Romain Huguet[1]; Min Du[2]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Lexington, MA*

ThP 577 **Intelligent Targeted MS Acquisition Achieves Seven-Order Dynamic Range in Oocyte Analysis**; Michael Baggio Lorenz[1]; Maria Wahle[1]; Tim Heymann[1]; Georg Wallmann[1]; Johanna Gassler[1]; Max Hoek[2]; Johannes Petzoldt[2]; Till Zickmantel[2]; Sophia Steigerwald[2]; Ankit Dwivedi[2]; Christian Hock[2]; Kikuë Tachibana[1]; Matthias Mann[1]; *[1]Max Planck Institute of Biochemistry, Martinsried, Germany; [2]Thermo Fisher Scientific, Bremen, Germany*

ThP 578 **Improving quantitative sensitivity for peptide analysis in plasma using a novel QTOF mass spectrometer**; Ebru Selen[1]; Eshani Galermo[1]; Rahul Baghla[1]; Jason Causon[2]; *[1]Sciex, Redwood City, CA; [2]SCIEX, Concord, ON*

ThP 579 **Comparison of Data-Dependent Acquisition, Data-Independent Acquisition, and Parallel Reaction Monitoring PASEF Methods for Bottom-up Histone LC-timsTOF MS/MS Analysis**; Marissa A. Carter[1]; Lilian Valadares Tose[1]; Francisco A. Fernandez-Lima[1]; *[1]Florida International University, Miami, FL*

ThP 580 **Development of a highly multiplexed PRM method on the Stellar MS to reduce instrument time and broaden CSF**

proteome coverage; Wes Rogers[1]; Sudipa Maity[1]; Yadira Perez Paramo[2]; Erin Tom[2]; Veronica G. Anania[2]; [1]*Thermo Fisher Scientific, San Jose, CA;* [2]*Genentech, South San Francisco, CA*

ThP 581 **Detuning FAIMS-CV of PRTC peptides improves the dynamic retention time feature for FAIMS-PRM on Orbitrap instruments**; Camille Lombard-Banek[1]; Marya Melkie[2]; Yeoun Jin Kim[2]; Steve Sweet[2]; [1]*Astrazeneca, Gaithersburg, MD;* [2]*AstraZeneca, Gaithersburg, MD*

ThP 582 **Verifying quadrupole isolation efficiency for both light and heavy peptides using appropriate controls is essential for accurate quantification in PRM**; Beom-Jun Kim[1]; Camille Lombard-Banek[1]; Mary Melkie[1]; Yeoun Jin Kim[1]; Steve M Sweet[2]; [1]*AstraZeneca, Gaithersburg, Maryland;* [2]*AstraZeneca, Gaithersburg, MD*

ThP 583 **Molecular Mops: An Innovative Approach to Synthetic Opioid Neutralization**; Jonathan Ferguson[1]; Amina Woods[2]; Milaan Thirukumaran[1]; Francine Yanchik-Slade[1]; Asher Brandt[3]; Masayuki Nishimura[1]; Nazim Nazim Boutaghou[1]; Scott Kuzdzal[1]; [1]*Shimadzu Scientific Instruments, Columbia, MD;* [2]*Amina Woods Consulting, Pikesville, Maryland;* [3]*University of Saint Joseph, West Hartford, CT*

ThP 584 **Developing and Evaluating Electrospray Ionization mass spectrometry Methods for the Discovery and Quantitative Analysis of Cyclic Peptide**; Tolulope Ogunsanya[1]; Ian Ferraro[1]; Kanwal Jeet[1]; Anna O'Brien[1]; Anyin Li[1]; [1]*University of New Hampshire, Durham, NH*

ThP 585 **An Automated Data Processing Pipeline for System Suitability QC in FAIMS-PRM Assays on the Exploris 480 Mass Spectrometer**; Lihe Zhang[1]; Wen Yu[1]; Xiaotao Qu[1]; Miaomiao Chen[1]; Yeoun Jin Kim[1]; Steve M Sweet[1]; [1]*AstraZeneca, Gaithersburg, Maryland*

ThP 586 **Optimizing PhosphopeptideTargeted Assays for Low Input Formalin-Fixed Paraffin-Embedded (FFPE) Samples: SureQuant vs DynRT, with and without FAIMS**; Lihe Zhang[1]; Marya Melkie[2]; Camille Lombard-Banek[2]; Stephanie Zalesak-Kravec[2]; David J Clark[2]; Yeoun Jin Kim[2]; Steve M Sweet[2]; [1]*AstraZeneca, Gaithersburg, MD;* [2]*AstraZeneca, Gaithersburg, Maryland*

ThP 587 **A Novel All-Ion Parallel Reaction Monitoring (AI-PRM) Methodology for Enhanced Sensitivity in High Throughput Targeted Proteomics Analysis**; Liulin Deng[1]; Leonard C. Rorrer III[1]; Lauren Royer[1]; Isabel Uribe[1]; Daniel DeBord[1]; [1]*Mobilion Systems Inc., Chadds Ford, PA*

ThP 588 **SureQuant-based targeted quantitation of phosphotyrosine-containing proteins inT cell receptor signaling pathway**; Firdous A Bhat[1]; Husheng Ding[1]; Dong-Gi Mun[1]; Jane A. Peterson[2]; M. Cristine Charlesworth[2]; Richard K. Kandasamy[1, 3, 4, 5]; Akhilesh Pandey[1, 5]; [1]*Department of Laboratory Medicine and Pathology, Mayo Clinic, Rochester, MN;* [2]*Proteomics Core, Mayo Clinic, Rochester, MN;* [3]*Department of Quantitative Health Sciences, Mayo Clinic, Rochester, MN;* [4]*Department of Immunology, Mayo Clinic, Rochester, MN;* [5]*Center for Individualized Medicine, Mayo Clinic, Rochester, MN*

ThP 589 **Absolute Quantitation of Phosphopeptides and Glycopeptides by Coulometric Mass Spectrometry (CMS) Without Using Standards**; Md. Tanim-Al Hassan[1]; Timothy Yaroshuk[1]; Arjun Sharma[1]; Bhavya Deshaboina[1]; Quentin Young[1]; Yongling Ai[1]; Howard D. Dewald[2]; Hao Chen[1]; [1]*Department of Chemistry and Environmental Science, New Jersey Institute of Technology, Newark, New Jersey;* [2]*Chemistry & Biochemistry Department, Ohio University, Athens, Ohio*

ThP 590 **Automated Quantitative Analysis of 1951 Subject Cancer Cohort Study in Multiple Reaction Monitor (MRM) LC-MS**; Jiana Duan[1]; Sangeet Adhikari[1]; Yong Zhou[1]; Isaiah Odoyo[1]; Hao Qian[1]; Wan-fang Chou[1]; Adam Poltorak[1]; Ranjan Bhadra[1]; Jessica Chan[1]; Jimmy Yi Zeng[1]; Robert Zawada[1]; Joon-Yong Lee[1]; Bruce Wilcox[1]; Phillp Ma[1]; [1]*Prognomiq, San Mateo, CA*

ThP 591 **Regulated Bioanalysis for Endogenous Glucagon-like Peptide-1 (GLP-1) and Synthetic Analog Therapeutic Peptide Quantitation in Biomatrix by LC–MS/MS**; Chunhai Ruan[1]; Kumar Shah[1]; Gus Hui[1]; M. Shane Woolf[1]; Moucun Yuan[1]; William R. Mylott Jr. [1]; [1]*PPD, part of Thermo Fisher Scientific, Richmond, VA*

ThP 592 **Enhanced Proteomics Quantitation with Stellar Mass Spectrometry for High-Throughput Applications**; Yuan Lin[1]; Jia Tang[2]; Runsheng Zhang[3]; Shanhua Lin[1]; [1]*Thermo Fisher Scientific, Sunnyvale, CA;* [2]*Thermo Fisher Scientific, San Jose, CA;* [3]*Thermo Fisher Scientific, Germering, Germany*

ThP 593 **A Novel Validated LC-MSMS Approach for Survodutide in Mouse Liver**; Xinfa Fu[1]; Yanfu Ren[1]; Zhiyu Li[2]; Lili Xing[2]; Yi Tao[2]; Liang Shen[2]; [1]*WuXi AppTec (Suzhou), Suzhou, China;* [2]*WuXi AppTec, Shanghai, China*

ThP 594 **Towards enrichment-free quantification of phosphopeptides from single-cells using targeted mass spectrometry**; Sofani T. Gebreyesus[1]; Nathaniel B. Axtell[1]; Ryan T. Kelly[1]; [1]*Brigham Young University, Provo, UT*

ThP 595 **Comprehensive workflow for Automated Cleanup and Sensitive Quantitation of Glucagon-like peptide-1 (GLP-1) Analogs from Plasma**; Xi Qiu[1]; David Wong[2]; Steve Murphy[2]; [1]*Agilent Technologies, Wilmington, DE;* [2]*Agilent Technologies, Santa Clara, CA*

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ThP 597 **Tackle the Challenges of Alpha-Gal Analysis in Therapeutic Proteins**; Yutian Gan[1]; Liz Johnson[1]; Vy Tran[1]; John Briggs[1]; Jeff Zhang[1]; Christian Schoneich[2]; Tomasz Baginski[1]; Feng Yang[1]; [1]*Genentech, Inc., South San Francisco, CA;* [2]*University of Kansas, Lawrence, KS*

ThP 598 **Develop and Validate an LC-MS/MS Assay for Neutralizing Antibody Evaluation of CPG2 in Human Serum to Support Clinical Studies**; Yudong Zhang[1]; Yu Xin[2]; Chenggang Li[1]; Min Meng[1]; Tinghe Yu[2]; Shugang Li[2]; Laixin Wang[1]; Yuhuan Ji[1]; [1]*Resolian, Chongqing, China;* [2]*Chongqing Kerun Biopharm Ltd. Co, Chongqing, China*

ThP 599 **Develop and Validate a Sensitive LC-MS/MS Assay for Accurate Quantitation of CPG2 in Human Serum**; Yuhuan Ji[1]; Yu Xin[2]; Min Yan[1]; Yudong Zhang[1]; Tinghe Yu[2]; Min Meng[1]; Shugang Li[2]; Laixin Wang[1]; [1]*Resolian, Chongqing, China;* [2]*Chongqing Kerun Biopharm Ltd. Co, Chongqing, China*

ThP 600 **Considerations for hybrid LC-MS assays for preclinical ADC bioanalysis**; Yifan Shi[1]; Daniel Anderson[1]; Shengsheng Xu[1]; Wenying Jian[1]; [1]*JOHNSON AND JOHNSON, Spring House, PA*

ThP 601 **Enhancing biotherapeutic characterization with an alternative MS/MS fragmentation technique and improved MS sensitivity**; Haichuan Liu[1]; Zoe Zhang[1]; Elliott Jones[1]; [1]*SCIEX, Redwood City, CA*

ThP 602 **Enhancing mAb Proteoform Detection Sensitivity on an icIEF-UV/MS system leveraging Zeno trap technology**; Scott Mack[1]; Jingwen Ding[1]; Maggie Ostrowski[1]; [1]*SCIEX, Fremont, CA, FREMONT, CA*

ThP 603 **Leveraging LC-MS for Routine Media and Feed Optimization in Continuous CHO Cell Cultures**; Diego Bertaccini; *EMD Serono, Corsier-sur-Vevey, Switzerland*

ThP 604 **Development of Quantitative cGMP Impurity Protein Assays Supporting Diverse Modalities: Discovery Analysis**; Gus H M F Souza[1]; Joshua Pacheco[1]; R. Jeremy Woods[1]; Michael J Nold[1]; [1]*KBI Biopharma Inc., Durham, NC*

ThP 605 **Mass spectrometry-based biodistribution of biotherapeutics: an alternative to radio-biodistribution**; Domenico Ravazza[1]; Sheila Dakhel Plaza[1]; Andrea Galbiati[1]; Andrea Ciamarone[1]; Samuele Cazzamalli[1]; Dario Neri[2, 3]; Ettore Gilardoni[1]; [1]*Philochem AG, Otelfingen, Switzerland;*

[2]*Philogen S.P.A, Sovicelle, Italy; [3]Swiss federal Institute of Technology, Department of Applied Biosciences, Zurich, Switzerland*

ThP 606 **Enhanced Selectivity in Proteomics: A Duel Immunocapture Approach Combining Protein and Peptide Level Enrichment for LC/MS Analysis**; Stephen Cusumano; *Boehringer Ingelheim, Ridgefield, CT*

ThP 607 **Enhanced Detection and Quantification of Host Cell Proteins using Protein Enrichment and LC-MS**; Konrad Winkels[1]; Oskar Knittelfelder[1]; Karin Yeoh[2]; Juliane Weißer[1]; Zuzana Demianova[2]; Guillaume Tremintin[3]; Christian Albers[1]; [1]*Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [2]PreOmics GmbH, Martinsried, Germany; [3]Bruker Scientific LLC, San Jose, California*

ThP 608 **A Robust And Versatile New Peak Detection Workflow to Facilitate the Multi-Attribute Method (MAM) Implementation From Research to Commercialization**; Francois Griaud[1]; Patrick Sascha Merkle[1]; Victor Le[1]; Michelle English[2]; Andrei Starikov[3]; Dominik Mertens[4]; Thomas Pohl[1]; [1]*Novartis Pharma AG, Basel, Switzerland; [2]Genedata Inc., Boston, MA; [3]Genedata GmbH, Munich, Germany; [4]Genedata AG, Basel, Switzerland*

ThP 609 **Assessment of Therapeutic Humanized IgG2 Antibody Concentrations in Human Plasma Using LC/PRM-MS and ELISA: A Comparative Study**; Claudia Gaither[1, 2]; Robert Popp[2]; Pradyumn Maheshwari[2]; Adeline Shanker[2]; Christoph Borchers[3]; [1]*Université de Montréal Saint-Hyacinthe Campus, Saint-Hyacinthe, QC; [2]MRM Proteomics Inc, Montreal, Quebec; [3]McGill University, Montreal, Québec*

ThP 610 **Generic reagent-free 2D-LC/MS platform for highly sensitive preclinical pharmacokinetics assessment of therapeutic proteins**; Yipei Zhang[1]; Mark G Qian[1]; Linlin Dong[1]; [1]*Takeda Pharmaceutical, Cambridge, MA*

ThP 611 **Ensure Selectivity of Signature Peptide of Therapeutic Proteins Analyzed by Immunoaffinity-capture LC-MS/MS Assay from Human Serum**; Yan-Ping Lin[1]; Liyun Zhang[1]; Shuyu Hou[1]; Tian-Sheng Lu[1]; [1]*Medpace, Cincinnati, OH*

ThP 612 **Quantitation of MMAE and the Antibody of the Antibody Drug Conjugate Anetumab-MMAE From Rat Plasma Using HPLC-MS/MS and HPLC-HRMS/MS**; Chad David Christianson[1]; Jason Scott Watts[1]; Jennifer S Zimmer[1]; Balaganesh Kuruba[1]; [1]*Alturas Analytics, Moscow, ID*

ThP 613 **Silk Nanoparticle Protein Corona Delineation for Brain Cancer Therapy**; Sawnaz Shaidani[1, 2]; Mynaja Ferguson[1]; Hom Rijal[1]; Rachel Muriph[1]; Charlotte Jacobus[2]; Shawn Cui[2]; Jason J. Evans[1]; David L Kaplan[2]; [1]*University of Massachusetts Boston, Boston, MA; [2]Tufts University, Medford, MA*

ThP 614 **Enhanced sequence variant and native mass spectrometry analyses of a bispecific antibody using a novel QTOF**; Eric Beil[1]; Michael Poltash[1]; Andy Mahan[1]; Haichuan Liu[2]; Zoe Zhang[2]; Hirsh Nanda[1]; [1]*JOHNSON AND JOHNSON, Spring House, PA; [2]SCIEX, Fremont, CA, FREMONT, CA*

ThP 615 **Proteome-scale molecular characterization of computationally-designed therapeutic proteins**; Catherine Sniezek[1]; Chelsea Lin[2]; Katarina Vlajic[2]; Chris McGann[2]; Green Ahn[3]; Ella Haefner[3]; Nora McNamara-Bordewick[3]; Thomas Schlichthaerle[4]; David Baker[3, 4, 5]; Devin Schweppe[2]; [1]*Genome Sciences, University of Washington, Seattle, WA; [2]University of Washington - Genome Sciences, Seattle, WA; [3]University of Washington - Institute for Protein Design, Seattle, WA; [4]University of Washington - Biochemistry, Seattle, WA; [5]Howard Hughes Medical Institute, University of Washington, Seattle, WA*

ThP 616 **Development and Validation of a Sensitive UHPLC-MS/MS Method for Teduglutide Analysis in Human Plasma on LCMS-8060RX**; Chaitanya Krishna Atmakuri[1]; Avinash Gaikwad[1]; Yogesh Arote[1]; [1]*Shimadzu Application Development Centre, Navi Mumbai, India*

ThP 617 **Detemir Plasma Quantification: Advanced LC-MS/MS Methodology with ShimadzuLC-MS/MS-8060RX**; Yogesh Gorakhnath Arote[1]; Avinash Gaikwad[1]; Chaitanya Krishna Atmakuri[1]; [1]*Shimadzu Application Development Centre, Navi Mumbai, India*

ThP 618 **Protein Centric Analysis with Top-N Quantification: Combining Byos Muti-Protein Quantitation Module and GraphPad Prism**; William Resager[1]; Vahid Golghalyani[1]; Antony Harvey[1]; [1]*Protein Metrics, LLC, Boston, Massachusetts*

ThP 619 **Drug-to-Antibody Ratio Analysis of Antibody Drug Conjugates using HIC-ADC Phenyl and Butyl columns**; Alan Bouskila; *Tosoh Bioscience LLC, King of Prussia, PA*

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ThP 621 **Using online microfluidic chip desalting for native MS and CD-MS**; Brian H Tran[1]; Austin Culberson[2]; Jim Filippini[2]; Mason Chilmonczyk[2]; Michael Thomas Marty[1]; [1]*University of Arizona, Tucson, AZ; [2]Andson Biotech Inc., Atlanta, GA*

ThP 622 **The Adventure of Hunting for a Membrane Protein Standard Expressed in Mammalian Cells for Cryo-EM**; Weijing Liu[1]; Xue Wang[2]; Aaron McBride[3]; Yihu Yang[4]; Qiwei Miao[4]; Feng Wang[4]; Joanna Geddes[3]; Leigh Foster[3]; Mahfuz Rahman[3]; Barbara Kaboord[3]; Rosa Viner[1]; Thomas Moehring[5]; [1]*Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Eindhoven, Netherlands; [3]Thermo Fisher Scientific, Rockford, IL; [4]Biortus USA, Woburn, Massachusetts; [5]Thermo Fisher Scientific, Bremen, Germany*

ThP 623 **Enrichment of transmembrane protein identification in mass spectrometry with the BeatBox sample homogenizer**; Paulo MARCELO[1]; Katrin Hartinger[2]; Zehan HU[2]; Silvia WUERTENBERGER[2]; Quentin ENJALBERT[2]; Julien SAINT-POL[3]; [1]*Plateforme d'Ingénierie Cellulaire & Analyses des Protéines ICAP Université de Picardie Jules Verne, Amiens, France; [2]PreOmics GmbH, Martinsried, Germany; [3]Univ. Artois, UR 2465, Blood-Brain Barrier laboratory (LBHE), Lens, France*

ThP 624 **A high-throughput platform for nanoscale cartography of the native membrane**; Caroline Brown[1, 2]; Snehasish Ghosh[1, 2]; Fiona Weaver[2]; Kallol Gupta[1, 2]; [1]*Department of Cell Biology, Yale School of Medicine, New Haven, CT; [2]Nanobiology Institute, Yale University, West Haven, CT*

ThP 625 **Membrane Proteomic Analysis of Extracellular Vesicles from Different Isolation Techniques**; Alexandria Gallagher[1]; Kenneth B Tomkovich[1]; Reihaneh Safavisohi[1]; [1]*Seton Hall Univeristy, South Orange Village, NJ*

ThP 626 **Using proteomic profiling and targeted proteomics to elucidate the mechanism of clinical phenotypes**; Jianshi Yu[1]; Christina Williams[2]; Nageswara Pilli[2]; Mehari Weldemariam[2]; Paul Trainor[3]; Alexander R Moise[4]; Andrew Wilkie[5]; Maureen A Kane[2]; [1]*University of Maryland at Baltimore, Baltimore, MD; [2]Department of Pharmaceutical Sciences, University of Maryland School of Pharmacy, Baltimore, Baltimore, MD; [3]Stowers Institute for Medical Research, Kansas City, MO; [4]Medical Sciences Division, Northern Ontario School of Medicine University, Sudbury, ON; [5]MRC Weatherall Institute of Molecular Medicine, University of Oxford, Oxford, United Kingdom*

ThP 627 **Analysis of Membrane Proteins under Native Conditions Using Capillary Electrophoresis Coupled to High-Resolution Mass Spectrometry**; Noah Gould[1]; Yunfan Gao[1]; Anne-Lise Marie[1]; Alexander R. Ivanov[1]; [1]*Northeastern University, Boston, MA*

ThP 628 **Multi-platform LC-MS analysis of the toxin arsenal of venomous organisms: cephalopods and cone snails**; Ioana Clotea[1]; Saurabh Attarde[2]; Mande Holford[2]; Beatrix Ueberheide[1]; [1]*NYU Langone Health, New York, NY; [2]CUNY Hunter College, New York, NY*

PROTEOMICS: NEW APPROACHES II
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ThP 629 **Evaluation Of A Novel, Automated Ion Source And Column Assemblies With Integrated Replaceable Emitters For Proteomics Data Acquisition**; Cornelia Boeser[1]; Katherine Walker[1]; Joshua A Silveira[1]; Runsheng Zheng[2]; Alec C Valenta[1]; Eloy R. Wouters[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Germering, Germany*

ThP 630 **Characterization of Key Performance Figures of Merit for PAMAF in Proteomics Applications**; Leonard C Rorrer, III[1]; Liulin Deng[1]; Lauren Royer[1]; Isabel Uribe[1]; Daniel Debord[1]; *[1]MOBILion Systems, Inc., Chadds Ford, PA*

ThP 631 **Comprehensive protein turnover mapping in cynomolgus monkey tissue**; Ghazaleh Yassaghi[1]; Liang Xue[2]; Robert J Seward[1]; Yasaman Jami[1]; Vahid Farrokhi[1]; Hendrik Neubert[1]; *[1]Pfizer Inc., Andover, MA; [2]Pfizer Inc., Cambridge, MA*

ThP 632 **Expanding Nanoparticle Enrichment applications for Deep Plasma Proteome Profiling of Understudied Animals**; Gustavo Diaz[1]; Dorathea Lee[1]; Karla Cureno Hernandez[2]; Margarita Herera-Alonso[2]; Corey D Broeckling[1]; *[1]Analytical Resources Core: Bioanalysis and Omics, Colorado State University, Fort Collins, CO; [2]Chemical and Biological Engineering, School of Advanced Materials Discovery, Colorado State University, Fort Collins, CO*

ThP 633 **Nanoparticle protein corona-assisted sample preparation for proteomics of early-stage zebrafish embryos with remarkably better proteome coverage**; Lance M Thorp[1]; Jose Cibelli[2]; William Poulos[2]; Liangliang Sun[2]; *[1]Michigan State University, East Lansing, MI; [2]Michigan State University, Department of Chemistry, East Lansing, MI*

ThP 634 **Systematic Profiling of N-terminal Acetylation in Extracellular Vesicles by a Novel SP3-based Approach**; Zhuojun Luo[1]; Yanyan Du[1]; William LeFever[2]; Marco Hadisurya[1]; W. Andy Tao[1, 2, 3, 4]; *[1]Department of Biochemistry, Purdue University, West Lafayette, IN; [2]Department of Chemistry, Purdue University, West Lafayette, IN; [3]Tymora Analytical Operations, West Lafayette, IN; [4]Purdue Institute for Cancer Research, West Lafayette, IN*

ThP 635 **PanPTM – towards a streamlined quantification of multiple PTMs from same sample without intermediary purification steps**; Johannes Trefz[1]; Frank Rolfs[1]; Giada Marino[1]; Till Kindel[1]; Dezbah Turnbald-Phillips[1]; Andreas Tebbe[1]; Christoph Schaab[1]; Nagarjuna Nagaraj[1]; *[1]Evotec International GmbH, Munich, Germany*

ThP 636 **Dynamic profiling of the cellular proteome in distinct metabolic environments**; Sui Seng Tee[1]; Yanbao Yu[2]; *[1]University of Maryland School of Medicine, Baltimore, MD; [2]University of Delaware, Newark, DE, DE*

ThP 637 **A Magnetic Bead based Approach for Mass Spec Sample Prep**; Michael Rosenblatt[1]; Zhiyang Zeng[2]; Wenhui Zhou[2]; Marjeta Urh[3]; *[1]Promega Corp, Madison, WI; [2]Promega Corporation, San Luis Obispo, CA; [3]Promega Corporation, Madison, WI*

ThP 638 **Complexome profiling workflow reveals mitochondrial protein interactions**; Marek Vrbacky[1]; Kristyna Cunatova[2, 3]; Tomas Mracek[1]; Rayyan Tariq Khan[1, 4]; Petr Pecina[1]; *[1]Institute of Physiology, Czech Academy of Sciences, Prague, Czech Republic; [2]Department of Biomedical Sciences, University of Padova, Padova, Italy; [3]Veneto Institute of Molecular Medicine, Padova, Italy; [4]Institute of Molecular Genetics, Czech Academy of Sciences, Prague, Czech Republic*

ThP 639 **Unraveling Proteomic Data Analysis Workflows: A Comparative Analysis of Byonic and FragPipe in Peptide Discovery and Spectral Matching**; Juan Pablo Galindo[1]; Casey Powers[1]; Fang Liu[1]; Garvey McKenzie[1]; Ryan Leib[1]; Allis S Chien[1]; *[1]Stanford University Mass Spectrometry, Stanford, CA*

ThP 640 **Using Adaptive Focused Acoustics (AFA) to Access the Protein Corona Around Nanoparticles in Preparation of LC-MS Analysis**; Jason J. Evans[1]; Rachel Muriph[1]; Mynaja Ferguson[1]; Hom Rijal[1]; Sawnaz Shaidani[1, 2]; *[1]University of Massachusetts Boston, Boston, MA; [2]Tufts University, Medford, MA*

ThP 641 **Protein Barcoding and Next-Generation Protein Sequencing™ for Multiplexed Protein Selection, Analysis, and Tracking**; Ajay Vashisht[1]; Mathivanan Chinnaraj[1]; Haidong Huang[1]; Sebastian Hutchinson[1]; Michael Meyer[1]; Douglas Pike[1]; Marco Ribezzi[1]; Sharmin Sultana[1]; Ghada Mansour[1]; Derrek Ocampo[1]; Fengling Ding[1]; Emily Sexton[1]; Meredith Carpenter[1]; Ilya Chorny[1]; John Vieceli[1]; *[1]Quantum-Si, Branford, CT*

ThP 642 **Deep mass spectrometric spatial mapping of murine kidney: The methodological evolution of nanosecond infrared laser-based tissue sampling with LC-MS/MS**; Manuela Moritz[1]; Annika Gerdes[1]; Antonia Gocke[1]; Hartmut Schlüter[1, 2]; Jan Hahn[1, 2, 3]; *[1]Section Mass Spectrometry and Proteomics, Center for Diagnostics, University Medical Center Hamburg-Eppendorf, Hamburg, Germany; [2]University Cancer Center Hamburg (UCCH), University Medical Center Hamburg-Eppendorf, Hamburg, Germany; [3]Mildred Scheel Cancer Center Career Center Hamburg HaTriCS4, University Medical Center Hamburg-Eppendorf, Hamburg, Germany*

ThP 643 **Sensitive, comprehensive, and hi-fidelity cellular proteome analysis using a simplified lysis procedure and nanoparticle-mediated automated sample preparation**; Maedeh Zamani[1]; Adam Brewer[1]; Ambika Sundaresan[1]; Shao-Yung Chen[1]; Xiaoyan Zhao[1]; Ryan Benz[1]; Aaron S. Gajadhar[1]; *[1]Seer, Inc, Redwood City, CA*

ThP 644 **Isolating the surface proteome: Optimizing surface proteomics using a model of ALK fusion positive lung cancer**; Jacelyn Greenwald[1]; Ju Hwan Cho[2]; Elizabeth Shockney[2]; Brian C Searle[3]; David P Carbone[2]; Vicki H Wysocki[1, 4]; *[1]Department of Chemistry and Biochemistry, The Ohio State University, Columbus, Ohio; [2]Division of Medical Oncology and the Pelotonia Institute for Immuno-Oncology, The Ohio State University Comprehensive Cancer Center, Columbus, Ohio; [3]Department of Biomedical Informatics, The Ohio State University, Columbus, Ohio; [4]School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, Georgia*

ThP 645 **Parallel-Accumulation Mobility-Aligned Fragmentation Enables Substantial Improvements to Speed and Sensitivity for QTOF-based Global Proteomics Analysis**; Isabel R. Uribe[1]; Leonard C. Rorrer[1]; Lauren Royer[1]; Liulin Deng[1]; Benjamin Orsburn[2]; Vadim Demichev[3]; Daniel DeBord[1]; *[1]MOBILion Systems, Inc., Chadds Ford, PA; [2]University of Pittsburgh, Pharmacology and Chemical Biology, Pittsburgh, PA; [3]Charité University Medicine, Berlin, Germany*

ThP 646 **Advances in next generation ion sources: Enhancing rigor, reproducibility, and robustness within the shared resource environment**; Daniel Jackson[1]; Alec C Valenta[2]; Casey A. Powers[3]; Fang Liu[3]; Katherine Walker[1]; Garvey McKenzie[3]; Juan Pablo Galindo[3]; Cornelia L Boeser[1]; Joshua A Silveira[1]; Eloy R. Wouters[1]; Ryan D Leib[3]; Allis S Chien[3]; *[1]Thermo Fisher Scientific, 355 River Oaks Pkwy, San Jose, California; [2]Thermo Fisher Scientific, Somerset, NJ; [3]Stanford University Mass Spectrometry, Stanford, CA*

ThP 647 **A Hybrid-DIA Approach for Simultaneous Targeted and Untargeted Analysis Using an Orbitrap Tribrid System**; David Bergen[1]; Jingjing Huang[2]; Rafael D Melani[2]; Vlad Zabrouskov[2]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, San Jose, California*

ThP 648 **Characterization of electron- and laser-based peptide fragmentation techniques using the Orbitrap-Omnitrap hybrid instrument, large datasets and deep learning modelling**; Nikita Levin[1]; Joel Lapin[2]; Cemil Can Saylan[2]; Yana Demyanenko[1, 3]; John Sidda[1, 3]; Mathias Wilhelm[2]; Shabaz Mohammed[1, 4, 5]; *[1]Rosalind Franklin Institute, Didcot, United Kingdom; [2]Technical University of Munich, Freising, Germany; [3]Department of Pharmacology, University of Oxford, Oxford, United Kingdom; [4]Department of*

Biochemistry, University of Oxford, Oxford, United Kingdom; [5]Department of Chemistry, University of Oxford, Oxford, United Kingdom

ThP 649 **Bayesian Confidence Intervals for Absolute Protein Quantification**; Vyas Pujari[1]; Meera Gupta[1]; Chirag Kumar[1]; Donovan Cassidy-Nolan[1]; Arjuna Subramanian[1]; Felix Keber[1]; Martin Wühr[1]; *[1]Princeton University, Princeton, NJ*

ThP 650 **Evaluation of nanoparticle-based Automated Sample Preparation Platform for Host Cell Proteins analysis**; Yue Guo[1]; Biao Shen[1]; Hui Xiao[1]; Ning Li[1]; *[1]Regeneron, Tarrytown, NY*

ThP 651 **Theoretical Investigation of Magnetic Material Usage During On-Bead Peptide Enrichment in Solution Systems**; Jerry Wang[1]; Quangqing Zhang[2]; Jenny Zhang[3]; Jingran Zhang[1]; Vincent Wen[3]; *[1]Agile Bio, Suzhou, China; [2]UCR, RIVERSIDE, CA; [3]Unified Separation Technologies Inc., Newark, DE*

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ThP 652 **Bioinformatics Analysis Of Proteomics Data Generated On Kidney Patients Impacted By Antibody-Mediated Rejection: A Retros**; Jordan Langston[1]; Alec Candib[1]; Manveen Sethi[1]; Joseph Zaia[1]; *[1]Boston University, Boston, MA*

ThP 653 **Changes of the liver proteome during morphine exposure**; Malgorzata Hopcias[1]; Piotr Suder[1]; Jolanta Helena Kotlinska[2]; *[1]AGH University of Krakow, Krakow, Poland; [2]Medical University of Lublin, Lublin, Poland*

ThP 654 **Mass Spectrometry-Driven Insights into Biochemical Shifts Revealing the Impact of Disrupted Meningeal Lymphatic Flow on Brain Function**; Zohaib Khan; *Weill Cornell Medicine, New York, NY*

ThP 655 **Bottom-up Identification of Detergent-Solubilized Transmembrane Proteins in Nervous Tissues and Hemolymph of the American Lobster Homarus americanus**; Zachary P Del Mundo[1]; Thao U Duong[2]; Vu Ngoc Huong Tran[1]; Lauren Fields[2]; Lingjun Li[1, 2]; *[1]School of Pharmacy, University of Wisconsin-Madison, Madison, WI; [2]Department of Chemistry, University of Wisconsin-Madison, Madison, WI*

ThP 656 **Systematic Quantitative Analysis of the Aging Rat Lung enabled by High-Throughput Extracellular Matrix Proteomics**; Anna G Towler[1]; Fei Wang[2]; Liam J Bandura[1]; Yanlong Zhu[3, 4]; Wayne Buck[5]; Lucy Phillips[2]; Lisa Hazelwood[5]; Annette Schwartz[2]; Kuniko Kadoya[6]; Yu Tian[2]; Yupeng He[5]; Ying Ge[1, 3, 4]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [2]AbbVie, Worcester, MA; [3]Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI; [4]Human Proteomics Program, University of Wisconsin-Madison, Madison, WI; [5]AbbVie, North Chicago, IL; [6]AbbVIe, Irvine, CA*

ThP 657 **Azo-Enabled Extracellular Matrix Proteomics for High-throughput Quantitative Analysis of Skin Tissue**; Liam Bandura[1]; Anna G Towler[2]; Andrew J Perciaccante[2]; Yanlong Zhu[3, 4]; Yupeng He[5]; Yu Tian[6]; Kuniko Kadoya[7]; Ying Ge[2, 3, 4]; *[1]Department of Chemistry, University of Wisconsin Madison, Madison, WI; [2]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [3]Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI; [4]Human Proteomics Program, University of Wisconsin-Madison, Madison, WI; [5]AbbVie Discovery Immunology, Chicago, IL; [6]AbbVie: Bioresearch Center: Development Biological Sciences, Worcester, MA; [7]AbbVie: Allergan Aesthetics R&D, Irvine, CA*

ThP 658 **Effects of Synaptamide Receptor GPR110 on the Hippocampal Proteome**; Bill Huang[1]; Mariam Melkumyan[1]; Hee-Yong Kim[1]; *[1]NIAAA/NIH, Rockville, MD*

ThP 659 **Post-mortem Alzheimer's Disease Brains Reveal Tau Interactome Changes in an APOE Genotype-Dependent Manner**; Lauren C Tang[1]; Manon Thierry[2]; Jackeline Ponce[1]; Mitchell Martà-Ariza[1]; Dominique Leitner[1]; Evgeny Kanshin[1]; Manor Askenazi[1, 3]; Eleanor Drummond[1]; Thomas Wisniewski[1]; Beatrix Ueberheide[1]; *[1]NYU Langone Health, New York, NY; [2]Paris Brain Institute, Paris, France; [3]Biomedical Hosting LLC, Arlington, MA*

ThP 660 **Evaluation of recent protein extraction methods on bone**; Timothy Cleland[1]; Laura Bergemann[2]; *[1]Smithsonian Institution, Suitland, MD; [2]New York University, New York, NY*

ThP 661 **Enhanced High-Sensitivity Spatial Tissue Proteomics for Pancreatic Cancer Progression Analysis**; Jongmin Woo[1]; Zhenyu Sun[1]; Yingwei Hu[1]; Decapite Christine[2]; Smith Katelyn[2]; Singhi Aatur[2]; Brand Randall[2]; Kay Li[1]; Ralph Hruban[1]; Hui Zhang[1]; *[1]Johns Hopkins University, Department of Pathology, Baltimore, Maryland; [2]University of Pittsburgh, Pittsburgh, PA*

ThP 662 **Mitochondrial Proteome Alterations in Adipose Tissue Thermogenesis and Cardiorenal Dysfunction in a High-Fat Diet-Induced Prediabetic Rat Model**; Judith Ijeoma Nwaiwu[1]; Monica S Makkar[2, 3]; Favour Chukwubueze[1]; Daramola Oluwatosin[1]; Esther O. Oji[1]; Odunayo O. Oluokun[1]; Ahmed El-Yazbi[4, 5]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX; [2]The Research and Innovation Hub, Alamein International University, Alamein, Egypt; [3]Department of Pharmaceutical Biochemistry, Faculty of Pharmacy, Alexandria University, Alexandria, Egypt; [4]Department of Pharmaceutical Biochemistry, Faculty of Pharmacy, Alexandria University, Egypt, Alexandria, Egypt; [5]Department of Pharmacology and Toxicology, Faculty of Pharmacy, Alexandria University, Alexandria, Egypt*

ThP 663 **Scaling-up low input spatial proteomics using Evosep Whisper Zoom on the timsTOF Ultra 2**; Melissa Klingeberg[1, 2]; Christoph Krisp[3, 4]; Anjali Seth[5]; Dorte Bekker-Jensen[6]; Ole Bjeld Hørning[6]; Nicolai Bache[6]; Gary Kruppa[7]; Fabian Coscia[1, 4]; *[1]Max Delbrück Center – Berlin Institute for Medical Systems Biology, Berlin, Germany; [2]Humboldt University Berlin, Berlin, Germany; [3]Bruker Daltonics GmbH & Co.KG, Bremen, Germany; [4]MDC-Bruker Center of Excellence for Single Cell Omics, Max Delbrück Center – Berlin Institute for Medical Systems Biology, Berlin, Germany; [5]Cellenion, Lyon, France; [6]Evosep Biosystems, Odense, Denmark; [7]Bruker s.r.o, Brno, Czech Republic*

ThP 664 **A DIA-MS based proteome map of the porcine heart**; Christof Lenz[1, 2, 3]; Lisa Neuenroth[1]; Brian Foo[1, 3]; Andrea Bähr[4]; Nikolai Klymiuk[4]; Stephan E Lehnart[1, 3]; Henning Urlaub[1, 2, 3]; *[1]University Medical Center Goettingen, Goettingen, Germany; [2]Max Planck Institute for Multidisciplinary Sciences, Goettingen, Germany; [3]Cluster of Excellence "Multiscale Bioimaging: from Molecular Machines to Networks of Excitable Cells" (MBExC), Goettingen, Germany; [4]Technical University of Munich, Munich, Germany*

ThP 665 **Proteome Changes in Rat Hippocampus and Prefrontal Cortex Tissue Following Glyphosate-Based Herbicide Exposure**; Abderrahmane Koraich[1]; Cristian D. Gutierrez-Reyes[1]; Jesús Chávez-Reyes[2]; Joy Solomon[3]; Mojibola Fowowe[1]; Moyinoluwa Adeniyi[1]; Yehia Mechref[1]; Bruno A Marichal-Cancino[2]; *[1]Texas Tech University, Lubbock,, TX; [2]Universidad Autonoma de Aguascalientes, Aguascalientes, Mexico; [3]Texas Tech University, Lubbock, TX*

ThP 666 **Scalable Proteomics of the Vertebrate Organizer: From Tissue to Cells**; Md Tarikul Islam[1]; Peter Nemes[1]; *[1]Department of Chemistry & Biochemistry, University of Maryland, College Park, 8051 Regents Drive, MD 20742*

ThP 667 **Identification of Canonical Pathways and Protein Interaction Networks Affected by Gonadectomy in a Glaucomatous Rat Model Through Mass Spectrometry-Based Proteomics**; Ammar Kapic[1]; Khadiza Zaman[1]; Vien Nguyen[1]; George C. Neagu[1]; Katalin Prokai-Tatrai[1]; Laszlo Prokai[1]; *[1]Department of Pharmacology & Neuroscience, University of North Texas Health Science Center, Fort Worth, TX*

ThP 668 **Spatially resolved, quantitative proteomics from laser capture microdissection for in vivo CRISPR screens in**

mouse cancer models; Jiaxi Peng[1, 2]; Brendon Seale[1]; Shifei Wu[1, 2]; Cassandra Wong[1]; Bhavisha Rathod[1]; Daniel Schramek[1, 2]; Anne-Claude Gingras[1, 2]; *[1]Lunenfeld-Tanenbaum Research Institute, Toronto, ON; [2]University of Toronto, Toronto, ON*

ThP 669 **AI-Guided precision Tumor Enrichment for efficient Histo-Proteomics**; Sudhanshu Abhishek[1]; David J Clark[2]; Anqi Tu[2]; Shichen Shen[2]; Andrew Chambers[2]; Steve Sweet[2]; Yeoun Jin Kim[2]; David Chain[2]; *[1]AstraZeneca, Gaithersburg, MD; [2]AstraZeneca, Gaithersburg, Maryland*

ThP 670 **Charting the Proteome Profiling of Human Brain Aging by Mass Spec**; Ernst Heinz V Pulido[1]; Emma Lundberg[2]; *[1]Stanford University, STANFORD, CA; [2]Stanford University, Stanford, CA*

ThP 671 **Proteomics-Based Identification and Validation of Biological Networks Impacted by Environmental Estrogens in the Freshwater Crustacean Hyalella azteca**; Marcel L Prokai[1]; Khadiza Zaman[2]; Vladimir Shulaev[1]; *[1]University of North Texas, Denton, TX; [2]University of North Texas Health Science Center, Fort Worth, TX*

ThP 672 **Nanoscale in situ extraction and digestion of FFPE.**; Chengqing Qu[1]; Francis Scott Heinemann[2]; Albert Siryaporn[3]; Paul Gershon[3]; *[1]Center for Engineering Mechanobiology, Washington University, St. Louis, MO; [2]Hoag Memorial Hospital Presbyterian, Newport Beach, CA; [3]UC-Irvine, Irvine, CA*

ThP 673 **In-cell processing and FAIMS-DIA-LC-MS/MS enable rapid and deep proteome analysis of single dorsal root ganglion**; Siyang Liao[1]; Yanbao Yu[1]; Austin Keeler[1]; *[1]University of Delaware, Newark, DE*

ThP 674 **Addressing cerebellum tissue heterogeneity with spatial proteomics at low input**; Chris Hsu[1]; Amber Nolan[1]; Christine C. Wu[1]; C. Dirk Keene[1]; Michael J MacCoss[1]; *[1]University of Washington, Seattle, WA*

ThP 675 **Overcoming Contamination Challenges in Tryptic Digests of Rat Placenta**; Brynn Nelson[1]; Mark Kristal[2]; Alexis Thompson[2]; Jean DiPirro[3]; Troy D Wood[4]; *[1]University at Buffalo, Amherst, NY; [2]Department of Psychology, University at Buffalo, Amherst, NY; [3]Department of Psychology, Buffalo State University, Buffalo, NY; [4]Department of Chemistry, University at Buffalo, Amherst, NY*

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ThP 676 **Optimized Single-Cell Proteomics Workflow for small cells analysis: Exploration of B lymphocyte subpopulations**; Pauline Perdu-Alloy[1, 2]; Charline Keller[1, 2]; Luc Matthieu Fornecker[1, 2, 3]; Delphine Rolland[1, 2, 4]; Christine Carapito[1, 2]; *[1]LSMBO, IPHC, CNRS, Strasbourg, France; [2]Infrastructure Nationale de Protéomique ProFI, Strasbourg, France; [3]Institut de Cancérologie Strasbourg Europe (ICANS), Strasbourg, France; [4]Hôpitaux Universitaire, Strasbourg, France*

ThP 677 **Benchmarking Performance in Single Cell Lipidomics by Low-Flow Liquid Chromatography Mass Spectrometry coupled with Flow Cytometry**; Ying Liu[1]; Alexandria R Van Grouw[2]; Erich I Williams[3]; Jared J Lutes[3]; Samuel G Moore[1]; Rahul Deshphande[4]; Facundo M Fernández[1, 2]; David A Gaul[1, 2]; *[1]Systems Mass Spectrometry Core, Petit Institute of Bioengineering and Bioscience, Georgia Institute of Technology, Atlanta, GA; [2]School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA; [3]Cellular Analysis and Cytometry Core, Petit Institute of Bioengineering and Bioscience, Georgia Institute of Technology, Atlanta, GA; [4]ThermoFisher Scientific, San Jose, CA*

ThP 678 **High-throughput single-cell metabolomics reveals distinct metabolic states of modulated CD4+ T cells**; Luisa Abreu[1, 2, 3]; Arne Müller[2]; Alexander Mattausch[2]; Theodore Alexandrov[1, 2, 4, 5]; *[1]Department of Pharmacology, University of California San Diego, San Diego, CA; [2]Molecular Systems Biology Unit, European Molecular Biology Laboratory, Heidelberg, Germany; [3]Collaboration for joint PhD degree between EMBL and Heidelberg University, Faculty of Biosciences, Heidelberg, Germany; [4]Department of Bioengineering, University of California San Diego, San Diego, CA; [5]DeepCyte Inc., San Diego, CA*

ThP 679 **Deep learning-assisted Single-Cell Data Processing Platform for Metabolite Profiling**; Felix Friedrich[1]; Cátia Marques[1]; Ingela Lanekoff[1]; *[1]Uppsala University, Uppsala, Sweden*

ThP 680 **Advancing Low Flow LC/MS for Single Cell Proteomics with Variable Flow and 50 cm Microfabricated Pillar Array Columns**; Jeff Op De Beeck[1]; Marcel Bühler[2]; Emin Araftpoor[2]; Julia Kraegenbring[3]; Bernard Delanghe[3]; Kris Gevaert[2]; Paul Jacobs[1]; *[1]Thermo Fisher Scientific, Ghent, Belgium; [2]UGent Gevaert Lab, Ghent, Belgium; [3]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

ThP 681 **Single Cell Spatial-Omics from Culture Using DESI-MS: Static imaging vs Dynamic mapping**; Emrys A Jones[1]; Alexandra Lee[1]; Mujeebatu Kadiri-Asamoah[1]; Michael Morris[1]; *[1]Waters Corporation, Wilmslow, United Kingdom*

ThP 682 **Large Panel Targeted Proteomics for Low-amount Samples Using an Enhanced LC/MS/MS Platform**; Linfeng Wu[1]; Daojing Wang[2]; PoYing Yeh[2]; Anding Fan[1]; *[1]Agilent Technologies, Santa Clara, CA; [2]Newomics Inc., Berkeley, CA*

ThP 683 **Accelerating Discovery: High-Throughput Single-Cell Proteomics with Rapid Analysis and Deep Protein Coverage**; Michael Krawitzky[1]; Jose Luis Marin Rubio[2, 3]; Megan S. Lim[2, 3]; Kojo S.J. Elenitoba-Johnson[2, 3]; *[1]Bruker Scientific LLC, Billerica, MA; [2]Human Oncology Pathogenesis Program, Memorial Sloan Kettering Cancer Center, New York, NY; [3]Department of Pathology and Laboratory Medicine, Memorial Sloan Kettering Cancer Center, New York, NY*

ThP 684 **Enabling scalable single-cell proteomics by utilizing the unique analytical properties of the Evotip Pure and Whisper Zoom methods**; Laurent Rieux[1]; Ole B. Hørning[1]; Nicolai Bache[1]; Dorte Bekker-Jensen[1]; *[1]Evosep, Odense, Denmark*

ThP 685 **Single Cell Fatty Acid Profiling in Cancer cells using Multiple Reaction Monitoring (MRM)-profiling and Charge Switch Derivatization**; Pooja Saklani[1]; Caitlin Randolph[1]; Harshit Arora[2]; Brianna Corman[3]; Connor H Beveridge[3]; Gaurav Chopra[3, 4, 5, 6, 7, 8, 9]; *[1]Purdue University, West Lafayette, IN; [2]Purdue University, West lafayette, Indiana; [3]Purdue Univeristy, West Lafayette, IN; [4]Department of Computer Science, Purdue University, West Lafayette, IN; [5]Purdue Institute for Drug Discovery, West Lafayette, IN; [6]Regenstrief Center for Healthcare Engineering, West Lafayette, IN; [7]Purdue Institute for Cancer Research, Purdue University, West Lafayette, IN; [8]Purdue Institute for Inflammation, Immunology, and Infectious Disease, West Lafayette, IN; [9]Purdue Institute for Integrative Neuroscience, West Lafayette, IN*

ThP 686 **Integrating spatial multiomics at 1 µm resolution in the same tissue to untangle the follicle stem cell niche using Dual-SIMS**; Hua Tian; *University of Pittsburgh, Pittsburgh, PA*

ThP 687 **HT SpaceM+IF: High-throughput single-cell metabolomics and multiplex protein imaging**; Sharath Krishnakumar Menon[1, 2, 3]; Andreas Eisenbarth[2]; Gargey B. Yagnik[4]; Kenneth J. Rothschild[4, 5]; Mark Lim[4]; Theodore Alexandrov[1, 6, 7]; *[1]Department of Pharmacology, University of California San Diego, San Diego, CA; [2]Molecular Systems Biology Unit, European Molecular Biology Laboratory, Heidelberg, Germany; [3]Collaboration for joint PhD degree between EMBL and Heidelberg University, Faculty of Biosciences, Heidelberg, Germany, Heidelberg, Germany; [4]AmberGen Inc., Billerica, MA; [5]Department of Physics and Photonics Center, Boston University, Boston, MA; [6]Department of Bioengineering, University of California San Diego, San Diego, CA; [7]DeepCyte Inc., San Diego, CA*

ThP 688 **Optimized High-Throughput Single-Cell Proteomics for Revealing Cellular Heterogeneity in Circulating Immune**

Cells Using TMT 32-Plex nanoPOTS and Dual-Column NanoLC system; Yumi Kwon[1]; James M. Fulcher[2]; Andrey V. Liyu[2]; Sarai M. Williams[2]; Daniel J. Orton[3]; Fengchao Yu[4]; Rashmi Kumar[2]; Ronald J. Moore[3]; Alexey I. Nesvizhskii[4, 5]; Ljiljana Pasa-Tolic[1]; *[1]Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA; [2]Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, Washington 99354; [3]Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA; [4]Department of Pathology, University of Michigan, Ann Arbor, MI; [5]Department of Computational Medicine and Bioinformatics, University of Michigan, Ann Arbor, MI*

ThP 689 **Establishing plasma cell clonality using single cell proteomics**; Dong-Gi Mun[1]; Joel-Sean Hsu[1]; Neha Joshi[2]; Kiran Kumar Mangalaparthi[1]; Richard K. Kandasamy[1, 3]; Wilson I. Gonsalves[4]; Shaji K. Kumar[4]; Leif Bergsagel[5]; Rafael Fonseca[5]; Akhilesh Pandey[1]; *[1]Department of Laboratory Medicine and Pathology, Mayo Clinic, Rochester, MN; [2]Mayo Clinic, Rochester, MN; [3]Department of Quantitative Health Sciences, Mayo Clinic, Rochester, MN 55905, USA., ROCHESTER, MINNESOTA; [4]Division of Hematology, Mayo Clinic, Rochester, MN, 55905, USA, Rochester, MINNESOTA; [5]Division of Hematology and Medical Oncology, Mayo Clinic, Phoenix, AZ 85054, USA, Phoenix, Arizona*

ThP 690 **Porous layer open-tubular (PLOT) columns in pressure- and electric field-driven nano-flow separations enhance proteomic and multi-omic analysis of limited samples**; Michal Gregus[1]; Yunfan Gao[1]; Anne-Lise I Marie[1]; Alexander R. Ivanov[1]; *[1]Northeastern University, Boston, MA*

ThP 691 **Multiplexed quantitation of post-translational modified peptides from single cells using triggered MS/MS combined with super heavy tandem mass tags**; Dong-Gi Mun[1]; Hiroshi Nishida[1]; Firdous A Bhat[1]; Anu Jain[1]; Akhilesh Pandey[1]; *[1]Mayo Clinic, Rochester, MN*

ThP 692 **Single-Cell Mass Spectrometry of Drosophila Ovaries Reveals Proteomic Signatures of Egg Development**; Merin M Rixen[1]; Margot Quinlan[1]; Rachel R. Loo[1]; Joseph A. Loo[1]; *[1]UCLA, Los Angeles, CA*

ThP 693 **Single-cell proteomic analysis of human brain organoids**; Reynaldo Magalhães Melo[1]; Natalia Chermont Dos Santos Moreira[2]; Daniela Turaca[2]; Lauro Thiago Turaca[2]; Luisa Bulcão Vieira Coelho[2]; Blake Tsu[2]; Alysson R. Muotri[2]; Aline M. A. Martins[1, 2]; John R. Yates[1]; *[1]Integrative Structural and Computational Biology Department, The Scripps Research Institute, La Jolla, CA; [2]Integrated Space Stem Cell Orbital Research (ISSCOR) Center / UCSD, San Diego, CA*

ThP 694 **HT SpaceM: Enhancing sample throughput and small molecule detection in Single-Cell Metabolomics**; Jeany Delafiori[1, 2]; Mohammed Shahraz[1, 2]; Andreas Eisenbarth[2]; Volker Hilsenstein[2]; Bernhard Drotleff[2]; Alberto Bailoni[2]; Bishoy Wadie[1, 2, 3]; Måns Ekelöf[2]; Alexander Mattausch[2]; Theodore Alexandrov[1, 2, 4]; *[1]University of California San Diego, San Diego, CA; [2]European Molecular Biology Laboratory, Heidelberg, Germany; [3]Heidelberg University, Heidelberg, Germany; [4]DeepCyte Inc., San Diego, CA*

ThP 695 **Constructing Quantitative Proteomic Panoramas in Single Cells of the Developing Human Brain**; Lihua Jiang[1]; Tianzhi Wu[2]; Ruiqi Jian[1]; Tiffany T Trinh[1]; Michael Snyder[1]; Jingjing Li[2]; *[1]Department of Genetics, Stanford University, Stanford, CA; [2]Department of Neurology, University of California, San Francisco, CA*

ThP 696 **Single Cell Proteomics of U2OS FUCCI Cells to Elucidate Cell Cycle-Dependent Dynamics**; Rong Chi[1]; Marina Brogley[1]; Emma Lundberg[1, 2, 3, 4]; *[1]Department of Bioengineering, Stanford University, Stanford, CA; [2]Department of Pathology, Stanford University, Stanford, CA; [3]Science for Life Laboratory, School of Engineering Sciences in Chemistry, Biotechnology and Health, KTH - Royal Institute of Technology, Stockholm, Sweden; [4]Chan Zuckerberg Biohub, San Francisco, CA*

ThP 697 **Development of a single-cell proteomic platform using LCM-based iCAB method**; Seok-Young Kim[1]; Taekyung Ryu[1]; Chan Hyun Na[1]; *[1]Department of Neurology, Institute of Cell Engineering, Johns Hopkin University School of Medicine, Baltimore, 21205*

ThP 698 **Enhanced sensitivity of a modified Orbitrap Astral mass spectrometer for deeper proteome coverage in single-cell proteomics applications**; Tabiwang N. Arrey[1]; Julia Kraegenbring[1]; Anjali Seth[2]; Bernard Delanghe[1]; Eduard Denisov[1]; Johannes Petzoldt[1]; Hamish Stewart[1]; Eugen Damoc[1]; *[1]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [2]Cellenion, Lyon, France*

SMALL MOLECULES: QUALITATIVE AND QUANTITATIVE ANALYSIS

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ThP 699 **A simple, sensitive and rapid LC-MS/MS method for simultaneous quantitation of Lurasidone and its three active metabolites in humanserum**; Shoko Ochiai[1]; Lei Shi[1]; Amber LaFayette[2]; Hiroyuki Nishikawa[1]; Yu-Luan Chen[1]; *[1]Sumitomo Pharma America, Inc., Marlborough, MA; [2]Labcorp, Madison, Wi*

ThP 700 **Simultaneous quantification of apalutamide and its N-desmethyl metabolite in human plasma by LC-MS/MS and a clinical application**; Yu-Luan Chen[1]; Sarah Lee[1]; Haoyu Wang[2]; Yuan-Shek Chen[2]; Solomiya Gumenyuk[1]; Hiroyuki Nishikawa[1]; *[1]Sumitomo Pharma America, Inc., Marlborough, MA; [2]QPS, LLC, Newark, DE*

ThP 701 **Comparison of Deuterium Incorporation Calculation Methods for Small Molecules**; Jay S Bhanot[1]; Corianne Randstrom[1]; Jessica Hoskins[1]; Cassie Yang[1]; Christopher Jones[1]; Russell Hertzler[1]; *[1]AbbVie, Inc., North Chicago, IL*

ThP 702 **Adaptation of two-dimensional correlation spectroscopy to mass spectrometry enables fragment/precursor identification from DART-MS and GC-MS of mixtures and extraterrestrial materials**; Elly Breves[1]; Garon H. Lowke[2]; Andrew Steele[3]; Robert B. Cody[4]; Caroline Freissinet[5]; Jacob T. Shelley[1]; *[1]Rensselaer Polytechnic Institute, Troy, NY; [2]Wingate University, Wingate, NC; [3]Carnegie Institution for Science, Washington, DC; [4]JEOL USA, Inc., Peabody, MA; [5]CNRS / LATMOS, Guyancourt, France*

ThP 703 **Investigation of Carryover in the Quantitation of Sunitinib and N-Desethylsunitinib in Human Plasma**; Moo-Young Kim[1]; Tyler D'Spain[1]; Ekram Hossain[1]; Melissa Mofikoya[1]; *[1]PPD, Middleton, WI*

ThP 704 **Quantitative Measurement of Ipratropium in Human Plasma using Column Switching and Tandem Mass Spectrometry**; Jingduan Chi[1]; Melissa Mofikoya[1]; *[1]Thermo Fisher Scientific Inc, Madison, WI*

ThP 705 **Optimizing the SQUAD Method Execution on Orbitrap Tribrid MS to Improve Acquisition Speed While Maintaining Mass Accuracy**; Xiao Wang[1]; Bashar Amer[1]; Brandon Bills[1]; Graeme McAlister[1]; Mike Senko[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

ThP 706 **CE-MS Analysis of Neurotransmitters in the Brain of Mice with Prenatal Morphine Exposure**; Chen Huang[1]; Elena V Romanova[2]; Jonathan Sweedler[2]; Mindy Reichelt[3]; Anna G Makela[4]; Kyle Cosby[4]; Brittany Smith[4]; *[1]University of Illinois at Urbana Champaign, Urbana, IL; [2]Department of Chemistry, University of Illinois Urbana-Champaign, Urbana, IL; [3]The Next Step Collaborative, Cincinnati, OH; [4]Department of Psychological Science at Northern Kentucky University, Highland Heights, KY*

ThP 707 **Development and Validation of a Simple and Rugged LC-MS/MS Method to Simultaneously Measure Carbidopa and Moxifloxacin in Human Plasma**; Nick Peng[1]; Jayce Brown[1]; Ardeshir Khadang[1]; *[1]Axis Clinicals, Dilworth, MN*

ThP 708 **A Sensitive LC-MS/MS Method for the Quantification of the Antiretroviral Islatravir in Rabbit Plasma**; Amanda P Schauer[1]; Craig Sykes[1]; Mackenzie L Cottrell[1]; Angela DM Kashuba[1]; *[1]University of North Carolina Chapel Hill, Chapel Hill, NC*

ThP 709 **Using chiral derivatization, LC-HRMS, and SFC-MS/MS to mitigate the bioanalytical selectivity issue caused by the presence of isobaric interferences**; Kasie Fang; *GSK, Collegeville, PA*

ThP 710 **An Ultra-sensitive and Selective Method for Quantification of Monomethyl auristatin E (MMAE) as ADC Payload in Human Plasma UsingHPLC-MS/MS**; Yan Luo[1]; Danyang Wang[1]; Hongfang Xue[1]; Min Meng[1]; Aihua Liu[1]; [1]*Resolian, Malvern, PA*

ThP 711 **Structure Elucidation of Xenobiotic Metabolites Using SWATH and Isotope Labels**; Suresh Annangudi[1]; Scott Greenwalt[1]; Jeffrey Simpson[1]; Heather Platt[1]; Ben Savage[1]; [1]*Corteva Agriscience, Indianapolis, IN*

ThP 712 **High-Throughput Quantitation of Carboxylate Enantiomers via a Novel Carboxyl-Reactive Isobaric Chemical Probe**; Yajing Lu[1]; Zicong Wang[1]; Lingjun Li[1]; [1]*University of Wisconsin - Madison, Madison, WI*

ThP 713 **Quantification of Dexmedetomidine in Equine Plasma and Red Blood Cells**; Jaclyn R. Missanelli[1, 2]; Youwen You[1, 2]; Rachel M. Proctor[1, 2]; Monica Midon[1]; Mary A. Robinson[1, 2]; [1]*University of Pennsylvania School of Veterinary Medicine, Kennett Square, PA;* [2]*Pennsylvania Equine Toxicology and Research Laboratory, West Chester, PA*

ThP 714 **Identification and sensitive quantitation of N-nitroso N-desmethyl orphenadrine impurity in orphenadrine citrate API**; Greg Roman[1]; Lakshmanan Deenadayalan[2]; Sashank Pillai[2]; Rahul Baghla[3]; Elliott Jones[3]; Eshani Galermo[3]; [1]*Sciex, Framingham, MA;* [2]*SCIEX - India, Bangalore, India;* [3]*Sciex, Redwood City, CA*

ThP 715 **Sensitive quantitation of N-nitroso N-desmethyl chloropyramine in chloropyramine hydrochloride API**; Paul Norris[1]; Sujata Rajan[2]; Sashank Pillai[2]; Rahul Baghla[3]; Elliott Jones[3]; Eshani Galermo[3]; [1]*Sciex, Framingham, MA;* [2]*SCIEX - India, Bangalore, India;* [3]*Sciex, Redwood City, CA*

ThP 716 **A sensitive method for the quantitation of perfluoroalkyl and poly-fluoroalkyl substances (PFAS) in a fluoro-pharmaceutical active pharmaceutical (f-API) ingredient**; Kevin He[1]; Ebru Selen[1]; Rahul Baghla[1]; [1]*Sciex, Redwood City, CA*

ThP 717 **Transforming quantitative sensitivity for small molecule analysis using a high-resolution workflow**; Elliott Jones[1]; Ebru Selen[1]; Rahul Baghla[1]; Jason Causon[2]; Eshani Galermo[1]; [1]*Sciex, Redwood City, CA;* [2]*SCIEX, Concord, ON*

ThP 718 **A Simple, High Throughput, and Sensitive Method for Quantification of Acalabrutinib and ACP-5862 in Human Plasma UsingHPLC-MS/MS**; Hongfang Xue[1]; Bo Yuan[1]; Jeff Cichalski[1]; Min Meng[1]; Aihua Liu[1]; [1]*Resolian, Malvern, PA*

ThP 719 **Evaluating Bond Dissociation Energies of Small Organic Molecules Using a Triple Quadrupole Mass Spectrometer**; Emilio S Rivera[1]; Philip Mach[1]; Wilton J. M. Kort-Kamp[2]; Ivana Gonzales[3]; Christopher Snyder[4]; [1]*Biochemistry and Biotechnology Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM;* [2]*Physics of Condensed Matter and Complex Systems Group (T-4), Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM;* [3]*Physics and Chemistry of Materals Group (T-1), Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM;* [4]*High Explosives Science and Technology Group, Los Alamos National Laboratory, Los Alamos, NM*

ThP 720 **Benefit of ultra-violet photodissociation (UVPD) in the analysis of structural isomers**; Yves Le Blanc[1]; Mircea Guna[2]; Eva Duchoslav[2]; [1]*SCIEX, Concord, On, ON;* [2]*SCIEX, Concord, ontario*

ThP 721 **Exploring Chemical Transformations in Ginger Tea through Ion Trap Liquid Chromatography-Mass Spectrometry**; Abide Mo[1, 2, 3]; Adnan A Kadi[2]; A F M Motiur Rahman[2]; [1]*Bangladesh International School English Section, Riyadh, Saudi Arabia;* [2]*King Saud University, Riyadh, Saudi Arabia;* [3]*Department of Biochemistry, University of Oxford, Oxford, United Kingdom*

ThP 722 **A Comparison Between LC-MS/MS and Microchip CE-MS/MS for Monitoring HIV Antiviral Adherence in Dried Blood Spots**; Craig Sykes[1]; Amanda P Schauer[1]; J. Scott Mellors[2]; J. Will Thompson[2]; [1]*UNC Chapel Hill, Chapel Hill, NC;* [2]*908 Devices, Inc., Morrisville, NC*

ThP 723 **Detection of N-nitrosamines and O-, S-, and C-nitroso compounds by using MS2 and MS3 experiments based on CAD**; Annika M Little[1]; Tuong V Nguyen[1]; David Toba Veloza[1]; Jack C Howard[1]; Daria T Tsoneva[1]; Hilkka I Kentämaa[1]; [1]*Purdue University, West Lafayette, IN*

ThP 724 **Simultaneous On-line Sample Pre-treatment and LC-MS/MS Analysis for Rapid and Sensitive Quantification of Eleven Cannabinoids in Biological Fluid**; Liangqiao Bian; *SCAAC, UT Arlington, Arlington, TX*

ThP 725 **Development of High Sensitivity LC/MS/MS Method With Formation of Hydrazone Derivative**; Xiaodong Zhu[1]; Jingguo Huo[1]; Steven Hoehne[1]; Xiaomei Bian[1]; Leimin Fan[1]; [1]*Worldwide Clinical Trials, Austin, TX*

ThP 726 **Analysis of N Nitroso Nebivolol, Nitroso Drug Substance Related impurity in Nebivolol 20 mg tablet formulation using LC-MS/MS system**; Prasanth Joseph[1]; Saikat Bhattacharya[1]; Vivek Dhyani[1]; Saikat Banerjee[1]; [1]*Agilent Technologies, BENGALURU, India*

ThP 727 **Analysis of carcinogenic Nitrosamines at ultra-trace levels among Terbinafine using LC/TQ**; Vikrant Goel[1]; Vivek Dhyani[2]; Saikat Banerjee[3]; [1]*Agilent Technologies, Gurgaon, India;* [2]*Agilent Technologies, Mumbai, India;* [3]*Agilent Technologies, Hyderabad, India*

ThP 728 **Quantitative analysis of 15 traditional nitrosamines in thalassemia drug at ultra-trace levels among using LC/TQ**; Vikrant Goel[1]; Vivek Dhyani[2]; Saikat Banerjee[3]; [1]*Agilent Technologies, Gurgaon, India;* [2]*Agilent Technologies, Mumbai, India;* [3]*Agilent Technologies, Hyderabad, India*

ThP 729 **Development of Quantification Method for Indomethacin and Indomethacin Glucuronide in mice gut samples via LC-MS**; Lazaro Antonio Toledo[1]; Aadra Bhatt[2, 3]; Brandie M Ehrmann[2]; [1]*UNC, Chapell Hill, NC;* [2]*University of North Carolina at Chapel Hill, Chapel Hill, NC;* [3]*Division of Gastroenterology and Hepatology, Department of Medicine and the Center for Gastrointestinal Biology and Disease, School of Medicine, Chapell Hill, NC*

ThP 730 **Validation of NAD+ measurements for human clinical studies: multi-method inter-laboratory standardization**; Jimmy P. XU[1]; Hennrique Taborda Ribas[1]; Nathaniel W. Snyder[2]; Clementina Mesaros[1]; [1]*University of Pennsylvania, Perelman School of Medicine, Philadelphia, PA;* [2]*Lewis Katz School of Medicine, Temple University, Philadelphia, PA*

ThP 731 **Extending the limits of linearity in Electrospray Ionization Mass Spectrometry by nanobubble addition**; George Joseph[1]; Bincy Binny[1]; Andre R Venter[1]; [1]*Western Michigan University, Kalamazoo, MI*

ThP 732 **LC-MS screening platforms to identify and quantify endogenous nucleoside ligands bound with high specificity to Bmp family transporters**; Ludmila Alexandrova[1]; Ryan D Leib[1]; Allis S Chien[1]; Qianqiao Liu[2]; Naima G. Sharaf[2]; [1]*Stanford University Mass Spectrometry, Stanford, CA;* [2]*Biology, Stanford University, Stanford, CA*

ThP 733 **An ultrasensitive LC-MS/MS method to monitor epigenetic alterations involving 5mdC and 5hmdC from limited number of TET2-mutation bearing cells**; Jinyong Kim[1]; Jisha Chandran[1]; Seul Kee Byeon[1]; Rahul R. Deshpande[2]; Susan S Bird[2]; Akhilesh Pandey[1]; [1]*Mayo Clinic, Rochester, MN;* [2]*ThermoFisher Scientific, San Jose, CA*

ThP 734 **Enhanced structural elucidation of conjugated xanthohumol metabolites with electron activated dissociation**; Jaewoo Choi[1]; Liping Yang[1]; Paige Jamieson[2, 3]; Claudia S. Maier[1]; Jan F. Stevens[2, 4]; [1]*Department of Chemistry, Oregon State University, Corvallis, OR;* [2]*Linus Pauling Institute, Oregon State University, Corvallis, OR;* [3]*College of Health, Oregon State University, Corvallis, OR;* [4]*Department of Pharmaceutical Sciences, Oregon State University, Corvallis, OR*

ThP 735 **Comparing Performance of Triple Quadrupole and Orbitrap Mass Spectrometers to Quantify Nitrosamines**

in Pharmaceuticals; Eric M Brown[1]; Tim Marzan[1]; Dan Berger[2]; Ee-Sunn Chia[2]; Obinna Ugwu-Oju[2]; Alicia Hoover[1]; Rachel Dunn[1]; Jingyue Yang[1]; *[1]U.S. Food and Drug Administration, St. Louis, MO; [2]U.S. Food and Drug Administration, Silver Spring, MD*

ThP 736 **Impact of In-Source Fragmentation on LC-HRMS Quantitation of Nitrosamine Drug Substance-Related Impurities in Pharmaceuticals**; Chioma Akor[1, 2]; Harmeet Chohan[1]; Md Abu Sufian[1]; Yen Vu[1]; Eric Brown[1]; Jinhui Zhang[3]; Dan Berger[3]; Ee-Sunn Chia[3]; Obbina Ugwu-Oju[3]; Alicia Hoover[1]; Rachel Dunn[1]; Tim Marzan[1]; Jingyue (Jan) Yang[1]; *[1]Food and Drug Administration, Saint Louis, MO; [2]AbbVie Inc, North Chicago, IL; [3]Food and Drug Administration, Silver Spring, MD*

ThP 737 **LC-MRM-MS Method for the Detection and Quantification of Six Nitrosamine Impurities in Sartan (ARB) Drugs**; James Turner[1]; Roxana Eggleston-Rangel[2]; *[1]Phenomenex, Torrance, California; [2]Phenomenex, Torrance, CA*

ThP 738 **Contribution of arachidonic acid availability and co-culture with macrophages for oxylipin production in SARS-CoV-2 infection**; Rosangela Silva Santos[1, 2]; YANNICK STAHL[3]; TIMO SACHSENHEIMER[2]; RALF BARTENSCHLAGER[3]; BRÜGGER BRITTA[2]; SAYURI MIYAMOTO[1]; *[1]University of Sao Paulo, Sao Paulo, Brazil; [2]Heidelberg University, Heidelberg, Germany; [3]Heidelberg University, Medical Faculty, Heidelberg, Germany*

ThP 739 **Improved linear dynamic range of small molecules on a novel Zeno TOF Instrument**; Suya Liu[1]; Doug Simmons[1]; Nic G Bloomfield[1]; *[1]SCIEX, Concord, ontario*

ThP 740 **Automated Tool for Optimal Quantitative Analysis Conditions Using mzCloud Spectral Library**; Gergő Bodnár[1]; Juraj Lutišan[1]; Marynka Ulaszewska[2]; Tim Stratton[3]; Michal Raab[1]; *[1]Thermo Fisher Scientific, Bratislava, Slovakia; [2]Thermo Fisher Scientific, Milano, Italy; [3]Thermo Fisher Scientific, Texas, Texas*

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ThP 741 **Phenylazothiazole Photoswitches on Macromolecules for Solar Energy Storage : Photoisomerization and Thermal Back-Isomerization Kinetics Parameters Determination by MS**; Gwendal Henrard[1]; Thomas Robert[2]; Thomas Robert[1]; Benjamin Tassignon[1]; Julien De Winter[1]; Jérôme Cornil[1]; Pascal Gerbaux[1]; *[1]University of Mons, Mons, Belgium; [2]University of Mons (UMons), Mons, Belgium*

ThP 742 **Could you please repeat that?: Fourier transform data analysis for polymer mass spectra with accurate-mass data and mass defect preprocessing**; Robert B Cody; *JEOL USA, Inc., Peabody, MA*

ThP 743 **Applications for Circular Distance Metric Analysis for Kendrick Mass Defect Analysis (KMD)**; Christopher Joseph Shaffer[1]; Cole Stapleton[1]; *[1]3M, Maplewood, MN*

ThP 744 **Detailed Characterization of Polymers and Microplastics by KMD Plots of Complex MS Spectra**; Arnd Ingendoh[1]; Volker Sauerland[2]; Kushal Modi[3]; Toshiji Kudo[4]; *[1]Bruker Daltonics, Bremen, Germany; [2]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [3]Bruker Inc, Billerica, MA; [4]Bruker Japan, Yokohama, Japan*

ThP 745 **Molecular Structure Rearrangements in Covalent Associative Networks Revealed by Multidimensional Mass Spectrometry**; Calum Bochenek[1]; Roberto Obregon[1]; Junpeng Wang[1]; Chrys Wesdemiotis[1]; *[1]The University of Akron, Akron, OH*

ThP 746 **Characterization of Highly Dispersed Polymers and Their End Groups by Combining SEC/MALDI-TOFMS and Kendrick Mass Defect Analysis**; Bryan Katzenmeyer[1]; Takaya Satoh[2]; Takafumi Sato[2]; Kumiko Ikuta[3]; Yuko Matsubuchi[3]; Takayasu Hirai[3]; Nobuyuki Kagawa[3]; Tetsuya Sugimoto[4]; Tsuneo Kobayashi[4]; *[1]JEOL, Peabody, MA; [2]JEOL Ltd., Akishima, Japan; [3]TOSOH Analysis and Research Center Co.,Ltd., Yokkaichi, Japan; [4]S.T. Japan Inc., Tokyo, Japan*

ThP 747 **Identifying molecular weight based on Nano-Projectile Secondary Ion Mass Spectrometry spectra**; Markus Langner[1]; Gregrey Swieca[1]; Won-Il Lee[2]; Shixian Ha[2]; Nikhil Tiwalee[3]; Chang-Yong Nam[2, 3]; Michael J. Eller[1]; *[1]California State University Northridge, Northridge, CA; [2]Stony Brook University, Stony Brook, NY 11794, USA, Stony Brook, NY; [3]Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, NY 11973,USA, Upton, Afghanistan*

ThP 748 **Comprehensive Analysis of Oligomeric Impurities, Monomer Composition, and End-Group Information in ArF Photoresist Block Copolymers Using Q-TOF High-Resolution Mass Spectrometry**; Guoqiang Liu[1]; Yue Song[1]; *[1]Agilent Technologies, Shanghai, China*

ThP 749 **Study of the cyanoacrylate fuming mechanism by electrospray ionization tandem mass spectrometry**; Mariska BANIDOL[1, 2]; Anais MONGE[1]; Hélène PIZZALA[1]; Laurence CHARLES[1]; *[1]Aix-Marseille University, MARSEILLE, France; [2]National Forensic Science Institute of the French Gendarmerie, Cergy-Pontoise, France*

ThP 750 **Fluoropolymer analysis by Thermodesorption/Pyrolysis-DART-FT-ICR-MS**; Frédéric Progent[1]; Pierre Pacholski[1, 2, 3]; Umut Ugur Ozkose[4, 5]; Bruno Ameduri[4]; Théo Voellinger[2]; Pierre Magri[2]; Sébastien SCHRAMM[2]; Frank David-Quillot[6]; Frédéric Aubriet[2]; *[1]CEA, Bruyères-le-Châtel, France; [2]Université de Lorraine, Laboratoire de Chimie et Physique-Approche Multi-échelles des Milieux Complexes (LCP-A2MC), Metz, France; [3]Université de Lille, CNRS, UMR 8523 - PhLAM - Physique des Lasers Atomes et Molecules, Lille, France; [4]Institut Charles Gerhardt (ICGM), Université de Montpellier, CNRS, ENSCM, Montpellier, France; [5]Piri Reis University, , Faculty of Science and Letters, Department of Chemistry, Tuzla, Turkey; [6]CEA, Le Ripault, France*

ThP 751 **HR/AM LC-MS and UHPLC Methods for Evaluating End-Group Purity of Silicone Oligomeric Crosslinker Material**; Patricia Harmon[1]; Andrew Hoteling[1]; *[1]Bausch + Lomb, Rochester, NY*

ThP 752 **Comprehensive Investigation of Polymer Oxidation using Interactive Visualizations and User Modified Libraries in PolyMatch Suite**; Wendi A Hale[1]; Jeremy P Koelmel[2]; Nicholas Oranzi[3]; David Weil[4]; Emma E. Rennie[4]; Paul Stelben[2]; Michael Kummer[5]; David Godri[6]; Jonathan Sparks[5]; Krystal J Godri Pollitt[2]; *[1]Agilent, Lexington, MA; [2]Yale University, New Haven, CT; [3]University of Florida, Gainesville, Florida; [4]Agilent Technologies, Santa Clara, CA; [5]Innovative Omics, Sarasota, FL; [6]3rd Floor Solutions, Caledon, ON*

ThP 753 **ToF-SIMS depth profiling of multilayered perovskite solar cells: a powerful approach to reveal structure-property relationships, but beware of artifacts**; Nico Fransaert[1]; Dirk Valkenborg[2]; Bart Cleuren[3]; Jean V. Manca[1]; Aslihan H. Babayigit[4, 5]; *[1]UHasselt, X-LAB, Agoralaan, 3590 Diepenbeek, Belgium; [2]UHasselt, Data Science Institute, Interuniversity Institute for Biostatistics and Statistical Bioinformatics, Center for Statistics, Agoralaan, 3590 Diepenbeek, Belgium; [3]UHasselt, Theory Lab, Agoralaan, 3590 Diepenbeek, Belgium; [4]UHasselt, Institute for Materials Research (IMO-IMOMEC), Agoralaan, 3590 Diepenbeek, Belgium; [5]EnergyVille, Thor Park 8320, 3600 Genk, Belgium*

ThP 754 **Understanding Property Changes in a Crosslinked Hydrogel Polymer Network using High Resolution Mass Spectrometry**; Michelle Piotrowski[1]; Patricia Harmon[1]; Andrew Hoteling[1]; *[1]Bausch+Lomb, Rochester, NY*

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ThP 755 **Impact of Quinone Derivatives, Environmental Pollutants, on the Architecture and Functionality of Human Red Blood Cells**; Neha .[1]; Santosh Kumar Mondal[2]; Amit Kumar Mandal[1]; *[1]Indian Institute of Science Education and Research, Kolkata, India; [2]All India Institute of Medical Sciences, Kalyani, Kolkata, India*

ThP 756 **Metabolomics and Lipidomics in Early Drug Development at Boehringer Ingelheim**; Joerg Thomas

Hannich[1]; Martin Pauers[1]; Federica Fiorini[1]; Svenja Mayer-Wrangowski[1]; Stefan Blech[1]; [1]*Boehringer Ingelheim, Biberach, Germany*

ThP 757 **Species-specific differences of per- and polyfluoroalkyl substances (PFAS) in benthic elasmobranchs along the coastal waters of the United States**; Qaim Mehdi[1]; Ines A Chambrier-Athias[1]; Lauren E Blackman[1]; Kady Lyons[2]; Jennifer T Wyffels[3, 4]; John A Bowden[1]; [1]*University of Florida, Gainesville, Florida;* [2]*Georgia Aquarium, Atlanta, GA;* [3]*Ripley's Aquariums, Myrtle Beach, South Carolina;* [4]*University of Delaware, Newark, DE*

ThP 758 **Sex-Specific Disruptions in Hepatic Lipid and Metabolite Profiles of Zebrafish Following Acute Bisphenol A Exposure**; Yoonjeong Jeon[1]; Sung-Gil Choi[1]; Won Noh[1]; Jong-wook Song[1]; Jong-Hwan Kim[1]; Jong-Su Seo[1]; [1]*Center for Environmental Safety Research, Korea Institute of Toxicology, Jinju, South Korea*

ThP 759 **Unraveling the Proteomic and Biochemical Impact of Acute Polystyrene Microplastic Exposure in Daphnia magna**; Young-Sang Kwon[1]; Chang-Beom Park[2]; Seung-Min Lee[1]; Jin-Woo Park[1]; Yeong-Jin Kim[1]; Jong-Su Seo[1]; [1]*Center for Environmental Safety Research, Korea Institute of Toxicology, Jinju, South Korea;* [2]*Center for Ecotoxicology and Environmental Future Research, Korea Institute of Toxicology, Jinju, South Korea*

ThP 760 **Irreversible Blood Protein Alterations Induced by Polyhexamethylene Guanidine Aerosol and Their Association with Lung Injury Severity**; Hee-Sung Ahn[1]; Jiyoung Yu[2]; Bokyung Kim[3]; Yelin Lee[3]; Minjoong Kim[3]; Jihyeon Kim[3]; Soo-Jong Hong[4]; Kyunggon Kim[2, 3]; [1]*AMC Sciences, Songpa-gu, South Korea;* [2]*Convergence Medicine Research Center, Asan Institute for Life Sciences, Asan Medical Center, Songpa-gu, South Korea;* [3]*Department of Digital Medicine, BK21 Project, University of Ulsan College of Medicine, Songpa-gu, South Korea;* [4]*Department of Pediatrics, Childhood Asthma Atopy Center, Humidifier Disinfectant Health Center, Asan Medical Center, University of Ulsan College of Medicine,, Songpa-gu, South Korea*

ThP 761 **Short Term Effects on Lipid Distributions in OPNA Poisioning and Treatment in a Humanized Mouse Model**; Ian Spears[1]; Seraiah Coe[2]; Benjamin Wadsworth[2]; C Linn Cadieux[2]; Caitlin M. Tressler[3]; [1]*Johns Hopkins University, Baltimore, MD;* [2]*CTR US Army USAMRICD, Baltimore, Maryland;* [3]*Johns Hopkin University, Baltimore, MD*

ThP 762 **Uptake of aerosolized organic acid and metal in a human lung cell co-culture model after binary mixture exposures**; Dinny Stevens[1]; Taylor Jefferis[1]; Christie M. Sayes[1]; [1]*Baylor University, Waco, TX*

ThP 763 **Short Term Metabolomic Effects of OPNA Poisoning and Treatment on a Humanized Mouse Model**; Ian Spears[1, 2]; Seraiah Coe[3]; Benjamin Wadsworth[3]; C Linn Cadieux[3]; Caitlin Tressler[1, 4]; [1]*Johns Hopkins AIMS Core, Baltimore, MD;* [2]*Johns Hopkin University, Baltimore, MD;* [3]*United States Army Medical Research Institute of Chemical Defense, Aberdeen Proving Ground, MD;* [4]*Johns Hopkins University, Baltimore, MD*

ThP 764 **Test for Posterbridge - Jennifer is presenter and submitting author**; Jennifer Anne Watson; *ASMS Office, Santa Fe, NM*

ThP 765 **Test for PosterBridge - Mike is the presenter and submitting author**; Mike Fenn; *Ativ Software, Philadelphia, PA*

MONDAY NETWORKING SESSION, 12:00 - 1:00 pm

Networking Session: Celebrating Women Mass Spectrometrists

Presiders: Tian (Autumn) Qiu, Prasanna Ashok Kumaar, Rosangela Silva Santos

Poster-Exhibit Hall, 12:00-1:00 pm

Come celebrate and be empowered by the journey and success of women mass spectrometrists in this networking event, organized in collaboration with Females in Mass Spectrometry!

- The session opens with a keynote presentation by a notable guest speaker, sharing career insights and stories of encouragement.
- The session continues with interactive discussions with the keynote speaker and invited guests from various career stages. Participants will have the opportunity to ask questions and to pose comments via an online platform or feel free to raise your hand!
- Of course, the session will feature networking time in small groups with trailblazers from the mass spectrometry community.

We invite all to join us in this 8th edition of the networking session on Celebrating Women Mass Spectrometrists – build meaningful connections and find inspirations to navigate your career.

MONDAY EVENING WORKSHOPS, 5:45 - 7:00 PM

01 Career Paths for Mass Spectrometrists: A Speed Networking Workshop

Career Development Interest Group

Presiders: Olya Vvedenskaya, Rosangela Silva Santos

Room 307-308

Career development in mass spectrometry offers diverse opportunities across academia, industry, government, and communication. However, navigating these paths and making informed career choices can be challenging for early career researchers.

This interactive workshop, organized in collaboration with the FeMS+ community, provides an opportunity to engage directly with professionals representing the following career trajectories:

- Government research - A senior research scientist working in a governmental agency – Dr. Maggie Tam
- Core facility management - A director of a mass spectrometry core facility – Dr. Prasanna Ashok Kumaar
- Science communication - A science communicator working in a biotech company – Dr. Olya Vvedenskaya
- Industry applications - A leader of an omics direction at a vendor company – Dr. Erica Forsberg
- Academic research - A postdoctoral researcher at a university – Dr. Duong Bui

The 90-minute session will begin with a brief introduction to the format, followed by five-minute presentations from each expert on their career journey and day-to-day responsibilities. Attendees will then participate in two 25-minute roundtable Q&A sessions, where they can rotate between speakers to ask questions. The event will conclude with a summary of key takeaways and networking opportunities.

This workshop is ideal for students, postdocs, and early-career scientists looking to explore different career options in mass spectrometry.

02 Real time Mass Spectrometry in Proteomics and Beyond

Independent

Presiders: Devin Schweppe**,** Nick Riley**,** William Barshop

Room 309-310

'Real-time mass spectrometry is the analysis or interpretation of spectral data in parallel with instrument acquisition to inform, optimize, or control future spectral acquisition.' The democratization of real-time instrument control is enabled by recent instrument application programming interfaces and has led directly to new methods for targeted (MaxQuant.Live, PRMlive, GoDig) and discovery proteomics (real-time search, real-time library search).

The purpose of this workshop is to provide a foundational demonstration of state-of-the-art real-time instrument control through short presentations (5-15 minutes) by invited experts. These presentations lay the groundwork for a panel discussion (30 minutes) that segues into an informal discussion on emerging topics for real-time instrument control (30 minutes). The format offers a unique and exciting opportunity to engage in open discussion, support junior researchers, and identify gaps in the current field that lab- or community-lead efforts can address. The workshop will establish avenues to improve open sharing of data, code, documentation, and methods for the continued development new real-time mass spectrometry tools.

03 Chemoproteomics: The Next Frontier for Drug Development (and More)

Independent

Presiders: Keriann Backus**,** Lindsay Pino

Room 314-317

Chemoproteomics has emerged as a critical discipline at the intersection of chemistry, proteomics, and drug development. As advances in chemical biology and mass spectrometry continue to accelerate, the opportunities for elucidating complex biological processes and identifying potential therapeutic targets have expanded tremendously. Building upon our 2024 workshop, we seek to bring together leaders and researchers in chemoproteomics from academia and industry to exchange knowledge, perspectives, and experiences. The workshop will focus on recent breakthroughs, methodologies, and technological innovations driving advancements in chemoproteomics and its application in the biomedical and drug discovery fields. The workshop will begin with a short introduction, "what is chemproteomics," by the presiders followed by a panel discussion with a mix of industry and academia experts giving their "hot takes" and debates on the topic. Panelists will focus on the state-of-the-art for chemoproteomics as well as ongoing challenges and opportunities, spanning chemical tools, sample preparation, and data acquisition and analysis. By exploring and discussing the latest developments in this dynamic field this workshop aims to foster collaboration, share insights, and spur future innovation.

04 Benchmarking Datasets for Untargeted Metabolomics and Exposomics and Compound Identification

Metabolomics Interest Group
Presiders: Corey Broeckling, Xiuxia Du
Ballroom II

Evaluation of software tools for untargeted mass spectrometry (MS)-based metabolomics and exposomics requires benchmarking datasets to ensure rigor and objectivity. This workshop will feature two datasets that have been created to address this need. The first dataset is for evaluating software tools that extract compound information from raw MS data. The second dataset is for the discovery and identification of molecules.

To produce the first benchmarking dataset, samples were prepared that consist of three pairs of reagents: (1) Standard mixtures of 96 pure analytes (96Mix); (2) Commercially available yeast cell extract containing separate 12C and uniformly 13C-labeled samples that were prepared in parallel; and (3) human plasma SRM 1950 paired with SRM 8231. These complex reagents have been mixed in a systematic and highly structured manner to enable objective heuristic rules to serve as ground-truths. All of the data were acquired on a Waters Acquity coupled to a Q-TOF and a UHPLC coupled with Orbitrap ID-X. Samples were separated using both HILIC and reverse phase chromatography, and profile data acquired in both positive and negative ionization mode. Data were acquired in MS only mode, and additional injections were performed in DDA MS/MS mode. The second benchmark dataset comprises the largest publicly available collection of high-quality labeled MS/MS spectra.

At this workshop, we will introduce these two datasets and conduct a survey to seek feedback from the audience to better understand the needs of the metabolomics and exposomics community to make metabolomics and exposomics informatics tools more rigorous and transparent.

05 Top-Down Proteomics: Software and Data Analysis Strategies for Getting the Most Out of Your Data

Top-Down Proteomics Interest Group
Presiders: Corinne Lutomski, Fanny Caroline Liu
Ballroom I

Despite ongoing advances in technology, the field of top-down proteomics (TDP) still faces significant challenges obstructing widespread adaptation. These obstacles span across all stages of the experimental workflow, including sample preparation, protein ionization/fragmentation, and data analysis. While efforts to democratize sample preparation and fragmentation have recently been published through community studies, data analysis remains a significant bottleneck in the widespread adaptation of TDP. A survey among the audience at the 2023 top-down proteomics workshop at ASMS indicated a critical challenge remains in software and data analysis.

This workshop will provide insight toward applying TDP to targeted analysis in biomedical, biopharmaceutical, and academic applications with a special focus on fully interpreting the complex data generated in TDMS experiments. The goal of the workshop is to provide perspectives from a range of experts in native and denatured top-down MS to provide a foundation for interpreting top-down spectra. The workshop will host six panelists, each panelist will give a short introduction about how they use top-down proteomics, the strategies they use to interpret top-down data, and the key metrics they look for. The audience will be directed toward resources for data analysis, including both free and commercial software packages.

06 Latest Developments in Open Data Standards Practices in Proteomics

Independent
Presiders: Douwe Schulte, Wout Bittremieux, Petr Novák
Ballroom III

The Proteomics Standards Initiative (PSI) has openly and collaboratively developed mass spectrometry data standards since 2002. This workshop will introduce some recent standards, ProForma 2.1, mzPAF, mzSpecLib, and Universal Spectrum Identifier (USI), and show their applicability to annotate MS2 spectra. The session will be closed with a discussion on the applicability and issues of the standards for the wider community.

The workshop will start with a plenary introduction of the ProForma notation. A notation to write down definitions of complex peptidoforms, explicitly supporting bottom-up, top-down and many other fields of mass spectrometry. We will address its recent update but focus on how to use it in common cases. This introduction will be alternated with hands on applying the introduced concepts in Annotator, a highly customisable fragmentation annotator for any proteomics MS data. By having these hands-on sections we can teach how to use ProForma in practice.

After the introduction of ProForma we will introduce Universal Spectrum Identifiers, which can be used to easily visualise publicly available mass spectra in the ProteomeXchange data ecosystem, e.g. the PRIDE database. This again will be alternating between plenary instruction and hands-on sections with the same software.

The session will end with a short recap of what was introduced and a discussion on the bottlenecks for applying the shown formats more generally. This section's goal is to find use cases for these formats not currently enacted and fields for which these formats do not have the necessary expressiveness to be of use.

07 Towards Guidelines for DIA Reporting Criteria

Data Independent Acquisition Interest Group
Presiders: Mike MacCoss, Michael Ford
Ballroom IV

The guidelines for reporting mass spectrometry proteomics data were outlined over twenty years ago and have provided a solid calibrator for the field since that time[1]. DIA specific guidelines were suggested in 2019[2]. It is our thought that an update to these guidelines may be necessary to include properties unique to evolving DIA workflows. The purpose of this workshop is to provide a forum for the discussion of DIA reporting guidelines. In an informal but structured setting of an ASMS workshop the community can engage in an open discussion about how the criteria may look and be applied. It is our intention to engage several experts in the field before the meeting to 1) establish a highly qualified list of speakers and 2) outline a set of goals/discussion points to ensure a focused conversation.

We hope for a lively discussion with community engagement. A framework for updating the reporting guidelines may emerge.

- The Need for Guidelines in Publication of Peptide and Protein Identification Data. Carr, Steven et al. Molecular & Cellular Proteomics, Volume 3, Issue 6, 531 - 533

MONDAY EVENING WORKSHOPS, 5:45 - 7:00 PM

- Initial Guidelines for Manuscripts Employing Data-independent Acquisition Mass Spectrometry for Proteomic Analysis. Chalkley, Robert et al. Molecular & Cellular Proteomics, Volume 18, Issue 1, P1-2

08 MS Outreach: Knowledge Share and Instrumentation Donations

Developing World Outreach Interest Group
Presiders: Hendrik Kersten, Giles Edwards
Room 336

The ASMS Interest Group "Developing World Outreach" aspires to bring together those who wish to share their ideas on how we as a society can assist in deploying mass spectrometry as a key analytical technique to address educational, health, environmental and economic issues in the Developing World.

The organizing committee of this group has shipped and installed a number of mass spectrometry products across the Globe for academia. If any ASMS members would like to contribute their engineering or applications based knowledge it would be gratefully received. The group aims to work out a strategy to utilize the skill set of ASMS members for outreach activities.

Recently, this group has setup a MS Online Seminar to facilitate academics, engineers and enthusiasts to share their research and mass spectrometry experience with others across the Globe (https://www.ipams.uni-wuppertal.de/de/startseite/workshops/conferences/online-ms-seminars).

The seminar sessions are free of charge and we would like to encourage ASMS members to join, present and get in touch with scientists around the globe who do not necessarily have the financial means to attend a conference like this one. Sharing is caring.

09 Taste to Targets: Food, Flavor and Fragrance Workshop

Flavor Fragrance & Foodstuff Interest Group
Presiders: David Schroeder, Devin Peterson,
Candice Ulmer Holland
Room 339-340

Food Flavor and Fagerance tools, techniques, and strategies discussion focused on applications.

Work Group discussion primers:

- Beer and coffee flavor analysis case studies for by Flavor Research and Education Consortium.
- USDA nutritional, residue chemistry, and Siluriformes
- Panel expertise SAFE, Dynamic Headspace, GC x GC, GC-MS/MS, GC-ToF LC-MS, LC-ToF

10 Nitrosamine Analysis in Pharmaceutics: Evolving Challenges and Emerging Solutions

Pharmaceuticals Interest Group
Presiders: Paolo Lecchi, Mack Shih, Jessica Hoskins
Room 341-342

Following the success of last year's workshop on nitrosamines, this session will provide an update on recent developments in the detection and quantification of nitrosamine impurities in pharmaceutical preparations. With evolving regulatory expectations and scientific advancements, the need for reliable analytical strategies remains critical.

This highly interactive workshop will foster open discussions and knowledge sharing among participants. Experts from various sectors will present the latest advancements in analytical methodologies, regulatory considerations, and industry best practices. Attendees will have the opportunity to engage in dynamic discussions, share experiences, and explore practical solutions to common challenges in nitrosamine analysis.

Through case studies, Q&A sessions, and group discussions, participants will engage in an open and interactive exchange on method development, validation, and risk assessment strategies. This session will provide a collaborative forum for discussing challenges, sharing experiences, and exploring current approaches to nitrosamine detection and quantification in pharmaceutical preparations.

11 Mass Spectrometry in Quality Control for Complex Biotherapeutics Modalities

Biotherapeutics Interest Group
Presiders: Sara Carillo, Sarah Rogstad
Room 343-344

The biotherapeutic landscape is seeing the rapid emergence of therapeutic formats more complex than traditional monoclonal antibodies as entities such as antibody drug conjugates (ADCs), bispecific antibodies (bsAbs), and fusion proteins. While these formats offer distinctive advantages in targeting diseases and are among the most promising drug classes in oncology, they pose new challenges from both design and quality control points of view.

Mass spectrometry techniques provide an attractive tool to decipher some of the critical quality attributes (CQAs) of these complex modalities and as such can be implemented in a Quality by Design (QbD) aspect of their development towards commercialization. However, minimal instances of mass spectrometry in QC have been approved for therapeutic proteins, and even fewer for complex modalities. When mass spectrometry has been implemented for these products, the specific approaches and CQAs analyzed have varied widely.

This workshop aims to: 1) understand current best practices in CQA analysis and monitoring for complex biotherapeutic modalities, 2) highlight the benefits of mass spectrometry-based analysis for ADCs, bsAbs, and fusion proteins, and 3) understand the technical and practical limits for their implementation in QC.

MONDAY EVENING WORKSHOPS, 5:45 - 7:00 PM

12 Photoionization MS: Where It Excels, Where It Falls Short, and How It Complements Other Methods

Photoionization MS Interest Group
Presiders: Christopher Rüger, Sven Ehlert, Patrick Mueller
Room 345-346

Photoionization mass spectrometry (PI-MS) has emerged as a powerful analytical tool, offering soft ionization with minimal fragmentation, high selectivity, and real-time analytical capabilities. It is particularly well-suited for volatile and semi-volatile compounds, allowing for direct analysis without the need for extensive sample preparation. However, its role within the broader landscape of ionization techniques remains a topic of active discussion. How does PI-MS compare to and complement traditional ionization techniques such as electron ionization (EI), electrospray ionization (ESI), and atmospheric pressure chemical ionization (APCI)? What are its limitations in terms of ionization efficiency, matrix effects, and compound coverage, and where does it offer unique analytical advantages?

This engaging workshop, hosted by the Photoionization Mass Spectrometry Interest Group, will feature three 5-minute flash talks offering focused insights into different aspects of PI-MS and its interplay with other ionization techniques. Discussions will explore hybrid ionization approaches, where PI-MS is coupled with complementary sources to enhance molecular coverage, as well as its application in real-time environmental monitoring, metabolomics, and high-throughput analysis.

A podium discussion will bring together experts to debate key topics, including ion source flexibility, selectivity vs. sensitivity trade-offs, and the integration of PI-MS into multi-technique workflows. Panelists will also deliver bold "Hot Takes" on the future of PI-MS, its evolving applications, and its potential role in next-generation analytical instrumentation.

The session will conclude with an open discussion and audience Q&A, offering attendees a unique opportunity to exchange ideas, discuss practical challenges, and explore innovative strategies for implementing PI-MS in modern analytical workflows.

13 Undergraduate Research: Strategies for Success

Undergraduate Research in MS Interest Group
Presiders: Mac Gilliland, Micah Donor
Room 347-348

Undergraduate research experiences can be exceedingly valuable, to both the students and their mentors, yet there are many unique challenges associated with them. In this workshop we will explore practical strategies for creating successful and productive undergraduate research experiences. From lab startup to regular operation, from project idea to publication, we will discuss key aspects of undergraduate research. This will include: making the most of limited time; working during the summer vs. during the academic year; recruiting and training new researchers; mentoring students with diverse backgrounds; developing independence; maintaining continuity from student-to-student; and involving students in the publication process. We expect that this workshop will be particularly useful to undergraduate students and anyone who mentors undergraduates - including PIs, postdocs, graduate students, and career scientists. This workshop will be highly interactive, with space for attendees to contribute their perspectives on these topics and participate in a discussion of how this group can best foster a strong culture of undergraduate research within ASMS.

14 Environmental Applications: You Are What You Eat and Breathe

Environmental Applications Interest Group
Presiders: Erin Baker, Carrie McDonough
Room 349-350

Chemicals in the environment have a massive impact on our health and well-being. For the many chemicals we are exposed to daily through ingestion, inhalation and dermal absorption, their health impacts are unknown. However, from Paracelsus we know that "the dose makes the poison", and any chemical, even water, can be toxic if consumed at high enough amounts. In this workshop, the audience will test their knowledge on the history and current state of chemicals of concern through an interactive quiz (with prizes!!). We will then have several short talks on current developments in environmental measurement approaches and applications, such as novel non-targeted analysis developments and computational workflows, which are allowing us to probe new chemicals of concern that we did not even know existed.

TUESDAY NETWORKING SESSION, 12:00 - 1:00 pm

Networking Session: Hispanics and Latinx in MS

Presiders: Adriana Zardini Buzatto, Rafael Montenegro Burke

Poster-Exhibit Hall, 12:00-1:00 pm

This networking session will act as the official Hispanics and Latinx in MS Special Interest Group meeting at the ASMS Conference. Last year in Anaheim, we held the second Hispanics and Latinx in MS meeting at ASMS (networking session), which was highly successful with over 70 attendees and strong engagement. During the networking session, we gave all candidates for our Executive Committee a chance to introduce themselves and why they were interested in serving the group. Additionally, we had short talks with members selected for an oral session. The elected leadership group, advised by the founders, is planning the next steps for the group, which includes the ASMS networking session. At this networking session, we will plan activities to allow for social, professional, and research exchanges and interactions. We will highlight our younger member's research by keeping the opportunity to present a short talk (we will solicit abstracts for selection). We feel this is important, as it is quite difficult to get a talk at the ASMS Conference, and this could give our younger members a boost in confidence to speak at a national meeting. Additionally, we will hold a career advisement session. Lastly, we would like to hold soft gathering Network Sessions to allow for more informal chats and research/professional advice meeting time.

TUESDAY EVENING WORKSHOPS, 5:45 - 7:00 pm

01 De Novo Peptide Sequencing: Ready For Prime Time?

Independent

Presiders: Justin Sanders, Wout Bittremieux, William Fondrie

Room 307-308

In recent years, deep learning-based de novo peptide sequencing has made significant advances, demonstrating remarkable performance in interpreting mass spectrometry data. Despite these successes, researchers still face numerous questions when applying these tools in practice. This workshop aims to demystify deep learning-based de novo sequencing, providing attendees with a clear understanding of the state of the field, best practices, and practical insights through interactive discussions and live demonstrations.

With a growing number of de novo tools and approaches available, researchers often find themselves asking:

- Which de novo tool should I use? With so many options available, selecting the right one can be challenging. We will present insights from a community-driven benchmarking effort comparing over a dozen de novo tools.
- What are the best practices for de novo sequencing? We will explore common pitfalls, practical considerations, and specific use cases, including immunopeptidomics and metaproteomics.
- How can I ensure confidence in my results? Unlike sequence database searches, de novo sequencing lacks well-established false discovery rate control methods. We will discuss best practices for assessing confidence and data quality.
- Can de novo sequencing solve my specific problem? We invite attendees to bring their own data and explore the power of de novo sequencing in real time. Through live analysis, we aim to uncover unexpected insights together.

Join us for an engaging session where we cut through the complexity and uncover the potential of deep learning-driven de novo peptide sequencing in mass spectrometry research!

02 Art, Museums and Archaeology

Art, Museums and Archaeology Interest Group

Presiders: Alba Alvarez Martin, Paul Haynes

Room 309-310

The study of archaeological specimens, artworks, and other cultural heritage objects by mass spectrometry requires the adaptation of techniques developed for biomedicine, forensics, or industrial and natural product research, to diverse fields such as anthropology, paleontology, archaeology, natural history, and art history. This introduces unique issues and challenges and often requires some creative problem-solving. Sharing information on some of the more unusual samples analyzed and projects undertaken is helpful for all fellows professionals in the fields, and it will be a unique and inspiring opportunity for other colleagues working on different topics.

This workshop will feature lightning talks selected from ASMS poster abstracts - students and fellows are encouraged to volunteer in advance by contacting the organizers.

Lightning talks will be followed by audience Q&A with a panel of academic, government, public museums and private institution scientists to discuss areas of interest in the field.

Topics may include such things as: ethics and permissions involved in analyzing culturally sensitive samples; considerations for historical and contemporary sample contamination; the risk of damage to objects as a result of analysis; the implementation of new minimal invasive sampling techniques; discerning the importance of chemicals identified from an analyte removed from context; sample-limited preparation and recovery approaches for rare and precious analytes; the significance of preservation and prediction of material degradation; the importance of a maintaining fluid communication with conservators and curators; employment, funding, and fellowship opportunities in the field; and much more.

TUESDAY EVENING WORKSHOPS, 5:45 - 7:00 pm

03 Spectral Library Basics - What is an Identification?

Mass Spectral Libraries Interest Group
Presiders: Tim Stratton, Douglas Slotta
Room 314-317

What information is available to provide for an identification? What is the value that should be placed on different pieces of information? How much information is required to provide a confident identification? What is the level of confidence that is required for a specific need? We will discuss viewpoints and potential answers around all of these questions through a series of presentations across a wide range of applications. Afterwards, we will hold a panel discussion between the experts and members of the audience. In addition, we will continue our interactive survey that we conduct every year.

04 Native MS: Strategies for Advancing Protein Characterization in Industry and Academia

Native Mass Spectrometry Interest Group
Presiders: Kristine Parson, Carter Lantz
Ballroom II

Native mass spectrometry (nMS) is a transformative analytical technique crucial for analyzing biomolecules, particularly proteins and protein complexes, while preserving their native conformations and non-covalent interactions under near-physiological conditions. This allows researchers to interrogate the structure, dynamics, and interactions with other biomolecules and compounds as they exist naturally. As a result, nMS has been able to provide valuable insights into complex biological processes like protein folding, ligand binding, and protein assembly formation. It is also instrumental in drug discovery and development, as it can provide relevant information on interactions between therapeutic compounds and targets including the specificity and efficacy of those interactions. The technique's capability to provide detailed molecular data enhances research rapidly and accurately in biochemistry, molecular biology, and pharmacology, confirming its indispensable role in life sciences.

This workshop will highlight recent advancements in nMS technology, focusing on how these innovations are applied across diverse research areas and how they are being used to solve complex problems. The workshop is designed to be informal and welcoming, serving as a valuable resource for both newcomers and those well-versed in nMS to ask questions and find inspiration for their own research.

Effectively using nMS requires technical expertise so the instrument can be optimized for the biological systems being studied. Traditionally, the workshop facilitates collaboration and knowledge exchange between academia and industry by featuring a diverse group of experts who provide brief presentations. The presentations, along with an open discussion led by the organizers, aim to promote productive dialogue among participants.

05 Young Mass Spectrometrist Workshop: Graduate School Through Early Career Forum

Young Mass Spectrometrists Interest Group
Presiders: John Stutzman, Jeremy Manheim
Ballroom I

The Young Mass Spectrometrist (YMS) Workshop has historically been an open forum for graduate students, post-docs, and early career scientists to question and receive career feedback from a diverse panel. A highlight of this workshop is the ability to ask direct questions and receive candid feedback, which has been a key piece of positive feedback from attendees. The YMS workshop at the 2025 ASMS conference will continue this practice with some minor changes based on attendee feedback from 2024. The two chairs (Jeremy Manheim and John Stutzman) will begin by gathering a diverse panel with considerations of career type (academia, government, industry) and position (technical support, researcher, project leader, hiring manager) as well as background (gender, race, culture). At the beginning of the workshop, approximately 15 minutes will be allocated for the panel to communicate a short introduction to the attendees. Once completed, the chairs will start questions from the attendees (approximately 60 minutes). 2024 feedback indicated that attendees wanted more time for Q&A, so condensing introductions and opening comments will ensure increased interaction. Attendees' questions may be asked directly through microphone or a question box. The chairs will have several preprepared topics and questions to help spark/facilitate discussion if the dialogue begins to slow. Preprepared topics will cover the spectrum of graduate school, post-doctoral positions, finding jobs, and early career topics. 2024 feedback also indicated a focus on graduate school and students, so there will be efforts to be inclusive over all early career mass spectrometrists.

06 Unlocking the Full Potential of Discovery and Early Development DMPK Support: Revolutionizing Efficiency, Innovation, and Integration with Mass Spectrometry

DMPK Interest Group
Presiders: HsinPin Ho**,** Yongle Pang
Ballroom III

In the pharmaceutical industry, bioanalytical outsourcing is common. However, companies may also maintain various portion of DMPK studies. This workshop delves into the scientific and operational aspects of supporting DMPK early discovery and preclinical stages, ensuring superior efficiency, cost-effectiveness, and data integrity.

Presenters will discuss strategic methodologies and innovative practices that enable companies to excel in DMPK and early development support. In addition, other insights for GXP support will be leveraged, allowing lab practices to adapt to new challenging technologies, focusing on risk-based approaches and prioritizing sustainability to ensure necessary compliance while technology advancements.

Attendees will gain a comprehensive understanding of DMPK support in the pharmaceutical industry, including embracing innovation, controlling data integrity with digital technologies, achieving expedited turnaround times, and maintaining seamless real-time knowledge exchange and proficient troubleshooting capabilities. The workshop will feature interactive discussions on strategies and practices that help pharmaceutical DMPK support, achieving unparalleled bioanalytical capabilities and driving scientific advancements.

TUESDAY EVENING WORKSHOPS, 5:45 - 7:00 pm

08 FTMS Community Resources: Access, Education, and Data Analysis

FTMS Interest Group
Presiders: Yury Tsybin, Martha Chacon-Patino
Room 336

Fourier transform mass spectrometry (FTMS), including FT-ICR, Orbitrap, and Charge Detection MS (CDMS), is a cornerstone of modern mass spectrometry, offering unparalleled resolution and accuracy. However, both newcomers and experts face challenges - newcomers in grasping fundamental principles and experts in staying updated with evolving methodologies, instrumentation access, and data analysis solutions.

The 2025 workshop aims to strengthen the FTMS community by fostering collaboration, sharing resources, and addressing key areas of interest. It will provide a platform to exchange insights, refine methodologies, and contribute to the development of next-generation FTMS applications.

Key Focus Areas:

1. Access to FTMS Instruments: We will explore global availability and accessibility, covering open-access FTMS facilities, project initiation at leading institutions, and international FTMS networks. The goal is to expand access and promote collaborative research.
2. Teaching FTMS Principles: We will focus on developing and sharing educational materials, including animations and tutorials, to enhance FTMS teaching at all levels. We aim to build a centralized repository of resources to support educators and learners.
3. Data Analysis Challenges & Solutions: Addressing the complexities of FTMS data processing, we will review available tools, discuss innovations, and identify gaps in existing workflows. The goal is to develop and share improved analytical pipelines.

Workshop Outcome:
Participants will collaborate on creating a centralized web-based resource featuring:

- A catalog of accessible FTMS instruments.
- Standardized educational materials.
- A repository of data analysis tools and best practices.

This initiative will strengthen the FTMS community, promoting engagement, education, and innovation in FTMS research and applications.

09 Process Considerations for Current Nucleic Acid Therapeutics and Emerging Modalities

Oligonucleaotides and Nucleic Acids Interest Group
Presiders: Varun Gadkari, Keeley Murphy, Robert Schuster
Room 339-340

This workshop proposal is submitted by Prof. Varun Gadkari (University of Minnesota), Keeley Murphy (Thermo Fisher Scientific), and Dr. Robert Schuster (GSK) for a workshop hosted by the ASMS Oligonucleotides and Nucleic Acids Interest Group.

Nucleic acids continue to be at the forefront of biomedical research across industry and academia. The annual ASMS workshop session allows the community to gather interested researchers in this space to exchange knowledge and ideas. This year, we will focus on the ever-challenging process development landscape within the nucleic acid therapeutic space.

As the investment in nucleic acid therapeutic research continues to increase, new challenges are emerging within process development and quality assurance, requiring unique analytical solutions that are often highly amenable with mass spectrometry. The resulting resurgence of interest in nucleic acid mass spectrometry and its applications in the pharmaceutical industry are being met with new process requirements, presenting new challenges for design and implementation. Furthermore, nucleic acid-based therapeutics themselves are rapidly evolving with new "next-generation" modalities emerging within this subfield. In this workshop we will host a panel of researchers from academia and industry to provide insight into the continuously evolving landscape of nucleic acid therapeutic product development. The discussion topics will focus on new process challenges, current best practices, and potential regulatory considerations when developing mass spectrometry-based processes for both 'traditional' nucleic acid therapeutics as well as emerging next-generation modalities. The aim is to include 4-6 panelists who will have ~7-10 minutes each to introduce themselves, outline their background and area of expertise, and provide a brief viewpoint on current therapeutic development challenges, mitigation strategies, and process considerations. The introductions will be followed by an open-planned discussion with the audience.

10 Fundamentals of Electrospray Ionization

Fundamentals Interest Group
Presiders: Rachel Loo, Cajetan Neubauer
Room 341-342

A generation after soft-ionization techniques have revolutionized mass spectrometry, advances in our ability to control the ionization of biological samples remain a critical challenge. In many experiments, the ionization process still fundamentally limits the scope and utility of the downstream mass spectrometric analyses.

The 2025 evening workshop will therefore revisit the physical chemical mechanisms of electrospray ionization (ESI), exploring both current knowledge and open questions: What are the known and unknown aspects of ESI mechanisms? How can a deeper understanding of ESI improve data quality in metabolomics, proteomics, and single-cell studies? What approaches are currently being explored to overcome the many limitations and artifacts of ESI? What are the major practical and theoretical challenges in ESI today? Could future approaches enable single-molecule sensitivity in mass spectrometry?

Presenters: Rachel Loo (UCLA), Lars Konermann (Western University, Canada), Anyin Li (University of New Hampshire), Derek Stein (Brown University), Alexander Makarov (Thermo Fisher Scientific). Short presentations are followed by an open forum panel discussion. Please feel free to email questions or other contributions for the discussion also in advance (rloo@mednet.ucla.edu and caj.neubauer@colorado.edu).

TUESDAY EVENING WORKSHOPS, 5:45 - 7:00 pm

11 Plastics, Polymers and Replacement Chemicals Part 1: Recycling, Deconstruction, and Redesign of Polymeric Materials

Energy & Biofuels, Exposomics, and Polymeric Materials Interest Groups
Presiders: Anthony Gies, David Stranz, Christopher Rüger
Room 343-344

This is part one of two-part workshop: (1) Polymers and Energy & Fuels interest groups will present the 1st workshop focusing on aspects of polymer/plastics recycling and (2) the Exposomics interest group will delve into the exposure aspects of these materials. The overall goal is to highlight the role of mass spectrometry in addressing complex challenges and growing environmental concerns over the waste streams of polymeric materials at the end of their life cycles, and how they can be reintroduced into new life cycles. In this first part, we will discuss strategies for recycling, upcycling, and redesign of polymeric materials. We will evaluate the role of advanced mass spectrometry techniques to enable this research area in the development of renewable materials.

This participatory workshop includes a series of short tutorial lectures. The lead talking points with the audience will include;

- What type of polymers/plastics can be reused and what are the current obstacles?
- Upcycling processes, including chemical and biological deconstruction of polymers
- Use of deconstructed products and analytical opportunities, including investigation of deconstruction chemistry and mechanisms to further this research.
- Circular polymer processes, such as replacement of petrochemically-derived feedstocks. Opportunities in application of advanced mass spectrometry to investigate reaction and degradation mechanisms to aid redesign of monomers for circular polymers.

Discussion panel will be composed of experts from variety of disciplines. They will be tasked with initiating discussions on challenges and potential solutions that mass spectrometry can offer in this economically impactful research area.

12 Proteomics Data Analysis: From Identification to Quantification

Bioinformatics MS Interest Group
Presiders: Fengchao Yu, Daniel Polasky
Room 345-346

This workshop aims to provide an overview of proteomics data analysis for anyone interested in proteomics, from novice to expert. The workshop will feature a brief overview of general principles of DDA and DIA data analysis, followed by a panel discussion of emerging trends and ongoing challenges. Participants will gain insights into key principles of peptide identification and quantification, exploring widely used computational tools and their applications in real-world research.

The session will begin with a brief overview of peptide identification and quantification for DDA and DIA data, covering the fundamental principles and introducing popular tools such as MaxQuant, DIA-NN, and MSFragger incorporated with FragPipe. Participants will learn how these tools process mass spectrometry data to accurately identify peptides and proteins, as well as the many approaches to quantitation and their key pros and cons. Emerging trends in the field, such as the role of machine learning and AI, will also be highlighted to seed discussion topics for the panel to follow. A second presentation on specialized applications of proteomics data analysis, including HLA peptidome and glycoproteomics research, will highlight key challenges in field that will serve as starting points for the panel discussion.

The panel discussion will aim to offer commentary on the current state of the field and provide interactive discussions with participants to enhance their understanding of advanced proteomics methodologies and gain practical knowledge to apply these techniques in their own studies.

13 Lab Management Software: Necessity or Luxury?

Analytical Lab Managers Interest Group
Presiders: Maryam Goudarzi, Caroline Chidley
Room 347-348

While lab management software is not a necessity for all labs, there has been an increase in demand for such software in service facilities across different sectors. The decision to invest in such software tools and which tool in specific is entirely dependent on each individual lab's operations, complexity of the offered services, staff and budget among other factors.

In this workshop we will discuss:

1. Popular commercial software solutions
2. Their pros and cons based on attendees' experiences
3. Points to consider when investing in a system, including key features
4. Staff training
5. Adoption and data migration

We will invite an open discussion with our attendees about their expectations from the software on:

1. Improved efficiency: Lab management software can automate many tasks, such as sample tracking, data entry, and report generation.
2. Reduced errors: Lab management software can help reduce errors by standardizing processes and
3. Increased compliance, including meeting regulatory requirements (i.e. FDA and HIPAA).
4. Improved Data management: Lab management software can help labs store and manage their data more effectively. This can make it easier to find, analyze data and collaborate on projects.

We will also discuss factors that lead to hesitation in adopting such systems in various labs, including software features, budget and getting buy-in from the staff.

WEDNESDAY NETWORKING SESSIONS, 12:00 - 1:00 pm

Two networking sessions will be held in different sections of the Poster-Exhibit Hall (look for signage)

Networking Session 01: SAMs (South Asians in Mass Spec): Career Transitions: Strategies for Growth and Success in Mass Spectrometry

Presiders: Presiders: Baljit Ubhi, Prasanna Ashok Kumar
Poster-Exhibit Hall, 12:00-1:00 pm

Navigating career transitions in mass spectrometry can be both challenging and rewarding, offering opportunities to explore diverse roles across academia, industry, consulting, and leadership. This workshop, hosted by South Asians in Mass Spectrometry (SAMS), aims to equip attendees - bench scientists as well as those seeking opportunities in consulting or commercial roles - with practical strategies for professional growth and success.

Our panel will feature distinguished professionals who have navigated significant career shifts, sharing personal experiences and lessons learned. Participants will gain insights into leveraging transferable skills, identifying new opportunities, and overcoming common challenges faced during transitions. The session will also emphasize the importance of diversity and inclusion, highlighting the unique experiences of South Asian professionals in the field.

The workshop includes an introduction to SAMS, outlining our mission to foster collaboration, promote innovation, and support professional development within the mass spectrometry community. An engaging panel discussion will be followed by an interactive Q&A, allowing attendees to connect directly with panelists. Additionally, an informal networking session will provide a platform for building meaningful professional relationships.

Ideal for students, early-career scientists, and seasoned professionals, this session offers valuable insights for anyone considering or navigating a career transition in mass spectrometry. Join us to explore new pathways, gain practical advice, and expand your professional network.

Key Highlights:
1. Diverse panel of experts from academia, industry, government and consulting
2. Networking opportunities with sponsored giveaways.

Networking Session 02: Career Opportunities for Chinese Students and Scholars

Presiders: Ling Hao, Hui Zhang
Poster-Exhibit Hall, 12:00-1:00 pm

With the rapid development of mass spectrometry technologies and the increasing applications to academic research, medicine, industry, and regulatory agencies, a growing number of mass spectrometrists including thousands of Chinese students and scholars are trained. The workshop for Career Development Opportunities for Chinese Students and Scholars aims to provide career perspectives to students and scholars to learn the career paths at different career stages. We will invite four speakers from academia, clinic, industry, and regulatory agencies to share their experiences for career development. We will also assemble a group of discussion panelists to answer questions from the audience. We believe the workshop is beneficial to both students and scholars of all ASMS members and potential employers. The workshop will provide opportunities for students and scholars to prepare for their career development during and after mass spectrometry training and help them to set up career goals in the field of mass spectrometry

WEDNESDAY EVENING WORKSHOPS, 5:45 - 7:00 pm

01 The Complementary Role of Ambient Ionization Methods in Analytical Science

Ambient Sampling & Ionization Interest Group
Presiders: Jacob Jordan, Chris Gill, Rabi Musah
Room 307-308

This workshop is intended to foster discussions about the topic of ambient ionization, a field that includes research, development and the application of many common methods of sampling and ionization for mass spectrometry. Prior workshop discussions have consistently brought up the question of how much validation is necessary for novel ambient ionization approaches and the complementary role of novel ambient ionization methods in analytical science with respect to the more widely used LC-MS approaches. We plan to continue these discussions in order to reach a consensus within the ambient ionization community and to demonstrate the complementary role of novel ambient ionization methods to those of LC-MS methods for routine measurements. The workshop will consist of lightning talks by students, professors, and industry experts in the field of ambient ionization and a panel discussion with experts that are involved in the validation and regulation process. The lightning talks will introduce attendees to cutting-edge developments in the field, whereas the panel discussion will aim to address the challenges and current solutions to addressing the barriers for validating and applying ambient ionization methods. We hope that these discussions will aid in identifying room for advancement in the very broad field of ambient ionization.

WEDNESDAY EVENING WORKSHOPS, 5:45 - 7:00 pm

02 The Interface of Biomarker Discovery, Clinical Algorithm Development and Regulatory Oversight

Clinical Chemistry Interest Group
Presiders: Timothy Collier, Matthew Crawford
Room 309-310

The increasingly multiplexable nature of liquid chromatography-mass spectrometry has made it a powerful tool for the discovery of not just single analyte biomarkers but also make possible the use of statistical algorithms to translate the simultaneous measurement of multiple analytes into indicators of patient health status and prognosis. As such, regulatory agencies including the NY State Department of Health and potentially the FDA, have begun to require descriptions of assay development processes, including the description of any statistical processes and software tools to derive analytical algorithms, from simple statistical approaches up to advanced artificial intelligence, machine learning, and/or natural language processing approaches. Regulatory agencies are also requiring detailed descriptions of discovery, test, and validation cohorts, power calculations to justify cohort sizes, and justification of said calculations.

These requirements have implications not only for commercial laboratories seeking to introduce a test to the market, but also for the academy, where most new biomarker discovery occurs. By encouraging discussion among workshop attendees and a panel of thought leaders in the field representing academic, government, and commercial laboratories, attendees should emerge with an understanding of new regulatory requirements on algorithms used in clinical measurements and what practices laboratories can adopt to meet these new requirements and enhance the translation of academic research into industry application.

03 Overcoming Challenges in Modern Ion Mobility

Ion Mobility MS Interest Group
Presiders: Christopher Chouinard, Elyssia Gallagher
Room 314-317

Ion mobility-mass spectrometry (IM-MS) has emerged as a powerful technique for chemical, biological, and environmental analysis over the last two decades. But despite significant advances in instrumentation, methods, and data analysis by commercial and academic researchers, there remain challenges to its routine implementation (i.e., sensitivity, resolution, data complexity, etc.). In this workshop, a brief opening presentation will describe the basics of modern ion mobility and highlight the biggest challenges in the field; we expect this presentation to be helpful for those hoping to learn more about ion mobility. Next, 4-5 speakers covering a variety of IM hardware/applications will present brief (~5 mins) research vignettes emphasizing new approaches to dealing with the highlighted challenges. Importantly, we aim for these presentations to spark curiosity amongst the audience members. Finally, the speakers will form a panel to motivate discussion of the future directions of ion mobility in light of these current challenges. We expect this format will encourage participation and learning for novice and expert users alike.

04 Single-cell proteomics by Mass Spectrometry: Best Practises and Current Challenges

Independent
Presiders: Erwin Schoof, Aline Martins, Samuel Payne
Ballroom II

With the mind-boggling pace of technical developments, single-cell proteomics by Mass Spectrometry (scp-MS) is a field poised for major discoveries across all life science in the very near future. As a field still very much in its infancy, there is an ever-increasing need for standardization, and clear communication about protocols, data acquisition parameters and performance statistics. This workshop will aim to gather some of the leading experts in the field, and run as a guided roundtable discussion to explore key aspects such as: 1) "labeled vs. label-free", 2) DIA library matching, friend or foe?, 3) Sample preparation options, 4) The future of scp-MS: throughput vs. depth and PTMs, 5) How we are going to apply scp-MS in the future - what real biological questions can we unlock using scp-MS?

We will recruit ~5-7 leading experts for the roundtable, with track record spanning all major aspects (technological developments, sample preparation, biological application and computational modeling), and prepare ample questions to be discussed in a facilitated manner and guided by the three listed workshop presiders. Industry representatives from e.g. Bruker, ThermoFisher, Cellenion, Evosep, etc. will also be invited to participate. Questions and feedback from the audience will be encouraged, to enable interactive and stimulating discussions on timely topics that are relevant for the field's future long-term success.

05 Ion Trap MS: Using Trapping Mass Analyzers Beyond Mass Analysis

Ion Trap MS Interest Group
Presider: Kenneth Lee
Ballroom I

Mass Spectrometry (MS) has evolved as an analytical technique to measure more chemical information than just mass. Various instrumental advances—including advances in ionization, gas-phase dissociation, and gas-phase chemistry—have provided unique experiments that position MS as a powerful tool for the analysis of chemical structures. A key player in these developments is the idea of trapping and interrogating ions. Primarily the 3D and linear quadrupole ion traps have demonstrated remarkable flexibility and utility in performing a wide variety of gas-phase measurements and experiments because of their ability to probe and analyze ions in one device. Recently, however, other trap-based mass analyzers that are typically viewed as only high-resolution mass analyzers have demonstrated similar capabilities of ion isolation and dissociation, as well as measure collision cross sections and perform charge deconvolution.

This workshop will feature research groups that are developing chemical analysis methods using trap-based mass analyzers. Some examples include measuring collision cross sections using an FT-ICR and single-ion charge measurements using an Orbitrap. Each group representative will provide a short overview of the method, followed by an open discussion with the presenters serving as panelists. The main discussion points will focus on looking back to what drove these unique ion trap innovations and looking forward to where ion trap innovation is progressing and where it could address unsolved analytical needs. The goals of this workshop are to first, provide context and perspective on the unique role ion traps in MS for those who are less familiar with ion trap MS, and second, provide an opportunity for discussion for potential future directions of ion traps beyond standard mass analysis.

06 Harmonizing Lipidomics through an Interactive Checklist

Lipids & Lipodomics Interest Group
Presiders: Jeff McDonald, Jace Jones
Ballroom III

The Lipidomics Minimal Reporting Checklist has been established and is continuously curated by the Lipidomics Standard Initiative (LSI) an interest group affiliated with the International Lipidomics Society (ILS). The checklist is based on consensus-driven guidelines for lipidomics implemented in a publicly available web-based questionnaire. Its main purpose is to describe all essential steps of lipidomic experiments in a standardized way. The checklist output, a PDF document, is intended to assist editors and referees in reviewing research studies containing lipidomic data. The checklist can be viewed as guideline on 'good lipidomics practice' for both new and experienced lipidomic investigators. The checklist covers preanalytics, lipid extraction, analytical platform, lipid identification and quantitation, quality control, method validation, and reporting summary. In addition to reviewing the ILS checklist, we will also provide examples of lipidomic reporting in literature highlighting the need for increased consensus and oversight for lipidomic research.

07 MS Imaging: Challenges and Recent Developments in Sample Preparation

Imaging MS Interest Group
Presiders: Andreas Roempp, Katerina Djambazova
Ballroom IV

Sample preparation is an integral part of any mass spectrometry imaging workflow. Approaches are very diverse and depend (among others) on the sample's characteristics, how it's prepared, and the employed MSI approach. We will cover the initial steps of the MS imaging workflow - from sample procurement and storage, up to tissue pre-treatment and matrix application (if any). Major topics will be tissue preservation/handling, sectioning, on-tissue modifications, and matrix application.

We are interested in discussing challenges that arise when developing protocols for the extraction of metabolites, lipids, glycans, and other analytes from biological specimens before MSI. Here, presenters are encouraged to share on negative results and failed experiments to encourage lively discussions among the workshop presenters and the audience.

This workshop aims to highlight established and novel methods that allow for the interrogation of historically understudied molecular classes, and/or samples that pose a challenge to standard MSI sample workflows.

Organization:
This workshop will be presented in two parts. First, multiple speakers will briefly describe their methodologies, including the pros and cons, for sample preparation in a series of flash talks. Second, the speakers will serve as a panel for a general discussion with the audience on the challenges that exist within the field, where they will identify opportunities and discuss future strategies. The audience is encouraged to come prepared with questions and ideas. An online tool will be used to ensure direct participation of the audience.

08 Metaproteomics: Less is (Balti)more

Independent
Presiders: Robert Hettich, Mary Lipton, Timothy Griffin
Room 336

Mass spectrometry-based metaproteomics research has experienced rapid growth due to its ability to help characterize complex microbial communities and is likely to become a central approach for understanding dynamic microbiome functions. Despite its value, metaproteomics offers analytical and bioinformatic challenges beyond those encountered in traditional, single-organism MS-based proteomics. Metaproteomics researchers who have participated in international metaproteomics conferences will initiate the brainstorming sessions to both inform and facilitate participation in a discussion about some specific opportunities to help propel this field forward. Various research groups attending the conference will also participate in the discussion. As a coordinated research effort, a global initiative has been developed for the dissemination of metaproteomics fundamentals and microbiome research applications. Members of the Metaproteomics Initiative (www.metaproteomics.org) will present updates on two recent CAMPI (Critical Assessment of Metaproteome Investigation) benchmark studies on sample preparation and functional annotations, and future projects that will be designed to propel this field forward. To highlight other on-going community effort in metaproteomics, panel members will also provide highlights on the International Metaproteomics Symposium and global challenges.

09 Cutting-Edge Structural Proteomics and Interactome Analysis: Advances in Covalent Labeling, Crosslinking, and Emerging Technologies

Covalent Labeling & Cross-Linking Interest Group
Presider: Saiful Chowdhury
Room 339-340

Crosslinking technology and covalent labeling have gained increasing popularity due to their ability to study protein structures and interactions in their native environments. While these techniques have primarily been applied in focused experimental settings, expanding their capabilities requires new tools and innovative applications. To push the boundaries of structural proteomics and interactome research, novel strategies must be explored.

This session will highlight emerging crosslinking and covalent labeling approaches and their role in advancing protein structural biology and interactome analysis. A particular emphasis will be placed on applications in in vivo settings, where these techniques offer unique advantages in capturing dynamic protein interactions within living systems. This year, we will explore how the combination of multiple complementary techniques can enhance our understanding of complex proteomes and biological networks. The session will begin with a series of short presentations featuring groundbreaking research and novel methodologies. These talks will be followed by an interactive discussion, facilitated by expert panelists who will provide insights into the latest advancements, technical challenges, and future directions of the field.

Attendees will have the opportunity to engage with leading researchers, ask questions, and contribute to discussions on how to further develop and integrate these technologies for broader applications. By bringing together experts in crosslinking, covalent labeling, and structural proteomics, this session aims to foster collaboration, inspire innovation, and shape the next generation of tools for studying protein interactions in complex biological systems.

10 Entrepreneurship in Mass Spectrometry: Non-Traditional Pathways for Scientific Innovation

Independent
Presiders: Lindsay Pino, Paula Burton
Room 341-342

Mass spectrometry (MS) has revolutionized fields such as drug discovery, diagnostics, and biomarker research. However, the entrepreneurial potential within MS remains underexplored by many scientists. This workshop aims to illuminate the opportunities for innovation and entrepreneurship in the MS field. Attendees will learn about pathways to commercializing MS technologies, from developing instrumentation and consumables to creating applications in healthcare, environmental science, and beyond.

The session will feature insights from successful MS entrepreneurs and experts who transitioned from academia to business. Topics will include navigating startup ventures, industry collaborations, intellectual property management, and funding strategies like grants and venture capital. The format will include short presentations followed by an interactive panel discussion with ample opportunities for audience engagement during Q&A and networking.

This workshop is ideal for those curious about translating their research into impactful business ventures or collaborating with industry partners. By demystifying the entrepreneurial process and sharing real-world experiences, the session will inspire attendees to explore new avenues for advancing science through entrepreneurship.

11 Plastics, Polymers, and Replacement Chemicals Part 2: Tracking the Right Compounds in Humans and the Environment

Energy & Biofuels, Exposomics, and Polymeric Materials Interest Groups
Presiders: Pablo Gago-Ferrero, Nina Zhao, Ruth Marfil-Vega
Room 343-344

This workshop will take a deep dive into the challenges and opportunities posed by plastics, polymers, and replacement chemicals to address sustainability and (eco-)toxicological effects. With growing concerns over the impact of emerging and unknown contaminants, we will critically examine whether we are looking at the right chemicals in exposomics research and connection with their fate in the environment.

Designed as a participatory workshop, the session will feature short, focused talks addressing key questions, followed by in-depth discussions. A major theme will be the role of databases in identifying plastic-associated compounds: what exists, what is used, where the gaps lie, and what is needed for the future. By bringing together experts from different disciplines, the session aims to foster critical dialogue and advance collaborative efforts in environmental exposomics.

12 Forensics & Homeland Security: Emerging Technology for the Forensic Chemist

Forensics & Homeland Security Interest Group
Presider: Ryan Bain
Room 345-346

Emerging technology which is nearing commercialization (or has recently been commercialized) which has been demonstrated on forensic and homeland security applications will be the focus of this session. Emphasis will be placed on breakout discussions focused on: A) emerging technology being embedded in the forensic laboratory, B) issues adapting workflows to emerging technology, C) particularly challenging analyses which are currently not being addressed, and D) measurements that could not be made previously which have been made possible by new mass spectrometry systems. There will be talks from those working on beta and first-generation versions of new instrumentation, applications of new sources on existing technology, and practical examples from forensic practitioners currently integrating these technologies.

13 Current Hot Topics in Bioanalysis from Hybrid Assays, Biomarker Assay Validation to AI

Regulated Bioanalysis Interest Group
Presiders: Jian Wang, Wenkui Li, Fabio Garofolo
Room 347-348

The RBIG workshop at ASMS this year will discuss current challenging topics in Bioanalysis with experts in Pharmaceutical and CRO industry and regulatory agencies to provide insights, guidance, and perspectives.

1. Update on hybrid LC-MS/MS assays: novel PK bioanalytical approaches in the bioanalysis of various ADCs (revisiting with new strategies) - bioanalytical strategies illustrated by case studies.
2. HRMS vs QQQ for Oligo/ASO analysis (Discovery to Regulated): There has been a recent explosion of interest in oligonucleotide therapeutics. This includes siRNA, antisense oligos (ASOs) and even oligo conjugates (ARCs/AOCs). This has led to an increased emphasis and need for developing sensitive and selective Bioanalytical methods.
3. FFP validation of biomarker assays.
4. Value of incurred samples in the bioanalytical method cross validations from the perspective of regulatory requirements and the operations in pharmaceutical and CRO companies.
5. Trackability of internal standards for small and large molecules.
6. AI - Using AI to help in data processing of LCMS data as well as report generation: AI can be a huge advantage in helping to improve efficiency and accuracy of bioanalytical data. This is a relatively new field and there are several companies working with various partners to investigate this area. Questions are should we centralize this effort (with various vendors - maybe similar to skyline) or do we let each company identify the best path forward and work independently with various providers. When is the right time to get involved or move forward with this area.

14 JASMS - The Life Cycle of a Manuscript and Joining the Reviewer Pipeline

Independent
Presiders: Jenny Brodbelt, Facundo Fernandez
Room 349-350

Launched in 1990, the Journal of the American Society for Mass Spectrometry (JASMS) is a premier science journal that covers all aspects of mass spectrometry, including fundamentals, instrumentation and applications of mass spectrometry in all fields (chemistry, biology, physics, geology, environmental science, and life sciences, among others). This Workshop will focus on the "nuts and bolts" of the manuscript submission and review pipeline of JASMS. It will cover how manuscripts are handled - from the time a manuscript is first submitted to the time the paper is published. The critical role of the reviewers in this process will be featured, including tips for being a great reviewer.