Welcome to the 64th ASMS Conference on Mass Spectrometry and Allied Topics. Conference program activities and exhibit booths are in the Henry B. Gonzalez Convention Center. Corporate Member hospitality suites are located in the Grand Hyatt Hotel.

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TABLE OF CONTENTS

Titles in the following sections are provided by authors. The complete abstracts are available online: www.asms.org

Registration is open 1:00 - 5:00 pm on Saturday, 10:00 am - 8:00 pm on Sunday, and 7:30 am - 5:00 pm on Monday - Thursday.

Attention Undergraduate Students and First Time (at ASMS) Graduate Students

4:00 - 5:00 pm, Sunday, Stars Ballroom 1, level 3
Plan Your Strategy: What to See and Do at ASMS

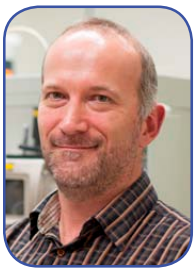
Sunday Tutorial Session, 5:00 - 6:30 pm

Hall 1, level 1

5:00 - 5:45 pm
Forensic Mass Spectrometry
#TellMeSomethingIDontKnow

Facundo Fernandez
Georgia Institute of Technology

Glen Jackson
West Virginia University



5:45 - 6:30 pm
An Analyte's Journey from Solution into the Gas Phase

Lars Konermann
University of Western Ontario

Sunday Conference Opening, 6:45 - 7:45 pm

Hall 1, level 1

Welcome

Vicki H. Wysocki
The Ohio State University
ASMS Vice President for Programs

A Molecular Arsenal Against Ebola Virus

Erica Ollmann Saphire
The Scripps Institute-La Jolla

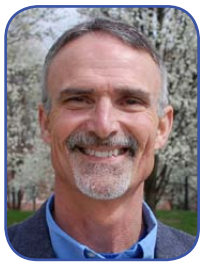
Sunday Welcome Reception, 7:45 - 9:00 pm

Poster/Exhibit Hall. Conference name badge is required.

PLENARY SESSIONS

Monday Award Lecture, 4:45 - 5:30 pm

Hall 1, level 1



Award for a Distinguished Contribution in Mass Spectrometry

Scott A. McLuckey
Purdue University

Tuesday Award Lecture, 4:45 - 5:30 pm

Hall 1, level 1

Biemann Medal

Kristina Håkansson
University of Michigan

Thursday Plenary Lecture, 4:45 - 5:30 pm

Hall 1, level 1

More than the Sum of its Parts: Collective Phenomena in Living Systems, from Single Molecules to Flocks of Birds

William Bialek
Princeton University

Don't miss

- **ASMS Meeting, Wednesday, 4:45 - 5:30 pm**
  Stars Ballroom 1, level 3
  Enjoy a beverage while you applaud awards, hear about new initiatives, and more!

- **Closing Event, Thursday, 6:30 - 9:00 pm**
  Briscoe Western Art Museum

Let's celebrate! Stroll to the Briscoe for a western barbecue under the live oak trees of the terrace overlooking the San Antonio Riverwalk. View the exhibits which preserve and interpret the art, history, and culture of the American West. The evening continues with music, dancing and karaoke. Ticket is required, $30.

Oral Sessions are 8:30 - 10:30 am and 2:30 - 4:30 pm Monday through Thursday.

Level 1
Session A (MOA, TOA, WOA, ThOA) ..... Hall 1
Level 2
Session B (MOB, TOB, WOB, ThOB)..... Room 221
Level 3
Session C (MOC, TOC, WOC, ThOC)..... Stars 1
Session D (MOD, TOD, WOD, ThOD)..... Stars 2-3
Session E (MOE, TOE, WOE, ThOE)..... Stars 4
Session F (MOF, TOF, WOF, ThOF)..... Hemisfair 3
Session G (MOG, TOG, WOG, ThOG)..... Hemisfair 2
Session H (MOH, TOH, WOH, ThOH)..... Hemisfair 1

Oral Presentations are projected from ASMS computers running Microsoft Office. Speakers are required to use the ASMS computers for their presentations.

Speakers must load presentations at least one day prior to their talks. The speaker room is 222, level 2. The room is open with a technician according to this schedule:

Sunday: 10:00 am - 8:00 pm
Monday through Thursday: 7:30 am - 2:00 pm

Posters and Exhibit Booths are in the Poster/Exhibit Hall. The Hall is open:

Sunday Reception.....7:45 pm - 9:00 pm
Monday - Wednesday .....7:30 am - 8:00 pm
Thursday .....7:30 am - 3:00 pm

Poster Set-Up is 7:30 am on the day scheduled. **Refer to the poster numbers in this final program for board assignments.** A counter for poster supplies is near the main entrance to the Hall.

Poster Sessions are 10:30 am - 2:30 pm, Monday through Thursday.

Poster Authors must be present at posters on scheduled days at these times.

10:30 am - 1:00 pm .....Odd-numbered posters
12:00 - 2:30 pm .....Even-numbered posters

Presenters who must leave a poster unattended should post a return time. Presenters should wear "Poster Presenter" badges which are available at the poster supply counter.

Posters should not be removed before 7:30 pm on Monday, Tuesday and Wednesday. Thursday posters should be removed at 2:30 pm.

Lunch Concessions in the Poster/Exhibit hall offer a variety of options to dine and network while taking a break from posters. Concessions are open 11:00 am - 2:00 pm, Monday through Thursday.

Exhibitors must staff exhibit booths as follows:

Sunday Reception.....7:45 pm - 9:00 pm
Monday - Thursday .....10:30 am - 2:30 pm

Workshops are 5:45 - 7:00 pm on Monday, Tuesday, and Wednesday. Light refreshments are provided in the pre-function areas on level 2 and level 3.

Dinner Break 7:00 - 8:00 pm is time for a breath of fresh air before the opening of hospitality suites at 8:00 pm.

Special Program for Undergraduate Students

- **Sunday, 7:30 - 9:00 pm, Poster competition**, Poster/Exhibit Hall
- **Monday, 11:30 am - 1:00 pm, Meet the Experts.** Lunch tables reserved for undergraduate students in the Poster/Exhibit Hall. Free vouchers for lunch will be provided at the tables. Arrive promptly at 11:30 am to obtain your voucher.

Free WiFi Access is provided in the Poster/Exhibit Hall. Computers are provided at stations throughout the convention center.

Conference Proceedings will be published online. Submission to the Proceedings does not constitute publication and does not jeopardize the rights of authors to publish contents of their submissions. **Speaker web casting slides will be printed to PDF and used for speakers who fail to submit an extended abstract.**

Web Casting includes tutorial lectures, plenary lectures, and oral sessions. Web casting will be available to conference attendees for three months after the conference. ASMS does not retain rights to material included in web castings. To access the presentations, go to www.asms.org and login. The link to "web casting" is on the annual conference page.

Corporate Hospitality Suites are open to all attendees from at least 8:00 - 11:00 pm Monday - Wednesday. Suites are also open during the day for one-on-one or small group meetings (no more than 25 people) by appointment only. Interested attendees should contact their sales representative for more information. Companies may also use their suites for breakfast seminars. Suites are located in the **Grand Hyatt Hotel**.

Career Center is located in the Poster/Exhibit Hall. The Career Center is open to all conference attendees. Applicants and employers must enter resumes and employment opportunities online. There are computers in the center for searching the database of candidates and positions. Interview rooms must be reserved one day in advance.

Sunday .....7:45 - 9:00 pm
Monday - Wednesday .....7:30 am - 5:00 pm
Thursday .....7:30 am - 2:30 pm

Guest Registration ($10) includes designated name badge and entrance to the Sunday evening reception. The badge does not gain entrance to oral sessions or the Poster/Exhibit Hall.

Single Use/Family Restrooms are available on each level.

Mother's Room is Room 215 (for mothers only). From the Ballroom Level proceed to the Hemisfair Ballroom foyer and take escalators down. Room 215 is on the right side of the foyer space.

Corporate Breakfast Seminars are located in the convention center and at the Grand Hyatt. Reservations are required and may be made at company exhibit booths.

MONDAY	
Company	**Convention Center Room**
Advanced Chemistry Development	Room 224
Agilent Technologies (at Grand Hyatt)	Lone Star Ballroom DEF
Bruker Daltonics	Room 225CD
LECO	Room 303A
Matrix Science	Room 302BC
SCIEX	Room 304A
SCIEX	Room 305
Shimadzu	Room 220
Thermo Fisher Scientific (at Grand Hyatt)	Republic ABC
Waters Corporation (at Grand Hyatt)	Texas Ballroom BC
Waters Corporation	Room 301BC
Waters Corporation	Room 301A
TUESDAY	
Company	**Convention Center Room**
Agilent Technologies (at Grand Hyatt)	Lone Star Ballroom DEF
Biotage	Room 225B
Bruker Daltonics	Room 225CD
GL Sciences	Room 301A
LECO	Room 303A
Matrix Science	Room 302BC
MilliporeSigma	Room 303BC
New Objective	Room 305
Prosolia	Room 224
SCIEX	Room 302A
SCIEX	Room 304A
SCIEX	Room 304BC
Shimadzu	Room 220
Thermo Fisher Scientific (at Grand Hyatt)	Republic ABC
Waters Corporation (at Grand Hyatt)	Texas Ballroom BC
Waters Corporation	Room 301BC
WEDNESDAY	
Company	**Convention Center Room**
Agilent Technologies (at Grand Hyatt)	Lone Star Ballroom DEF
Bruker Daltonics	Room 225CD
LECO	Room 303A
New Objective	Room 305
SCIEX	Room 302A
SCIEX	Room 304A
SCIEX	Room 304BC
Shimadzu	Room 220
Thermo Fisher Scientific (at Grand Hyatt)	Republic ABC
Waters Corporation (at Grand Hyatt)	Texas Ballroom BC
Waters Corporation	Room 301BC
THURSDAY	
Company	**Convention Center Room**
SCIEX	Room 304A
Shimadzu	Room 220
Thermo Fisher Scientific	Room 225CD

Media Events are scheduled for members of the press and financial institutions. All will be held in the Grand Hyatt Hotel.

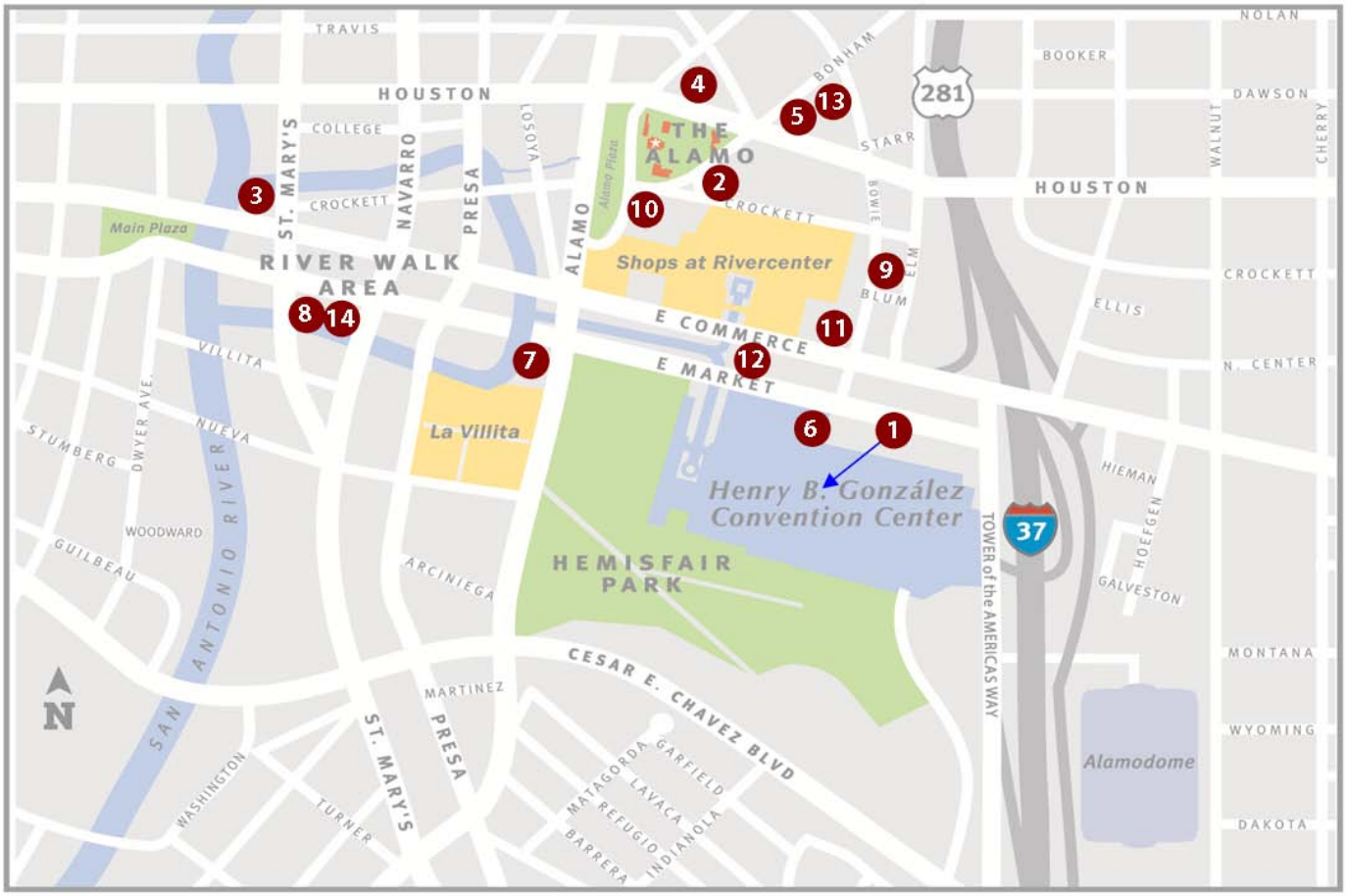
Company	Monday	Grand Hyatt Hotel Location
Bruker	8:00-9:00 am	Texas Ballroom A
Shimadzu	9:30-10:30 am	Texas Ballroom EF
SCIEX	11:00-12:00 pm	Lone Star Ballroom ABC
Agilent Technologies	1:30-2:30 pm	Lone Star Ballroom DEF
Thermo Fisher Scientific	3:00-4:00 pm	Texas Ballroom D
Waters Corporation	4:30-5:30 pm	Texas Ballroom BC

Conference Regulations

- **Name badge is required** for all conference sessions, including the Poster/Exhibit Hall and the employment center.
- **No smoking** is permitted in the convention center.
- **All devices** must be silenced and screens darkened in oral sessions.
- **No photography** or recording is allowed in oral sessions or in the poster/exhibit Hall.
- **Parents.** Planned conference sessions and hospitality suites may not be appropriate for children. Please respect the interests of your colleagues by allowing them to attend activities without disruption and without concern for the safety of children. Strollers, child backpack carriers or similar devices for child transport are prohibited in the Poster/Exhibit Hall and hospitality suites.
- **Material presented or displayed** at the ASMS Conference, including but not limited to orals, posters, workshops, exhibit booths and hospitality suites, is the intellectual property of the presenter and may not be recorded, photographed, quoted, disseminated or transmitted by summary in any form without express written authority of the author.
- **The placement of advertising** in the meeting area is prohibited. There are poster boards and tables in the Poster/Exhibit Hall for approved announcements.
- **Hardware, accessories or any items for sale** may be displayed only in corporate exhibit booths and hospitality suites.
- **Designated publisher tables** in the conference registration area are for the display of books and journals and must be reserved in advance.
- **There are tables in the registration area for authors** who wish to display their books. Authors may use a table to promote their books, sign copies, and speak with members. Table space must be reserved at conference registration.
- **No organized activities (even off-site)** other than those approved by ASMS are allowed during the conference week (5:00 pm on Sunday through 6:00 pm on Thursday).
- **Corporate hospitality suites** may be used during the daytime hours of 8:00 am – 8:00 pm for one-on-one and small group meetings (no more than 25 persons per organization) by appointment only (no walk-ins). No music, programs, seminars, or refreshments may be included in these private, business meetings.
- **Corporate or institutional logos** on slides or posters may appear only one time in the presentation.

Hotel	Telephone
1. Convention Center	(210) 207-8500
2. Crockett Hotel	(210) 225-6500
3. Drury Inn & Suites Riverwalk	(210) 212-5200
4. Emily Morgan	(210) 225-5100
5. Fairfield Inn & Suites	(210) 212-6262
6. Grand Hyatt San Antonio	(210) 224-1234
7. Hilton Palacio del Rio	(210) 222-1400

Hotel	Telephone
8. Homewood Suites by Hilton	(210) 222-1515
9. La Quinta Inn & Suites	(210) 222-9181
10. Menger Hotel	(210) 223-4361
11. Marriott Rivercenter	(210) 223-1000
12. Marriott Riverwalk	(210) 224-4555
13. Springhill Suites San Antonio	(210) 222-2121
14. Westin Riverwalk	(210) 224-6500



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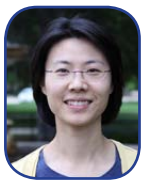

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to these members who were elected to the ASMS Board

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Jennifer Watson
Cindi Pettit, Lola Priest, Miquela Sena
Marin Walker, Brent Watson

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Bioinformatics for MS	Sangtae Kim Meena Choi
Biotherapeutics	Damian Houde Ashley Ruth
Clinical Chemistry	Tim Garrett Brian Rappold
Data Independent Acquisition	Ludovic Gillet Jarrett Egertson
Drug Metabolism & Pharmacokinetics	Kevin Bateman Philip Tiller
Energy, Petroleum & Biofuels	Mark Barrow Lateefah Stanford
Environmental Applications	Marc Engel Chris Gill
Exposomics	David Balshaw Anthony Macherone
Flavor, Fragrance and Foodstuff	Walter Hammock David Schroeder
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FTMS	David Kilgour Don Smith
Fundamentals	Alessandra Ferzoco Michael Van Stipdonk
H/D Exchange, Covalent Labeling & Cross Linking	Joshua Sharp David Weis
Imaging MS	Vilmos Kertesz Raf Van de Plas
Ion Mobility MS	Erin Baker Stephen Valentine
Ion Trap MS	Daniel E. Austin Zheng Ouyang
Lipids & Lipodomics	Christer Esjing Todd Mitchell
LC/MS Related Topics	Michael Bereman Brent Dixon
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Metal Ion Coordination Chemistry	Cheng Lin Alex Shvartsburg
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Pharmaceuticals	Christine Gu Matthew Schenauer
Photoionization MS	Jack Syage Ralf Zimmerman
Polymeric Materials	Stephen Rumbelow Gyorgy Vas
Regulated Bioanalysis	Jian Wang
Undergraduate Research in MS	Elaine Marzluff Megan Gessel
Young Mass Spectrometrists	Violet Lee Kristin Wildsmith

Committees

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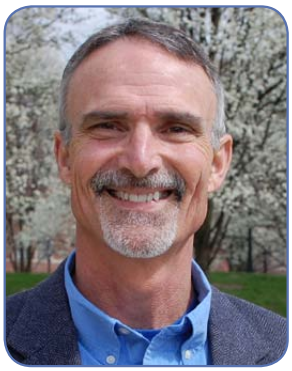
Education	Igor Kaltashov, Chair Allessandra Ferzoco Damian Houde Dil Ramanathan Elizabeth Stemler
Nominating	Gary Glish, Chair Ben Garcia Michael Easterling Ljiljana Pasa-Tolic David Tabb
Publications	Facundo Fernandez, Chair Lorna De Leoz Leslie Hicks Richard Perry Will Thompson Joseph Loo (*ex officio*)
Sanibel Conference	Erin Baker, Chair Fanyu Meng Victor Ryzhov Patrick Griffin

AWARD FOR A DISTINGUISHED CONTRIBUTION IN MASS SPECTROMETRY
2016 Recipient: Scott A. McLuckey
Award Lecture: 4:45 pm Monday, Hall 1, level 1



Dr. Scott A. McLuckey is the recipient of the 2016 ASMS Award for a Distinguished Contribution in Mass Spectrometry for his pioneering contributions to the understanding of the gas-phase ion/ion reactions of polyatomic molecules and their applications in analytical mass spectrometry.

Gas-phase ion chemistry has played a central role in mass spectrometry since its inception. Unimolecular and ion/neutral reactions, for example, have been observed, studied, and used throughout the entire history of molecular mass spectrometry. While the study of ion/ion reactions originated with J.J. Thomson and has been pursued within the context of plasma chemistry, atmospheric chemistry, and chemistry in the interstellar medium, ion/ion reactions have not been exploited in mainstream mass spectrometry until relatively recently. Keys to this development have been the introduction of techniques capable of generating multiply charged ions, electrospray being chief among them, and the use of electrodynamic ion traps, which can store efficiently oppositely charged ions in overlapping time and space. McLuckey and co-workers, beginning at Oak Ridge National Laboratory in the mid-1990s and continuing at Purdue University since 2000, initiated and sustained a line of research employing electrospray and ion traps that has revealed a wide and expanding array of ion/ion reactions that significantly expand the scope of tandem mass spectrometry, particularly in biological mass spectrometry.

Dr. McLuckey's efforts in this area have focused both on understanding the dynamics of ion/ion reactions and on developing ion/ion reactions for analytical applications. He and his co-workers demonstrated that ion/ion reactions in ion traps can be both highly efficient and fast. Furthermore, ion/ion reactions are universal in that some form of reaction will occur for any combination of oppositely charged ions. Dr. McLuckey's initial work was focused on proton transfer, and to a lesser extent, electron transfer reactions. Proton transfer reactions have been demonstrated to be particularly useful for charge state manipulation and have been used for mixture analysis, concentrating charge, inverting ion charge, etc. Electron transfer has proved to be particularly useful for generating structural information. For example, the discovery in Donald Hunt's lab of reagent anions that transfer electrons to peptide and protein cations led to the development of electron transfer dissociation. These developments, which leveraged much of what was known about proton transfer ion/ion reactions in ion traps, catalyzed the commercial introduction of ion/ion reactions tools that rely on electrospray and ion traps.

In recent years, McLuckey's group has expanded ion/ion chemistry to include selective metal ion insertion/removal and functional group specific covalent bond formation. Collectively, these chemistries, along with proton and electron transfer, significantly expand the power of MS/MS in characterizing peptides, proteins, oligonucleotides and lipids. The wide-ranging efforts of McLuckey and his colleagues in instrumentation, fundamentals, and applications of ion/ion reactions over the past two decades constitute a distinguished contribution to mass spectrometry.

Dr. Scott A. McLuckey is the John A. Leighty Distinguished Professor of Chemistry at Purdue University, West Lafayette, IN.

RON A. HITES AWARD Outstanding Research Publication in *JASMS*
Award Presentation: ASMS Meeting, 4:45 pm Wednesday, Stars Ballroom 1, level 3

The Ron Hites Award recognizes an outstanding publication of original research, based on a paper's innovative aspects, technical and presentation quality, likely stimulation of future research and impact on future applications. The award is named to honor Professor Ron Hites of Indiana University, who led the creation of *JASMS* in 1988 while president of ASMS. The award includes $2,000 and a certificate for each author.

The 2016 award recognizes Kevin Pagel, Max Planck Society Berlin, and, co-authors Waldemar Hoffmann and Johanna Hofmann for their paper Energy-Resolved Ion Mobility-Mass Spectrometry: A Concept to Improve the Separation of Isomeric Carbohydrates: *JASMS* (2014) 25, 471-479.

Left to right Johanna Hofmann, Kevin Pagel, and Waldemar Hoffmann

BIEMANN MEDAL
2016 Recipient: Kristina "Kicki" Håkansson
Award Lecture: 4:45 pm Tuesday, Hall 1, level 1

Dr. Kristina "Kicki" Håkansson has been awarded the 2016 Biemann Medal for her contributions related to her work to develop and elucidate the mechanisms of electron-based activation methods, including electron capture dissociation, electron detachment dissociation, and electron induced dissociation. She has applied these electron-based activation methods to identify and characterize biological molecules from a number of classes, including peptides, oligonucleotides, and oligosaccharides.

The challenges associated with structural characterization of increasingly complex biological molecules has inspired the development of many new activation methods. Ones involving the attachment or detachment of an electron to an ion have shown great promise and have motivated renewed interest in gas-phase radical ion chemistry, both areas which are hallmarks of the Håkansson group. Dr. Håkansson has focused on deciphering the mechanisms of electron-activated dissociation and shown the outstanding utility of these methods for analysis of nucleic acids, oligosaccharides, and peptides including ones with labile modifications like phosphorylation. Negative ion electron capture dissociation (discovered in the Håkansson laboratory) in particular has shown excellent performance for characterization of phosphorylated and sulfated peptides ionized in the negative mode. Her group has also shown that electron-activated dissociation methods are gentle enough to allow preservation of higher order structures of nucleic acids.

Dr. Håkansson is a professor in the Department of Chemistry at the University of Michigan in Ann Arbor.

2016 RESEARCH AWARDS
Award Presentation: 4:45 pm Tuesday, Hall 1, level 1

The Research Awards are fully funded by Thermo Fisher Scientific and Waters Corporation in the amount of $35,000 each.

Sponsored by
Thermo Fisher Scientific

Ronghu Wu
Georgia Institute of Technology

Sponsored by
Waters Corporation

Etienne Garand
University of Wisconsin-Madison

2016 POSTDOCTORAL AWARDS

Award Presentation: ASMS Meeting, 4:45 pm Wednesday, Stars Ballroom 1, level 3

Four awards in the amount of $10,000 each are intended to promote the professional career development of postdoctoral fellows in the field of mass spectrometry. Activities funded by these awards include conference and workshop attendance, travel to other mass spectrometry laboratories, purchase of books and/or software. The awards are open to ASMS members who are postdoctoral fellows within three years of completing a Ph.D. or equivalent degree. Applicants must be currently appointed as a postdoctoral fellow in North America (e.g., in academia, industry, a government or national laboratory or at a research institute). Details and an application are posted to asms.org.

John Cahill
Oak Ridge National Laboratory

Andrew DeBlase
Purdue University

Catherine Going
Stanford University

Pengyuan Liu
The Wistar Institute

2016 STUDENT AWARDS

Award Presentation: ASMS Meeting, 4:45 pm Wednesday, Stars Ballroom 1, level 3

ASMS supports up to ten awards of $1,000 for graduate students and ten awards of $500 for undergraduates. Applications and details for these awards are posted to asms.org. The deadline for submission is January 15.

Graduate Student Awards

Xibei Dang, Florida State University

Zachery Gregorich, University of Wisconsin-Madison

Nathan Hendricks, University of California, Riverside

Johanna Hofman, Max Planck Society

Ramsunder Iyer, University of Tennessee

Brent Kuenzi, University of South Florida

Anumita Saha-Shah, Indiana University

Stephen Sciuto, The University of Toronto

Candice Ulmer, University of Florida

Yejing Weng, Chinese Academy of Sciences

Undergraduate Student Awards

Willem Duckworth, Clarkson University

Carlo Eikani, Saint Mary's College of California

Matthew Kazaleh, University of Florida

Yekaterina Kori, University of Massachusetts Amherst

Rebecca Marin, Florida International University

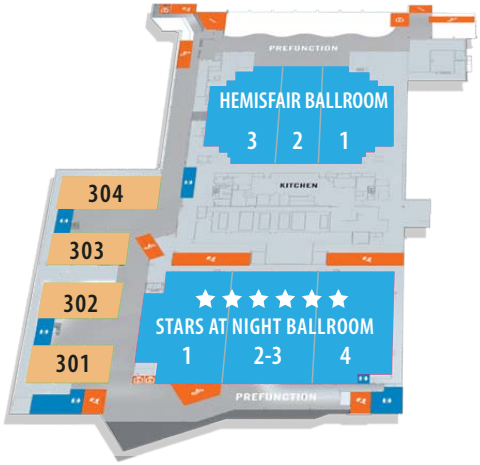
Rachel Martini, University of Michigan

Evan Perez, Duquesne University

LEVEL 3 - BALLROOM LEVEL

Sessions C (Stars 1)
Session D (Stars 2-3)
Session E (Stars 4)
Session F (Hemisfair 3)
Session G (Hemisfair 2)
Session H (Hemisfair 1)

Workshops, Breakfast Seminars (Rooms 301 - 305



LEVEL 2 - MEETING LEVEL

Sessions B (Room 221)

Workshops, Breakfast Seminars (Rooms 220 - 225)

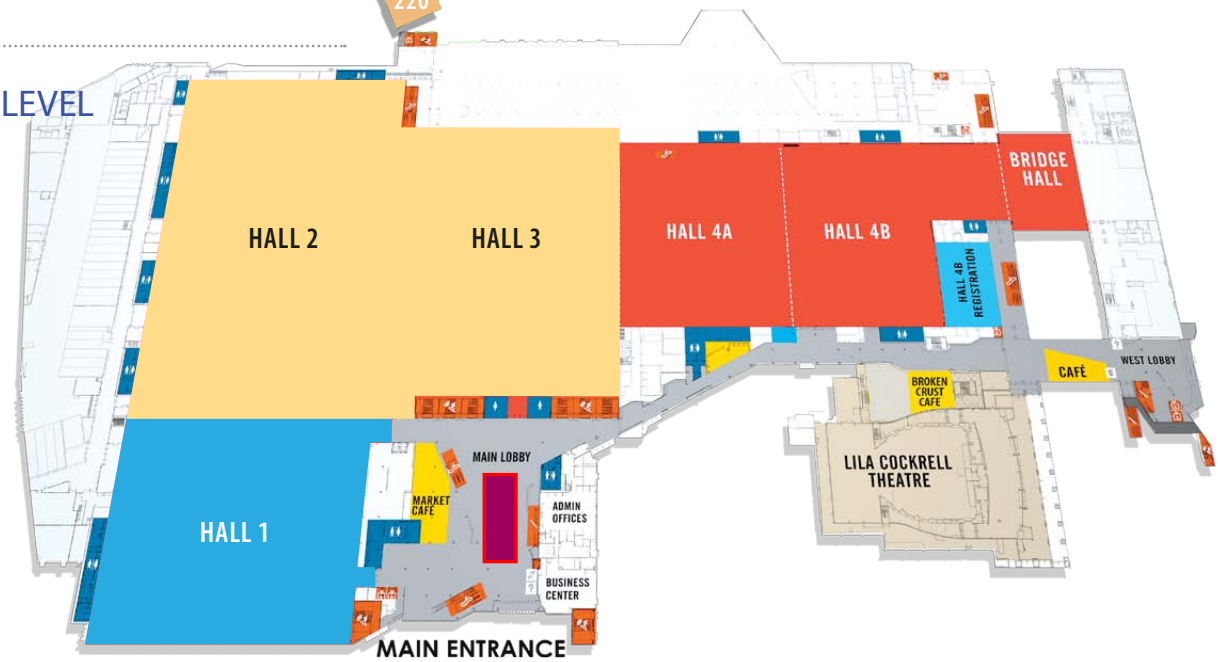
Speaker Room (Room 222)

LEVEL 1 - STREET LEVEL

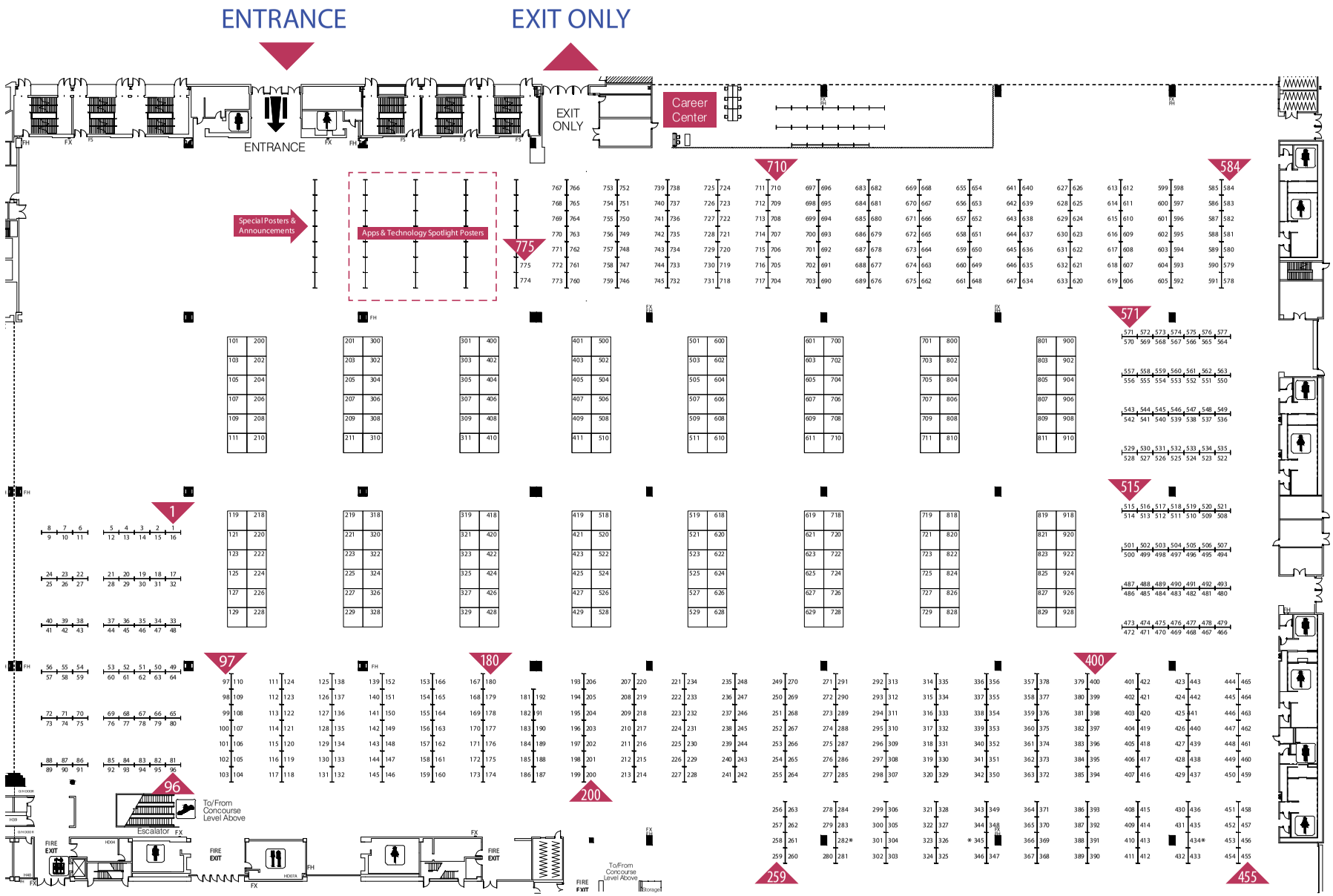
Posters, Exhibits, Career Center (Halls 2 - 3)

Session A, Plenary Sessions (Hall 1)

Registration



Market Street


ENTRANCE
EXIT ONLY
ENTRANCE
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Career Center
Special Posters & Announcements
Apps & Technology Spotlight Posters
710
584
775
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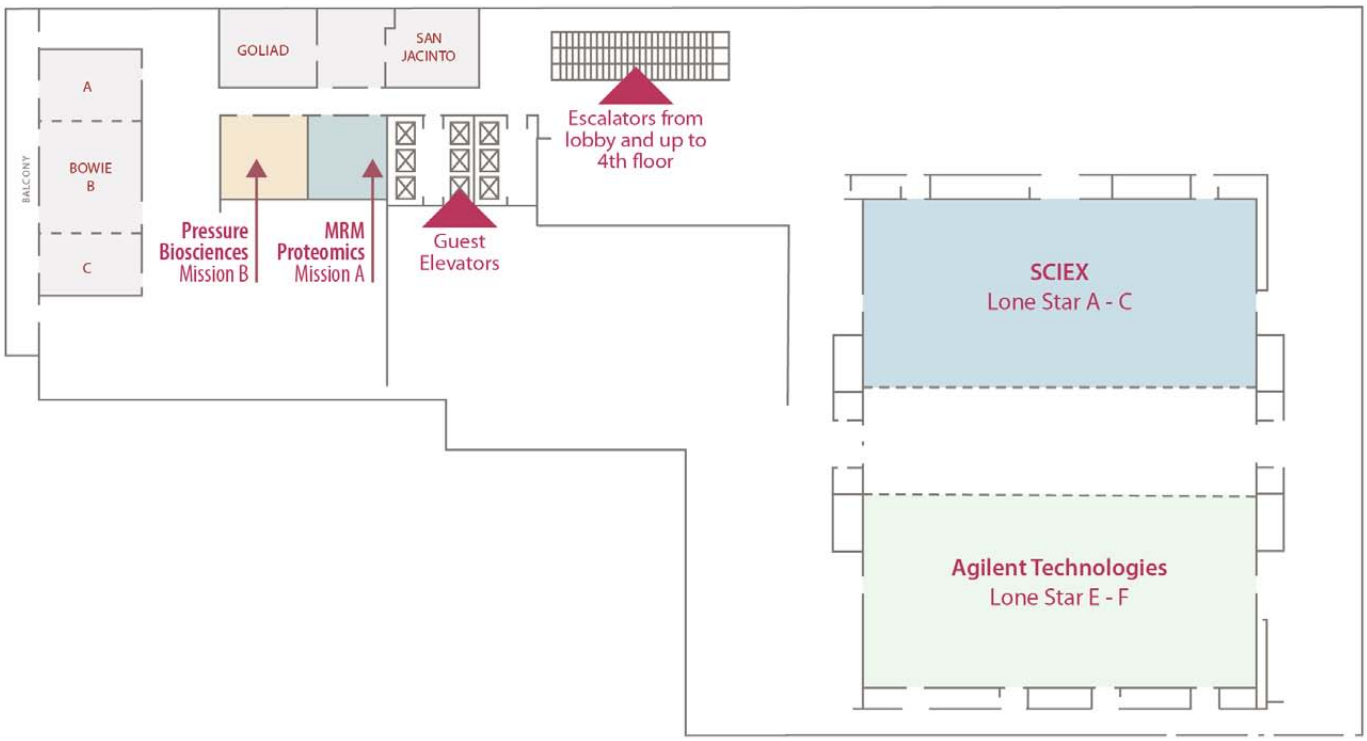
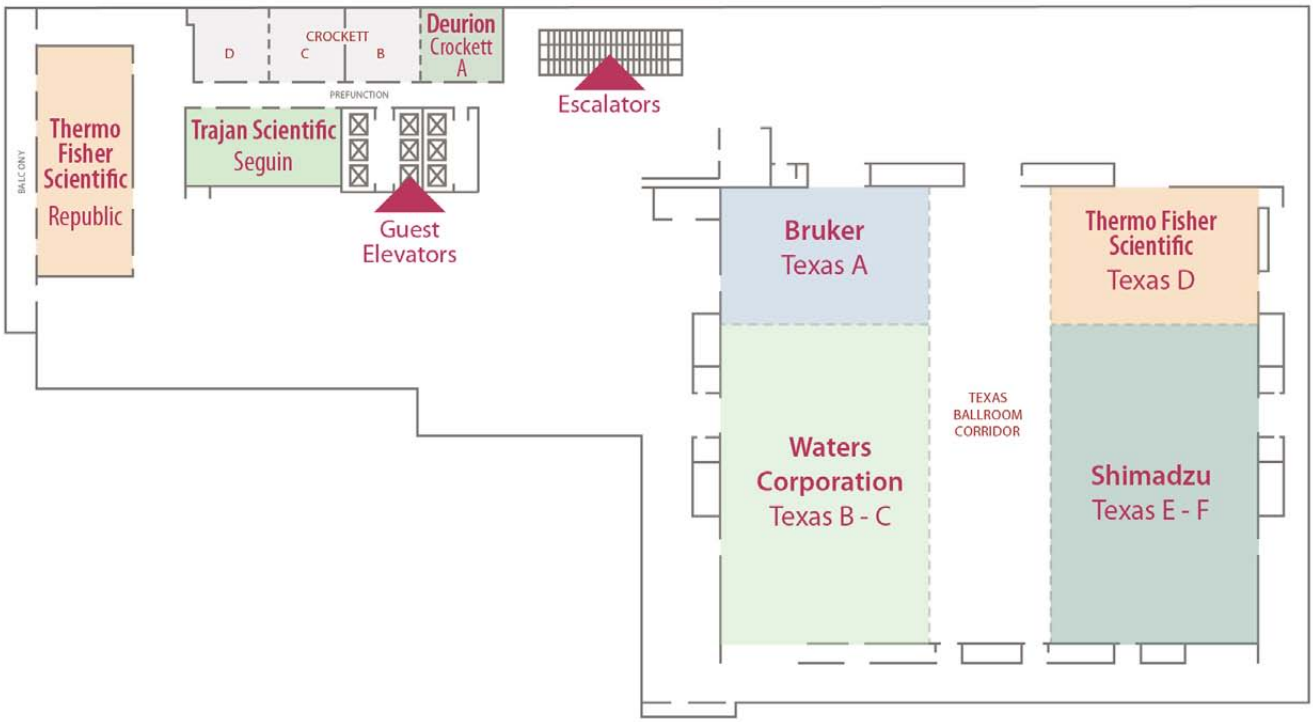
180
400
96
200
259
455
To/From Concourse Level Above
Escalator
FIRE EXIT

Grand Hyatt, 2nd Floor



Grand Hyatt, 4th Floor



COMPANY	POSTER / LIBRARY	BOOTH	SUITE IN GRAND HYATT HOTEL	BREAKFAST
1st Detect		424		
908 Devices		503		
ACS Publications	Library			
Adeptrix Corporation	Poster	304		
Advanced Chemistry Development (ACD/Labs)	Poster	701		Room 224, Mon (6/6)
Advanced Chromotography		519		
Advanced Energy		219		
Advion Inc.		811		
Agilent Technologies	Poster	200	Lone Star Ballroom DEF	Lone Star Ballroom DEF, Mon-Wed (6/6-6/8)
Alliance Pharma, Inc.		411		
Analytical Parts Supply, LLC		421		
Analytical Sales and Services, Inc.	Poster	107		
Analytical Scientific Instruments		208		
Anasys Instruments		527		
Anest Iwata		703		
Antec		700		
Apricot Designs, Inc.		621		
Ardara Technologies LP		629		
Avanti Polar Lipids, Inc.		427		
BioChromato, Inc.		809		
BIOCRATES Life Sciences AG		121		
Biognosys	Poster	209		
Bioinformatics Solutions Inc.	Poster	318		
Biotage		300		Room 225B, Tue (6/7)
Bonna-Agela Technologies, Inc.	Poster	709		
Bruker Daltonics		329	Texas Ballroom A	Room 225CD, Mon-Wed (6/6-6/8)
Cambridge Isotope Labs		800		
Canadian Life Science	Poster	301		
Cayman Chemical Company		801		
Cerno Bioscience		129		
Chemyx, Inc.		523		
CMP Scientific, Inc.		610		
Compare Networks	Library			
CovalX		501		
Covance		607		
Cryoxtract	Poster	420		
CSS Analytical Co. Inc.		520		
CTC Analytics AG		409		
Denator AB		526		

COMPANY	POSTER / LIBRARY	BOOTH	SUITE IN GRAND HYATT HOTEL	BREAKFAST
Detector Technology, Inc.		500		
Deurion	Poster		Crockett A	
Digital Proteomics	Poster	601		
Drummond Scientific		507		
EBARA Technologies		622		
Edwards Vacuum		504		
Elforlight Ltd.		928		
El-Mul Technologies		810		
e-MSion, Inc.		821		
ESI Source Solutions		328		
ETP Electron Multipliers/Ion Detect		326		
Excellims Corporation		705		
Extrel	Poster	223		
Fluid Management Systems		611		
Fortis Technologies Ltd	Poster	125		
Genedata		207		
Genetic Engineering & Biotechnology News	Library			
Genovis	Poster	600		
GenTech Scientific, Inc.		506		
GERSTEL, Inc.	Poster	625		
GL Sciences Inc.		111		Room 301A, Tue (6/7)
Golden West Biologicals, Inc.		202		
Grenova	Poster			
Hamamatsu Corporation	Poster	327		
Hamilton Robotics	Poster	605		
Harris Corp	Poster	711		
HighChem		528		
Horizon Technology, Inc.		628		
HTX Technologies, LLC		829		
HVM Technology		720		
IDEX Health & Science	Poster	400		
iLab Solutions		404		
IMCS		718		
Imtakt USA		211		
Institute for Systems Biology		805		
INTAVIS Bioanalytical Instruments AG		307		
International Ceramic Engineering		719		
International Equipment Trading Ltd.		410		
International Labmate	Library			
ionBench		419		
IonSense, Inc.	Poster	119		

COMPANY	POSTER / LIBRARY	BOOTH	SUITE IN GRAND HYATT HOTEL	BREAKFAST
ION-TOF GmbH	Poster	518		
IsoSciences		406		
JEOL USA, Inc.		229		
JPT Peptide Technologies		405		
LEAP Technologies		623		
LECO Corporation	Poster	305		Room 303A, Mon-Wed (6/6-6/8)
Linden CMS GmbH		123		
Mac-Mod Analytical		828		
Markes International	Poster	728		
MasCom Technologies		508		
MassTech Inc.		429		
Matrix Science		221		Room 302BC, Mon-Tue (6/6-6/7)
Matsusada Precision Inc.		320		
McKinley Scientific		323		
MeCour Temperature Control		729		
MestreLab Research		502		
Microliter Analytical Supplies (A WHEATON Company)		604		
MilliporeSigma	Poster	721		Room 303BC, Tue (6/7)
Mo Bio Laboratories		222		
Moeller Medical GmbH		524		
MRM Proteomics Inc			Mission A	
MS Noise		529		
mSPEC group		309		
MStm		306		
nanoLiter, LLC	Poster	426		
Nest Group, The	Poster			
New England Peptide, Inc.		227		
New Objective, Inc.	Poster	321		Room 305, Tue-Wed (6/7-6/8)
NIST		308		
Oerlikon Leybold Vacuum		509		
Omni Enclosures		522		
Omni International		511		
OPOTEK, Inc.		606		
Optimize Technologies, Inc.	Poster	608		
Optys Tech Corporation		425		
Owlstone, Inc.		407		
Pall Laboratory		204		
Parker Balston/Hannifin		418		
PEAK Scientific	Poster	619		
Peeke Scientific		624		
Perfinity Biosciences		127		
PerkinElmer		428		

COMPANY	POSTER / LIBRARY	BOOTH	SUITE IN GRAND HYATT HOTEL	BREAKFAST
Pfeiffer Vacuum	Poster	310		
Phenomenex		226		
Phoenix S&T, Inc.		303		
PHOTONIS	Poster	401		
Physical Electronics	Poster	228		
Phytronix Technologies, Inc.		203		
Presco Incorporated		727		
Pressure BioSciences, Inc.		819	Mission B	
Promega Corporation		618		
Prosolia, Inc.	Poster	423		Room 224, Tue (6/7)
Protea Biosciences, Inc.		325		
Protein Metrics Inc.		510		
Proteome Sciences	Poster			
Proteome Software Inc.		322		
Proton Onsite		105		
PTM Biolabs, Inc.		521		
PurSpec Technologies, Inc.		408		
Pursuits Instrument Limited		803		
Qioptiq, An Excelitas Technologies Co		707		
Rapid Novor Inc.	Poster	206		
Restek Corporation		627		
Resyn Biosciences		704		
RMI Laboratories		224		
Samin Science Co., Ltd		910		
Science/AAAS	Library			
Scientific Instrument Services	Poster	218		
Scientific Systems, Inc.		722		
SCIEX		101	Lone Star Ballroom ABC	Room 302A, Tue-Wed (6/7-6/8) Room 304A, Mon-Thu (6/6-6/9) Room 304BC, Tue-Wed (6/7-6/8) Room 305, Mon (6/6)
Shimadzu Scientific Instruments, Inc.	Poster	210	Texas Ballroom EF	Room 220, Mon-Thu (6/6-6/9)
Shimifrez Inc.		708		
Sierra Analytics		422		
Silantes GmbH		603		
Sound Analytics		702		
Spark Holland		525		
SpectralWorks Limited	Poster	205		
Spectroscopy		402		
Spectroswiss		311		
Spellman High Voltage		620		

COMPANY	POSTER / LIBRARY	BOOTH	SUITE IN GRAND HYATT HOTEL	BREAKFAST
Springer Science + Business Media				
SunChrom GmbH		710		
Superior Technical Ceramics		626		
SYFT Technologies	Poster	609		
Tecan	Poster	220		
The Analytical Scientist	Library			
Thermo Fisher Scientific		319	Texas Ballroom D and Republic ABC	Room 225CD, Thu (6/9) Republic ABC, Mon-Wed (6/6-6/8)
Tofwerk AG		225		
Tosoh Bioscience		324		
Trajan Scientific and Medical	Poster	403	Seguin AB	
Veritomyx		818		
VICI Valco Instruments		109		
VRS		103		
VUV Analytics		900		
Waters Corporation	Poster	201	Texas Ballroom BC	Room 301A, Mon (6/6) Room 301BC, Mon-Wed (6/6-6/8) Texas Ballroom BC, Mon-Wed (6/6-6/8)
Wiley	Library			
XPC Corporation		302		
Zef Scientific Inc.		602		
Zhejiang Haochuang Biotech Co., Ltd	Poster	826		

Vice President for Programs

Vicki H. Wysocki
The Ohio State University
Vice President for Programs

Student Assistants

Graduate students assist with many aspects of the conference, including registration, oral and poster sessions, and the employment center. The students each receive a stipend to help with their conference travel expenses.

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Sebastian Boecker
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Joshua Coon
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Naidong Weng
Michael Westphall
Si Wu
Yang Yuan
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Erin Baker
Mark Barrow
Nuno Bandeira
Kevin Bateman
Michael Bereman
Andrey Bondarenko
Achille Cappiello
Allis Chien
Brent Dixon
Meena Choi
Eric Deutsch
Dawn Dufield
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Christer Ejsing
Jarrett Egertson
Marc Engel
Alessandra Ferzoco
Valerie Gabelica
Hongying Gao
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Megan Gessel
Ludovic Gillet
Ying Ge
Chris Gill
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Christine Gu
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Anthony Macherone
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Violet Lee
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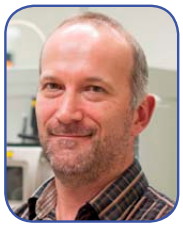
Gyorgy Vas
Jian Wang
Laixin Wang
Kristin Wildsmith
Christine Wu
Stephen Valentine
Raf Van de Plas
Michael Van Stipdonk
Gyorgy Vas
Guido F. Verbeck
David Weis
Nathan Yates
Ralf Zimmerman

Saturday

9:00 AM - 4:30 PM	Short Courses
1:00 - 5:00 PM	Registration

Sunday

9:00 AM - 4:30 PM	Short Courses
10:00 AM - 8:00 PM	Registration
4:00 - 4:45 PM	**Attention: First-time Graduate Students and Undergraduate Students** **Plan your Strategy: What to See and Do at ASMS, Stars Ballroom 1, level 3**
5:00 - 6:30 PM	**Tutorial Lectures**, Hall 1, level 1  **5:00 - 5:45 pm** **Forensic Mass Spectrometry #TellMeSomethingIDontKnow** **Facundo Fernandez** Georgia Institute of Technology  **Glen Jackson** West Virginia University  **5:45 - 6:30 pm** **An Analyte's Journey from Solution into the Gas Phase** **Lars Konermann** University of Western Ontario
6:45 - 7:45 PM	**Conference Opening**, Hall 1, level 1 **Vicki Wysocki (The Ohio State University),** *ASMS Vice President for Programs*  **A Molecular Arsenal Against Ebola Virus** **Erica Ollmann Saphire** The Scripps Institute-La Jolla
7:45 - 9:00 PM	**Welcome Reception in the Poster/Exhibit Hall** Undergraduate Student Poster Competition

Monday

7:30 AM - 5:00 PM	**Registration**
8:30 - 10:30 AM	**Oral Sessions** • MOAam: Synthetic Polymers, Hall 1, level 1 • MOBam: Fundamentals: Ion-Ion and Ion-Neutral Interactions, Room 221, level 2 • MOCam: Ion Mobility: Small Molecules, Pharmaceuticals, and DMPK, Stars Ballroom 1, level 3 • MODam: Instrumentation: FTMS, Stars Ballroom 2-3, level 3 • MOEam: Diagnostic Clinical Chemistry, Stars Ballroom 4, level 3 • MOFam: Informatics: Discovery Proteomics, Hemisfair Ballroom 3, level 3 • MOGam: Metabolomics: Untargeted Profiling, Hemisfair Ballroom 2, level 3 • MOHam: Membrane Protein MS, Hemisfair Ballroom 1, level 3
10:30 AM - 2:30 PM	**Poster Session and Exhibits,** Monday Posters, Poster/Exhibit Hall, level 1 Odd-number posters present 10:30 am - 1:00 pm. Even-number posters present 12:00 - 2:30 pm. 11:30 – 1:00 pm: **Undergraduate students** – look for reserved tables and free lunch vouchers to ***Meet the Experts***
2:30 - 4:30 PM	**Oral Sessions** • MOApm: Food Safety and Chemistry: Foodomics, Allergens, Bacteria, Foods, Hall 1, level 1 • MOBpm: Fundamentals: Ion Spectroscopy, Room 221, level 2 • MOCpm: Instrumentation: New Developments in Ionization and Sampling, Stars Ballroom 1, level 3 • MODpm: Antibodies and Antibody Drug Conjugates, Stars Ballroom 2-3, level 3 • MOEpm: Data Independent Acquisition: Innovative Methods and Applications, Stars Ballroom 4, level 3 • MOFpm: Informatics: Metabolomics, Hemisfair Ballroom 3, level 3 • MOGpm: Nucleic Acid MS, Hemisfair Ballroom 2, level 3 • MOHpm: Covalent Labeling and Chemical Crosslinking, Hemisfair Ballroom 1, level 3
4:45 - 5:30 PM	**Award Lecture**, Hall 1, level 1 **Award for a Distinguished Contribution in Mass Spectrometry**  **Scott A. McLuckey** Purdue University
5:45 - 7:00 PM	**Workshops** There are light refreshments in the common areas. 01 Top-Down Proteomics: Ready for Primetime? Room 220, level 2 02 Next Generation LC-MS: Critical Insights & Future Perspectives, Room 221, level 2 03 Art and Cultural Heritage Mass Spec Applications, Room 225A, level 2 04 Bioinformatics: Challenges & Opportunities in Proteogenomics (Bioinformatics for MS), Room 225B, level 2 05 Environmental Analysis: Emerging Topics (Environmental Applications Interest Group), Room 225C, level 2 06 Metal Cationization in MS/MS of Biomolecules (Metal Ion Coordination Chemistry Interest Group), Room 225D, level 2 07 Proteomics Informatics for the Trans-Proteomic Pipeline, Room 301A, level 3 08 Metabolomics: Emerging Technologies for Continued Innovation (Metabolomics Interest Group), Room 301BC, level 3 09 Polymer MS Technology: Advancements and Discussion (Polymeric Materials Interest Group), Room 302A, level 3 10 MS Analysis of Antibody-Drug Conjugates (Pharmaceuticals Interest Group), Room 302BC 11 Protocol Repositories for Proteomics and Metabolomics (Analytical Lab Managers Interest Group), Room 303A, level 3 12 Miniaturization of Ion Traps and Related Devices (Ion Trap Interest Group), Room 303BC 13 MS Career Options: How to Kick-Start your Career (Young Mass Spectroscopists Interest Group), Room 304, level 3 14 System Performance: Tracking through Statistical QC Monitoring (LC/MS & Related Topics Interest Group), Room 305, level 3
7:00 - 8:00 PM	**Dinner Break**
After 8:00 PM	**Corporate Hospitality Suites,** Grand Hyatt Hotel

Tuesday

7:30 AM - 5:00 PM	**Registration**
8:30 - 10:30 AM	**Oral Sessions** • TOAam: Energy, Petroleum, and Biofuels: Instrumentation and Method Development, Hall 1, level 1 • TOBam: Fundamentals: Metal Ion Cationization, Metal-Ligand Interactions and Catalysis, Room 221, level 2 • TOCam: HRMS for Quantitation in Drug Discovery, Development and Beyond, Stars Ballroom 1, level 3 • TODam: Imaging: Instrumentation & Method Development, Stars Ballroom 2-3, level 3 • TOEam: Quantitative Proteomics in Systems Biology, Stars Ballroom 4, level 3 • TOFam: Instrumentation: non-FT based Analyzers, Hemisfair Ballroom 3, level 3 • TOGam: Lipids and Profiling, Hemisfair Ballroom 2, level 3 • TOHam: Native MS in Structural Biology, Hemisfair Ballroom 1, level 3
10:30 AM - 2:30 PM	**Poster Session and Exhibits,** Tuesday Posters, Poster/Exhibit Hall Odd-number posters present 10:30 am - 1:00 pm. Even-number posters present 12:00 - 2:30 pm.
2:30 - 4:30 PM	**Oral Sessions** • TOApm: Environmental: New Instrumentation and Approaches, Hall 1, level 1 • TOBpm: New Developments in Ion Detection, Room 221, level 2 • TOCpm: Quantitative Analysis in Drug Discovery and Development, Stars Ballroom 1, level 3 • TODpm: Ion Mobility, FAIMS & DMS: New Developments & Applications, Stars Ballroom 2-3 • TOEpm: Qualitative and Quantitative Analysis of Post-translational Modifications, Stars Ballroom 4, level 3 • TOFpm: Imaging: Computational Methods and Analysis, Hemisfair Ballroom 3, level 3 • TOGpm: Metabolomics: New Technologies and Applications, Hemisfair Ballroom 2, level 3 • TOHpm: Protein-Ligand Interactions, Hemisfair Ballroom 1, level 3
4:45 - 5:30 PM	**Award Lecture,** Hall 1, level 1  **Kristina "Kicki" Håkansson** University of Michigan
5:45 - 7:00 PM	**Workshops** There are light refreshments in the common areas 01 Glycoproteomics: Site Specific Glycan Analysis, Room 220, level 2 02 Ion Mobility: How to Interpret the Data (Ion Mobility MS Interest Group), Room 221, level 2 03 H/D Exchange, Covalent Labeling & Cross-Linking (H/D Exchange, Covalent Labeling & Cross-Linking Interest Group), Room 225A, level 2 04 Food Safety & Security: HRMS Applications (Flavor, Fragrance & Foodstuff Interest Group), Room 225B, level 2 05 Microcontrollers and Microcomputers: Emerging Technologies, Room 225C, level 2 06 DNA/RNA Adducts: Assay Development in Detection and Quantification (Oligonucleotides and Nucleic Acids Interest Group), Room 225D, level 2 07 Petroleum and Biofuels: Handling the Data (Energy, Petroleum & Biofuels Interest Group), Room 301A, level 3 08 Metabolism of Biotherapeutics: When, Why and How? (DMPK Interest Group), Room 301BC, level 3 09 Modification of Commercial Instruments for Fundamental Research (Fundamentals Interest Group), Room 302A, level 3 10 Lipidomics in the Era of Systems Biology: The Big Fat Challenges (Lipids and Lipidomics Interest Group), Room 302BC, level 3 11 Undergraduate Research in Mass Spectrometry (Undergraduate Research in MS Interest Group), Room 303A, level 3 12 The Chorus Project: Sustainable Cloud Solution for MS Data, Room 303BC, level 3 13 Data Independent Acquisition (Data Independent Acquisition Interest Group), Room 304, level 3 14 Good Manufacturing Practice (GMP); Mass Spectrometric Instrument Qualification, Room 305
7:00 - 8:00 PM	**Dinner Break**
After 8:00 PM	**Corporate Hospitality Suites,** Grand Hyatt Hotel

Wednesday

7:30 AM - 5:00 PM	**Registration**
8:30 - 10:30 AM	**Oral Sessions** • WOAam: Energy, Petroleum and Biofuels: Structure, Quantification, and Data Analysis, Hall 1 level 1 • WOBam: Fundamentals: Energetics and Mechanisms of Uni and Bimolecular Reactions, Room 221, level 2 • WOCam: Imaging: Pharmaceuticals and Metabolites, Stars Ballroom 1, level 3 • WODam: Instrumentation: Miniaturization of MS, Stars Ballroom 2-3, level 3 • WOEam: Biomarkers: Qualitative Analysis, Stars Ballroom 4, level 3 • WOFam: Informatics: Multiomics Integration and Application, Hemisfair Ballroom 3, level 3 • WOGam: MS in the QC Lab, Hemisfair Ballroom 2, level 3 • WOHam: Macromolecular Complexes, Hemisfair Ballroom 1, level 3
10:30 AM - 2:30 PM	**Poster Session and Exhibits,** Wednesday Posters, Poster/Exhibit Hall Odd-number posters present 10:30 am - 1:00 pm. Even-number posters present 12:00 - 2:30 pm.
2:30 - 4:30 PM	**Oral Sessions** • WOApm: Exposomics: Targeted, Untargeted and Bioinformatics Methodologies, Hall 1, level 1 • WOBpm: Fundamentals: Molecular Modeling and Quantum Mechanical Calculations in IM and MS, Room 221, level 2 • WOCpm: Environmental: Emerging Contaminants, Stars Ballroom 1, level 3 • WODpm: Imaging: Biomedical Applications, Stars Ballroom 2-3, level 3 • WOEpm: Top Down Protein Analysis, Stars Ballroom 4, level 3 • WOFpm: MS in the Regulatory Environment, Hemisfair Ballroom 3, level 3 • WOGpm: Carbohydrates, Hemisfair Ballroom 2, level 3 • WOHpm: New Separations Approaches Coupled to MS, Hemisfair Ballroom 1, level 3
4:45 - 5:30 PM	**ASMS Meeting,** Stars Ballroom 1, level 3: Awards, board reports, wine, beer, soft drinks - and more!
5:45 - 7:00 PM	**Workshops** There are light refreshments in the common areas. 01 Bioanalysis: Current Status of Strategy and Practice of a Tiered Approach (Regulated Bioanalysis Interest Group), Room 220, level 2 02 Large-Scale Analysis of MS Big Data: From Data to Knowledge and Back, Room 221, level 2 03 FTMS: Day-to-Day Concerns for High Resolution Mass Analysis (FTMS Interest Group), Room 225A, level 2 04 Novel Mass Spectrometry Instrumentation: Moving into the Hands of Practitioners (Forensics & Homeland Security Interest Group), Room 225B, level 2 05 Photoionization: New Developments (Photoionization MS Interest Group), Room 225C, level 2 06 The NIH Review and Funding Process, Room 225D, level 2 07 Entrepreneurship: Creating a Job in Mass Spectrometry, Room 301A, level 3 08 Protein Quantitation (Absolute) by LC-MS: Biomarker and Biotherapeutic, Room 301BC, level 3 09 Isomeric Glycans: Characterization & Quantitation, Room 302A, level 3 10 Protein Therapeutics: Characterization using MS (Biotherapeutics Interest Group), Room 302BC, level 3 11 The Exposome: MS-based Metabolomic Workflows to Characterize the Exposome (Exposomics Interest Group), Room 303A, level 3 12 Biomarker Translation: Quality Control & Quality Assurance (Clinical Chemistry Interest Group), Room 303BC, level 3 13 Imaging MS: Present and Future of Multimodal Studies (Imaging MS Interest Group), Room 304, level 3 14 Galaxy for Proteomics Data Analysis: An Interactive Demonstration, Room 305, level 3
7:00 - 8:00 PM	**Dinner Break**
After 8:00 PM	**Corporate Hospitality Suites,** Grand Hyatt Hotel

Thursday

7:30 AM - 5:00 PM	**Registration**
8:30 - 10:30 AM	**Oral Sessions** • ThOAam: New Concepts for Forensic MS, Hall 1, level 1 • ThOBam: Fundamentals: Photodissociation, Room 221, level 2 • ThOCam: New Developments in Ionization and Sampling for DMPK, Stars Ballroom 1, level 3 • ThODam: Translational Success with MS, Stars Ballroom 2-3, level 3 • ThOEam: Glycopeptides and Glycoproteins, Stars Ballroom 4, level 3 • ThOFam: Informatics: Targeted Proteomics and DIA, Hemisfair Ballroom 3, level 3 • ThOGam: Application of Stable Isotope Labeling in MS, Hemisfair Ballroom 2, level 3 • ThOHam: Ion Mobility: Structure, Hemisfair Ballroom 1, level 3
10:30 AM - 2:30 PM	**Poster Session and Exhibits,** Thursday Posters, Poster/Exhibit Hall Odd-number posters present 10:30 am - 1:00 pm. Even-number posters present 12:00 - 2:30 pm.
2:30 - 4:30 PM	**Oral Sessions** • ThOApm: Food Safety and Chemistry: Non-targeted Screening, Hall 1, level 1 • ThOBpm: Fundamentals: Ion Activation and Dissociation, Room 221, level 2 • ThOCpm: MS Solutions for Drug Metabolism Challenges, Stars Ballroom 1, level 3 • ThODpm: Ambient Ionization: Instrumentation & Applications, Stars Ballroom 2-3, level 3 • ThOEpm: Biomarkers: Quantitative Analysis, Stars Ballroom 4, level 3 • ThOFpm: Informatics: Peptide and Protein Identification, Hemisfair Ballroom 3, level 3 • ThOGpm: Lipidomics: New MS Technologies and Applications, Hemisfair Ballroom 2, level 3 • ThOHpm: Hydrogen-Deuterium Exchange MS, Hemisfair Ballroom 1, level 3
4:45 - 5:30 PM	**Plenary Lecture,** Hall 1, level 1  **More than the Sum of its Parts: Collective Phenomena in Living Systems, from Single Molecules to Flocks of Birds** **William Bialek** Princeton University
6:30 - 9:00 PM	**Closing Event** **Briscoe Western Art Museum.** Ticket required

SUNDAY EVENING, 4:00 - 9:00 PM

4:00 – 4:45 PM, SUNDAY
Attention First-time Graduate Students and Undergrads
Plan your Strategy: What to See and Do at ASMS
Elaine Marluff and JC Poutsma, presiding
Stars Ballroom 1, level 3

5:00 – 6:30 PM, SUNDAY
TUTORIAL SESSION
Vicki Wysocki (The Ohio State University) presiding
Hall 1, level 1

5:00 – 5:45 pm
Forensic Mass Spectrometry
#TellMeSomethingIDontKnow

Facundo Fernandez
Georgia Institute of Technology

Glen Jackson
West Virginia University

5:45 – 6:30 pm
An Analyte's Journey from Solution into the Gas Phase

Lars Konermann
University of Western Ontario

6:45 – 7:45 PM, SUNDAY
CONFERENCE OPENING
Vicki Wysocki (The Ohio State University) presiding
Hall 1, level 1

Welcome, Vicki H. Wysocki (The Ohio State University)
ASMS Vice President for Programs

A Molecular Arsenal Against Ebola Virus

Erica Ollmann Saphire
The Scripps Institute-La Jolla

7:45 – 9:00 PM, SUNDAY
WELCOME RECEPTION
Poster/Exhibit Hall
Conference name badge is required.

MONDAY MORNING ORAL SESSIONS

8:30-10:30 am MONDAY
SYNTHETIC POLYMERS
Paul Kowalski (Bruker Daltonics, Inc.)
Hall 1, level 1

MOA am 08:30 **Mechanistic Studies of Hafnocene Catalyzed Olefin Polymerization**; Anthony Paul Gies[1]; Roger Kuhlman[2]; Cristiano Zuccaccia[3]; Alceo Macchioni[3]; *[1]Dow Chemical Company, Freeport, TX; [2]Univation Technologies, Freeport, TX; [3]Dipartimento di Chimica, Biologia e Biotecnologie and CIRCC, University of Perugia, Perugia, Italy*

MOA am 08:50 **Analytical Characterization of PEG and PEG conjugates by Mass Spectrometry**; Guanghui Han[1]; Wilson Phung[1]; Whitney Shatz[1]; Julie Q. Hang[1]; Justin Scheer[1]; Paul Schnier[1]; Wendy Sandoval[1]; *[1]Genentech Inc, South San Francisco, CA*

MOA am 09:10 **The Use of Iodo-functionalized Polydisperse Polymers as Mass-defect Tuned Calibrants**; Joseph A. Giesen[1]; Jennifer L. Marple[1]; Scott M. Grayson[1]; *[1]Tulane University, New Orleans, LA*

MOA am 09:30 **Sequence and Conformational Analysis of Recombinant Polypeptide-Polymer Conjugates**; Sahar Sallam[1]; Bradford A Paik[2]; Xinqiao Jia[2]; Chrys Wesdemiotis[1]; *[1]The University of Akron, Akron, OH; [2]University of Delaware, Newark, DE*

MOA am 09:50 **Using MS/MS to Design Information-Encoded Synthetic Copolymers**; Laurence Charles[1]; Jean-François Lutz[2]; *[1]Aix-Marseille University, Marseille Cedex 20 , PACA; [2]Institut Charles Sadron, Strasbourg, France*

MOA am 10:10 **Peptoid Fragmentation -The Bias toward Y-Ion Formation**; Jianhua Ren[1]; Yuan Tian[2]; Ekram Hossain[2]; Michael Connolly[3]; Ronald Zuckermann[3]; *[1]University of the Pacific, Stockton , CA; [2]University of the Pacific, Stockton, CA; [3]Lawrence Berkeley National Laboratory, Berkeley, CA*

8:30-10:30 am MONDAY
FUNDAMENTALS: ION-ION AND ION-NEUTRAL INTERACTIONS
John E. P. Syka (Thermo Fisher Scientific)
Room 221, level 2

MOB am 08:30 **Preparation of a Dianion with the Highest Known Proton Affinity: Ortho-Diethynyl Benzene**; Berwyck Poad[1]; Nicholas Reed[2]; Christopher Hansen[2]; Adam Trevitt[2]; Stephen J Blanksby[1]; Emily Mackay[3]; Michael Sherburn[3]; Bun Chan[4]; Leo Radom[4]; *[1]Queensland University of Technology, Brisbane, Australia; [2]University of Wollongong, Wollongong, Australia; [3]Australian National University, Canberra, Australia; [4]The University of Sydney, Sydney, Australia*

MOB am 08:50 **Evaluating Gas-Phase Folding of Protein Ions Using Cation to Anion Proton Transfer**; Kenneth J. Laszlo[1]; Eleanor B. Munger[1]; Stephanie C. Heard[2]; Matthew F Bush[1]; *[1]University of Washington, Seattle, WA; [2]Kalamazoo College, Kalamazoo, MI*

MOB am 09:10 **Selective Oxidation via Ion/Ion Reactions: Characteristic Chemistries for Methionine Residues and Cysteine Post-Translational Modifications**; Alice Pilo[1]; Scott A McLuckey[1]; *[1]Purdue University, West Lafayette, IN*

MOB am 09:30 **Identification of Carboxylic Acids in Protonated Drug Metabolites by using Ion-molecule Reactions in a Linear Quadrupole Ion Trap Mass Spectrometer**; Joann Max[1]; Xin Ma[2]; Rashmi Kumar[3]; Hilkka I Kenttamaa[3]; *[1]Purdue University, West Lafayette, IN; [2]Purdue University-Department of Chemistry, West Lafayette, IN; [3], West Lafayette, IN*

MOB am 09:50 **Ultraviolet Photodissociation of Native Proteins Following Proton Transfer Reaction in an Orbitrap Elite Mass Spectrometer**; Dustin D Holden; Jennifer Brodbelt[1]; *[1]The University of Texas, Austin, TX*

MOB am 10:10 **High-throughput Proteomics with Negative Electron Transfer Dissociation (NETD)**; Nicholas Riley[1]; Michael S Westphall[1]; Joshua J Coon[1]; *[1]University of Wisconsin-Madison, Madison, WI*

8:30-10:30 am MONDAY
ION MOBILITY: SMALL MOLECULES, PHARMACEUTICALS, AND DMPK
Cris Lapthorn (University of Greenwich)
Stars Ballroom 1, level 3

MOC am 08:30 **Highly Accurate Collision Cross Section Measurements for Comprehensive High Throughput Applications**; John Fjeldsted[1]; Ruwan T Kurulugama[1]; Alex Mordehai[1]; Emma E Rennie[1]; Ed Darland[1]; George C Stafford[1]; Jody May[2]; Sarah M Stow[2]; John A McLean[2]; Tim Causon[3]; Teresa Mairinger[3]; Stephan Hann[3]; Erin Baker[4]; *[1]Agilent Technologies, Santa Clara, CA; [2]Vanderbilt University, Nashville, TN; [3]Universität für Bodenkultur, Vienna, Austria; [4]Pacific Northwest National Lab, Richland, WA*

MOC am 08:50 **Stereoisomer Separation by Ion Mobility – Mass Spectrometry of Multivalent Cation-Chiral Small Molecule Complexes**; Christopher Chouinard[1]; Robin HJ Kemperman[1]; Nicholas M Oranzi[1]; Harrison M King[1]; Richard A Yost[1]; *[1]University of Florida, Gainesville, FL*

MOC am 09:10 **High-throughput Screening Strategy for Tracking Synthetic Biology Variants Libraries using Robotic Platforms and Colormetric Assays Combined with Fast LC-IM MS**; Cunyu Yan[1]; Mark Dunstan[2]; Nicholas Rattray[2]; Perdita Barran[2]; *[1]University of Manchester, Manchester, Manchester; [2]University of Manchester, Manchester, UK*

MOC am 09:30 **Amino Acid Separation using Different Drift Gases in an RF-Confining Drift Cell**; Kimberly Davidson[1]; Matthew F Bush[1]; *[1]University of Washington, Seattle, WA*

MOC am 09:50 **Structural Characterization of Monomers and Oligomers of D-Amino Acid Containing Peptides using Linear and Nonlinear Ion Mobility Separations**; Xueqin Pang[1]; Chenxi Jia[1]; Matthew Baird[2]; Zhengwei Chen[3]; Alexandre A Shvartsburg[2]; Lingjun Li[1, 3]; *[1]School of Pharmacy, University of Wisconsin Madison, WI; [2]Wichita State University, Wichita, KS; [3]Department of Chemistry, UW-Madison, WI*

MOC am 10:10 **Preparative Ion Mobility Spectrometry using an Inline Periodic Focusing Differential Mobility Analyzer (PFDMA)**; Kent Gillig[1]; Chung-Hsuan Chen[2]; *[1]Academia Sinica, Taipei, Nankang, Section 2, Taipei 115; [2]Academia Sinica, Genomics Research Center Taipei, Taiwan*

8:30-10:30 am MONDAY
INSTRUMENTATION: FTMS
Hilkka Kenttamaa (Purdue University)
Stars Ballroom 2-3, level 3

MOD am 08:30 **New Gated Approach for Coupling Trapped Ion Mobility Spectrometry to Fourier Transform Ion Cyclotron Mass Spectrometry**; Mark Ridgeway[1]; William Danielson[2]; Jeremy Wolf[1]; Melvin Park[1]; *[1]Bruker Daltonic, Billerica, MA; [2]Danielson Software Consulting, Richland, WA*

MOD am 08:50 **Multi-CRAFTI: Simultaneous Measurement of Relative Collision Cross Sections for Multiple Ions Measured using Fourier Transform Ion Cyclotron Resonance Linewidths**; David V. Dearden[1]; Anupriya Anupriya[1]; *[1]Brigham Young University, Provo, UT*

MOD am 09:10 **21 Tesla FT-ICR Mass Spectrometer for Ultrahigh Resolution Analysis of Complex Mixtures**; Donald F. Smith[1]; David C. Podgorski[1, 2]; Yuri E Corilo[1, 2]; Christopher L. Hendrickson[1]; *[1]National High Magnetic Field Laboratory, Tallahassee, FL; [2]Future Fuels Institute, FSU Tallahassee, FL*

MOD am 09:30 **Surface Induced Dissociation (SID) of Protein Complexes in a Hybrid FT-ICR**; Jing Yan[1]; Mowei Zhou[2]; Gilbert Joshua[1]; Jeremy J. Wolff[3]; Randall E. Pedder[4]; Arpad Somogyi[5]; Royston S. Quintyn[1]; Lindsay Morrison[1]; Michael L. Easterling[3]; Ljiljana Pasa-Tolic[2]; Vicki H. Wysocki[1]; *[1]Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH; [2]Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA; [3]Bruker Corporation, Billerica, MA; [4]Ardara Technologies L.P., Ardara, PA; [5]OSU Mass Spectrometry & Proteomics Facility, The Ohio State University, Columbus, OH*

MOD am 09:50 **Construction of a Dual-Detector Fourier Transform Electrostatic Linear Ion Trap Utilizing In-Trap Potential Lift**; Eric Dziekonski[1]; Robert Santini[1]; Scott A McLuckey[1]; *[1]Purdue University, West Lafayette, IN*

MOD am 10:10 **Influence of Ion Clouds Micromotion on FTICR Mass-Spectrometer Performances in Ultrahigh Resolution Mode of Operation**; Eugene Nikolaev[1]; Gleb Vladimirov[2, 1]; Goekhan Baykut[3]; Roland Jertz[3]; *[1]Institute for Energy Problems of Chemical Physics, Moscow, Russia; [2]Skolkovo Institute of Technology, Moscow, Russia; [3]Bruker Daltonic GmbH, Bremen, Germany*

8:30-10:30 am MONDAY
DIAGNOSTIC CLINICAL CHEMISTRY
Heather C. Kuiper (CDC)
Stars Ballroom 4, level 3

MOE am 08:30 **Intraoperative Diagnosis of Gliomas using Desorption Electrospray Ionization Mass Spectrometry: A Review of Clinical Cases**; Valentina Pirro[1]; Alan K. Jarmusch[2]; Zane R. Baird[2]; Clint Alfaro[2]; Eyas Hattab[3]; Aaron Cohen-Gadol[3]; Graham R Cooks[2]; *[1]Purdue University, West Lafayette, Indiana; [2]Purdue University, West Lafayette, IN; [3]Indiana University School of Medicine, Indianapolis, IN*

MOE am 08:50 **DESI-MSI-based Diagnostics of Cirrhotic Liver Diseases**; Anna Mroz[1]; Francesca Rosini[1]; Alex Pechlivanis[1]; Luisa Doria[1]; Evaggelia Liaskou[2]; Gideon Hirschfield[2]; Simon Taylor-Robinson[1]; David Jones[3]; Robert Goldin[1]; Elaine Holmes[1]; Zoltan Takats[1]; *[1]Imperial College London, London, United*

Kingdom; [2]University of Birmingham, Birmingham, UK; [3]Newcastle University, Newcastle upon Tyne, UK

MOE am 09:10 **On-demand Disease Diagnosis using 3D Microfluidic Paper-based Analytical Devices Capable of On-chip Mass Spectrometry**; Abraham Kwame Badu Tawiah[1]; Suming Chen[1]; Deidre E Damon[1]; *[1]Ohio State University, Columbus, OH*

MOE am 09:30 **Clinical Diagnosis of Botulism with Mass Spectrometry**; Suzanne R. Kalb[1]; Dongxia Wang[1]; Jakub Baudys[1]; Kaitlin Hoyt[2]; Kathryn Pigg[2]; John R Barr[1]; *[1]CDC, Atlanta, GA; [2]Battelle Memorial Institute, Atlanta, GA*

MOE am 09:50 **Typing of Bacterial Strains using Ultrahigh Resolution MALDI-FTICR-MS**; Frank Fleurbaaij[1]; Margriet E.M. Kraakman[2]; Eric C. J. Claas[2]; Wilco C. Knetsch[2]; Hans C. van Leeuwen[2]; Yuri E.M. van der Burgt[1]; Karin Ellen Veldkamp[2]; Wil Goessens[3]; Bart J. Mertens[4]; Ed J. Kuijper[2]; Paul J. Hensbergen[1]; Simone Nicolardi[1]; *[1]Center for Proteomics and Metabolomics, LUMC, Leiden, NL; [2]Department of Medical Microbiology, LUMC, Leiden, NL; [3]Department of Medical Microbiology and Infectious Disease, Erasmus MC, Rotterdam, NL; [4]Department of Medical Statistics, LUMC, Leiden, NL*

MOE am 10:10 **The Necessity for Liquid Chromatography in Drug of Abuse Analysis for Resolution of Opiate-Derived Interferences**; Brian Rappold; *Essential Testing, Collinsville, IL*

8:30-10:30 am MONDAY
INFORMATICS: DISCOVERY PROTEOMICS
Xiaowen Liu (Indiana University)
Hemisfair Ballroom 3, level 3

MOF am 08:30 **Enabling Massive Blind Database Search using Multiple Enzyme Proteomics**; Laurence E. Bernstein[1]; Seungjin Na[1]; Nuno Bandeira[2, 3, 4]; *[1]University of California San Diego, San Diego, CA; [2]Center for Computational Mass Spectrometry, University of California San Diego, La Jolla, CA; [3]Computer Science and Engineering, University of California San Diego, La Jolla, CA; [4]Skaggs School of Pharmacy, UC San Diego, La Jolla, CA*

MOF am 08:50 **Embracing Complexity and Diversity: Discovery Metaproteomics of Multiple Microbiomes using the Galaxy Framework**; Pratik Jagtap[1]; Brian Sandri[2]; Somaieh Afiuni-Zadeh[2]; Kevin Viken[2]; Kristin Boylan[2]; Jim Johnson[3]; Thomas F McGowan[3]; Maneesh Bhargava[2]; Chris Wendt[2]; Amy Skubitz[2]; Joel Rudney[2]; Tim Griffin[2]; *[1]Center for Mass Spectrometry and Proteomics, UMN, St.Paul, MN; [2]University of Minnesota, Minneapolis, MN; [3]University of Minnesota Supercomputing Institute, Minneapolis, MN*

MOF am 09:10 **Maximizing Shotgun Proteomics Isobaric Tagging Data Output using MS/MS Multi-Objective Optimization Algorithm**; John Corthésy[1]; Kostantinos Theofilatos[2]; Seferina Mavroudis[2, 3]; Ornella Cominetti[1]; Mona Remlawi[4]; Francesco Ferraro[4]; Antonio Núñez Galindo[1]; Ivan Montoliu[1]; Martin Kussmann[1]; Spiros Likothanassis[2,5]; Loïc Dayon[1]; *[1]Molecular Biomarkers Core, Nestlé Institute of Health Sciences, Lausanne, Switzerland; [2]InSybio Ltd., London, United Kingdom; [3]Department of Social Work, School of Sciences of Health and Care, Technological Educational Institute of Patras, Patras, Greece; [4]Bio System Informatics, Nestlé Institute of Health Sciences, Lausanne, Switzerland; [5]Department of Computer Engineering and Informatics of the University of Patras, Patras, Greece*

MOF am 09:30 **Real-Time Informatics: A Database Search Increases Depth and Accuracy of Isobaric Label Quantitation in Discovery Proteomics**; Christopher Michael Rose[1]; Derek J Bailey[2]; Joao Paulo[1]; Jeremy D O'Connell[1]; David P Nusinow[1]; Joel M Chick[1]; Steven P Gygi[1]; *[1]Harvard Medical School, Boston, MA; [2]Thermo Fisher Scientific, San Jose, CA*

MOF am 09:50 **An informatic Framework for Defining Multi-Proteoform Complexes (MPCs) by Native Top-Down Mass Spectrometry**; Nicole A Haverland[1]; Owen S Skinner[1]; Pierre C Havugimana[1]; Luca Fornelli[1]; Bryan P Early[1]; Joseph B Greer[1]; Ryan T Fellers[1]; Kenneth R Durbin[1]; Luis H. F. Do Vale[2]; Rafael D Melani[1]; Henrique S Seckler[1]; Micah Nelp[3]; Richard D LeDuc[1]; Vahe Bandarian[3]; Philip D. Compton[1]; Neil L Kelleher[1]; *[1]Northwestern University, Evanston, IL; [2]University of Brasilia, Brasilia, Brazil; [3]University of Arizona, Tucson, Arizona*

MOF am 10:10 **TargetSeeker-MS: A Bayesian Inference Approach for Drug Target Discovery using Protein Fractionation Coupled to Mass Spectrometry**; Mathieu Lavallée-Adam[1]; Alexander Pelletier[1, 2]; Jolene K. Diedrich[1, 3]; William Low[3]; Michael Petrascheck[1]; James J. Moresco[1, 3]; John R. Yates III[1, 3]; *[1]The Scripps Research Institute, La Jolla, CA; [2]UCSD, La Jolla, CA; [3]The Salk Institute, La Jolla, CA*

8:30-10:30 am MONDAY
METABOLOMICS: UNTARGETED PROFILING
Corey D. Broeckling (Colorado State University)
Hemisfair Ballroom 2, level 3

MOG am 08:30 **Automated Solid Phase Extractions Coupled with Ion Mobility-Mass Spectrometry Analyses Allow Rapid Metabolomic Screening of Complex Plasma and Urine Samples**; Erin S. Baker[1]; Xing Zhang[2]; Xueyun Zheng[1]; Kristin E. Burnum-Johnson[1]; Jennifer E Kyle[1]; Young-Mo Kim[1]; Erika M. Zink[1]; Matthew E Monroe[1]; Yehia M Ibrahim[1]; Daniel J Orton[1]; Justin G. Teeguarden[1]; Thomas O Metz[1]; Richard D. Smith[1]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]University of Colorado, Denver, CO*

MOG am 08:50 **Untargeted Profiling with Single-cell MS Uncovers Small-Molecule Cell Heterogeneity along the Left-Right Body Axis in the Frog Embryo**; Rosemary Masu Onjiko[1]; Sydney E Morris[1]; Sally A Moody[2]; Peter Nemes[1]; *[1]Department of Chemistry, The George Washington University, Washington, DC; [2]Department of Anatomy & Regenerative Biology, The George Washington University, Washington DC, DC*

MOG am 09:10 **Metabolomics: Elemental Composition from Ultrahigh Resolution FT-ICR MS; Structure from Two-Dimensional 1H/13C NMR Spectroscopy**; Alan G. Marshall[1]; Lidong He[2]; Lissa C Anderson[3]; Christopher L Hendrickson[3]; Cheng Wang[4]; Lei Bruschweiler Li[4]; Dawei Li[4]; Rafael Bruschweiler[4]; *[1]Ion Cyclotron Resonance Prog, Tallahassee, FL; [2]Florida State University, Tallahassee, Florida; [3]National High Magnetic Field Laboratory, Tallahassee, FL; [4]Ohio State University, Columbus, OH*

MOG am 09:30 **High-Throughput Discovery of New Natural Products and Their Biosynthetic Gene Clusters using a Metabologenomics Approach**; Anthony Goering[1]; Ryan A McClure[2]; James R Doroghazi[3]; Kou-San Ju[3]; Jessica C. Albright[2]; Nicole Haverland[2]; Yongbo Zhang[2]; Regan J Thomson[2]; William W Metcalf[3]; Neil L Kelleher[2]; *[1]Northwestern University,*

Chicago, IL; [2]Northwestern University, Evanston, IL; [3]University of Illinois at Urbana-Champaign, Urbana-Champaign, IL

MOG am 09:50 **Untargeted Stable-isotope Tracing of Folate-mediated 1-C Trafficking in Cancer Cells and an *in vitro* 3Dmodel of Neural Tube Closure**; Qiuying Chen[1]; Amanda K Vaughn[2]; John W Steel[2]; Robert M Cabrera[2]; Richard H Finnell[2]; Steven Gross[1]; *[1]Weill Medical College of Cornell, New York, NY; [2]University of Texas at Austin, Austin, TX*

MOG am 10:10 **Integration of Personal Metabolome and other Omes: Application to the Onset of Type 2 Diabetes**; Kevin Contrepois[1]; Michael Snyder[2]; *[1]Stanford University, Stanford, California; [2]Stanford University School of Medicine, Palo Alto CA*

8:30-10:30 am MONDAY
MEMBRANE PROTEIN MS
Nina Morgner (Johann Wolfgang Goethe-University)
Hemisfair Ballroom 1, level 3

MOH am 08:30 **Ion Mobility-Mass Spectrometry Reveals the Stoichiometry and Structures of Lipid Bound Amyloidogenic Peptide Complexes within Nanodiscs**; Richard A Kerr[1]; Jukyung Kang[1]; Anna Schwendeman[1]; Brandon T Ruotolo[1]; *[1]University of Michigan, Ann Arbor, MI*

MOH am 08:50 **Surface Induced Dissociation Provides Insight into Membrane Protein-Lipid Interactions**; Sophie Harvey[1, 2]; Yang Liu[3]; Wen Liu[3]; Vicki Wysocki[1]; Arthur Laganowsky[3]; *[1]The Ohio State University, Columbus, Ohio; [2]University of Manchester, Manchester, United Kingdom; [3]Texas A&M Health Science Center, Houston, Texas*

MOH am 09:10 **Identification and Characterization of Small Membrane Protein Complex Subunits Presenting Challenges for Routine Mass Spectrometric Analysis**; Julian Langer[1]; Anja Resemann[2]; Martin Kohlstaedt[1]; Detlev Suckau[2]; Schara Safarian[1]; Hartmut Michel[1]; *[1]MPI for Biophysics, Frankfurt Am Main, Germany; [2]Bruker Daltonic GmbH, Bremen, Germany*

MOH am 09:30 **XL-FASP: A New Integrated Cross-Linking Workflow to Study Extra Large Membrane Protein Complexes**; Martial Rey[1]; Eric Durand[2, 1]; Eric Cascales[2]; Rémi Fronzes[1]; Julia Chamot-Rooke[1, 3]; *[1]Institut Pasteur, Paris, France; [2]Institut de Microbiologie de la Méditerranée, CNRS, Marseille, France; [3]CNRS, Paris, France*

MOH am 09:50 **Top-down and Middle-down High-Resolution Mass Spectrometry of Lipidated Proteins**; Julian Whitelegge[1]; Joseph Capri[1]; Whitaker Cohn[1]; Don Puppione[1]; Pasqual Liaux[2]; Frederic Halgand[3]; *[1]University of California, Los Angeles Los Angeles, CA; [2]Ruhr University Bochum, Bochum, Germany; [3]University Paris Sud, Orsay, France*

MOH am 10:10 **Monitoring the Dynamic N-linked Cell Surface Glycoproteome by Quantitative Proteomics**; Christian Eberl[1]; Mathias Kalxdorf[1]; Stephan Gade[1]; Marcus Bantscheff[1]; *[1]Cellzome GmbH a GSK company, Heidelberg, Germany*

10:30 AM – 2:30 PM, MONDAY
MONDAY POSTER SESSION
Poster/Exhibit Hall
Lunch Concessions are open 11:00 am - 2:00 pm
Odd-number posters present 10:30 am - 1:00 pm
Even-number posters present 12:00 - 2:30 pm

11:30 am – 1:00 pm
Undergraduate Students
Meet the Experts at tables reserved for you in Poster/Exhibit Hall.

2:30-4:30 pm MONDAY
FOOD SAFETY AND CHEMISTRY: FOODOMICS, ALLERGENS, BACTERIA, FOODS
Katherine L. Fiedler (U.S. FDA)
Hall 1, level 1

MOA pm 02:30 **SWATH vs. MRM for Food Safety -Using Advanced MS to Verify the Gluten-free Status of Barley**; Michelle Lisa Colgrave[1]; Keren Byrne[1]; Gregory Tanner[2]; Crispin Howitt[2]; *[1]CSIRO Agriculture, Brisbane, Australia; [2]CSIRO Agriculture, Canberra, Australia*

MOA pm 02:50 **Analyses of Human Milk Oligosaccharides Discover Factors that Enhance and Diminish Infant Growth**; Jasmine C. C. Davis[1]; Sarah Totten[2]; Lauren D. Wu[1]; Sridevi Krishnan[1]; Mark R. Charbonneau[3]; Michael J. Barratt[3]; Jeffrey I. Gordon[3]; Angela M. Zivkovic[1]; Carlito B Lebrilla[1]; *[1]University of California, Davis, Davis, CA; [2]Stanford University School of Medicine, Palo Alto CA; [3]Washington University in St. Louis, St. Louis, MO*

MOA pm 03:10 **Risk Verses Benefits for Cadmium, Lead and Mercury Exposure From Seafood Consumption**; Marc E. Engel; *FDACS, Tallahassee , FL*

MOA pm 03:30 **Chemical Changes in a Gamma Ray-Irradiated Rodent Diet Revealed by nanoLC-MS/MS**; Jeevan K Prasain[1]; Landon Wilson[1]; Clinton J Grubbs[1]; Stephen Barnes[1]; *[1]University of Alabama at Birmingham, Birmingham, AL*

MOA pm 03:50 **Investigation of Sample Preparation and Data Acquisition Effects on Non-Targeted Screening of Food Matrices Using LC/HR-MS**; Ann M Knolhoff[1]; Caitlin Kneapler[1]; Timothy R Croley[1]; *[1]FDA/CFSAN, College Park, MD*

MOA pm 04:10 **Forensic Analysis of a Mass Poisoning in Mozambique Associated with a Homebrewed Beverage using LC-HRAM MS and DART-MS**; Sara Kern[1]; Travis M. Falconer[1]; Jennifer L Brzezinski[1]; Brian L Boyd[1]; James A Turner[1]; Jonathan J Litzau[1]; *[1]US FDA, Cincinnati, OH*

2:30-4:30 pm MONDAY
FUNDAMENTALS: ION SPECTROSCOPY
Thomas Rizzo (École Polytechnique Fédérale de Lausanne (EPFL))
Room 221, level 2

MOB pm 02:30 **Structural Transitions in Gas Phase Proteins Investigated via IR Spectroscopy: from Native to Helical to Unzipped**; Isabel Gonzalez[1]; Eike Mucha[1]; Jongcheol Seo[1]; Waldemar Hoffmann[1]; Stephan Warnke[1]; Kevin Pagel[1, 2]; Gert Von Helden[1]; *[1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany; [2]Freie Universität Berlin, Berlin, Germany*

MOB pm 02:50 **Understanding Structures of Amino Acid Cluster Ions in the Gas Phase: Solved and Unsolved Problems**; Xianglei Kong; *Nankai University, Tianjin*

MOB pm 03:10 **Conformation-specific IR-UV Double-resonance Spectroscopy and Structural Analysis of Sodiated Leucine Enkephalin**; Nicole Burke[1]; Christopher Harrilal[1]; Andrew DeBlase[1]; Timothy Zwier[1]; Scott A McLuckey[1]; *[1]Purdue University, West Lafayette, IN*

MOB pm 03:30 **Action-Excitation Energy Transfer for the Structural Characterization of Proteins**; Nathan Hendricks[1]; Ryan R Julian[2]; *[1]University of California, Riverside, Riverside, CA; [2]University of California, Riverside Riverside, CA*

MOB pm 03:50 **Gas-phase VUV Photoionization and Photofragmentation of Geometrically Well-Defined Coinage Metal Nanocluster Cations**; Richard A. J. O'hair[1]; Steven Daly[2]; Athanasios Zavras[8]; Laurent Nahon[4]; Jiaye Li[5]; Alexandre Giuliani[4]; Rodolphe Antoine[2]; Philippe Dugourd[2, 6]; *[1]University of Melbourne, Victoria, Australasia; [2]Université Lyon, Lyon, France; [3]University of Melbourne, Melburne, Australia; [4]SOLEIL, l'Orme des Merisiers, St Aubin, Gif sur Yvette Cedex, France; [5]University of Melbourne, Victoria, Australia; [6]CRNS, Lyon, France*

MOB pm 04:10 **Near-UV Water Splitting by Gas-Phase Copper(bipy) Complexes**; Andy Dang[1]; Frantisek Turecek[1]; Christopher J Shaffer[2]; Victor Ryzhov[3]; Michael Lesslie[3]; John Lawler[3]; *[1]University of Washington, Seattle, WA; [2]Valspar, Minneapolis, MN; [3]Northern Illinois University, DeKalb, IL*

2:30-4:30 pm MONDAY
INSTRUMENTATION: NEW DEVELOPMENTS IN IONIZATION AND SAMPLING
W. Alexander Donald (University of New South Wales)
Stars Ballroom 1, level 3

MOC pm 02:30 **Measuring Masses of Single Bacterial Whole Cells with Laser Induced Acoustic Desorption Plasma Charge Detection Quadrupole Ion Trap Mass Spectrometer**; Shao-Yu Liang[1]; Chou-Hsun Han[1]; Dineshkumar Yograj Turkar[1]; Avinash Adhikrao Patil[1]; Szu-Wei Chou[1, 2]; Wen-Ping Peng[1]; *[1]National Dong Hwa University, Shoufeng Hualien, Taiwan; [2]AcroMass Technologies, Inc. Taipei, Taiwan*

MOC pm 02:50 **Near Field Ablation High Lateral Resolution Sampling for Mass Spectrometry**; Fan Cao[1]; Fabrizio Donnarumma[1]; Kermit K Murray[1]; *[1]Louisiana State Univeristy, Baton Rouge, LA*

MOC pm 03:10 **Ultra-Soft Picosecond Laser Extraction of Biological Compounds from Water and Tissue for Mass Spectrometry**; Wesley Robertson[1]; Yinfei Lu[1]; Cornelius L Pieterse[1]; Frederik Busse[1]; R.J.Dwayne Miller[1]; *[1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany*

MOC pm 03:30 **Automated High Throughput Identification of Microorganisms using Rapid Evaporative Ionisation Time of Flight Mass Spectrometry (REIMS-ToF-MS)**; Zsolt Bodai[1]; Daniel Simon[2]; Schaffer Richard[2]; Frankie Bolt[1]; Tamas Karancsi[2]; Julia Balog[2]; Tony Rickards[1]; Adam Burke[1]; Simon Cameron[1]; Kate Hardiman[1]; Monica Rebec[1]; Zoltan Takats[1]; *[1]Imperial College, London, United Kingdom; [2]Waters Research Center, Budapest, Hungary*

MOC pm 03:50 **A Robotic Trapping Column Exchanger for Increasing Clinical Assay Throughput by Capillary Liquid Chromatography-Mass Spectrometry**; Sandra E. Spencer[1]; Huilin Shi[2]; Thomas N. Corso[3]; Michael J MacCoss[2]; *[1]Univ. of North Carolina at Chapel Hill, Chapel Hill, NC; [2]University of Washington, Seattle, WA; [3]CorSolutions, LLC., Ithaca, NY*

MOC pm 04:10 **Open Probe Fast GC-MS – Combining Ambient Sampling, Ultra-Fast Separation and In-Vacuum Ionization for Real Time Forensic Analysis**; Uri Keshet[1]; Aviv Amirav[2]; Alexander B Fialkov[1]; Tal Alon[1]; *[1]Tel Aviv University, Tel Aviv, Israel; [2]Tel-Aviv University, Tel-Aviv, Israel*

2:30-4:30 pm MONDAY
ANTIBODIES AND ANTIBODY DRUG CONJUGATES
Shawna Hengel (Seattle Genetics, Inc.)
Stars Ballroom 2-3, level 3

MOD pm 02:30 **Leveraging Antibody Structure Analysis via Data Multiplexing in Top-Down Targeted Protein analysis**; Kristina Srzentic[1]; Konstantin Nagornov[2]; Anton N Kozhinov[2]; Yury O Tsybin[2]; *[1]Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland; [2]Spectroswiss Sàrl, Lausanne, Switzerland*

MOD pm 02:50 **Extending the Middle-Down HDX-MS Method for Residue-Level Structural Characterization of Antibody-Antigen Complexes**; Jingxi Pan[1]; Suping Zhang[2]; Christoph H. Borchers[1, 3]; *[1]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [2]MRM Proteomics, Inc., Victoria, BC, Canada; [3]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada*

MOD pm 03:10 **A Modular and Adaptive Mass Spectrometry-Based Platform for Support of Bioprocess Development toward Optimal Host Cell Protein clearance**; Feng Yang[1]; Donald E. Walker[1]; Joseph Carver[1]; David A. Michels[1]; Christopher Yu[1]; *[1]Genentech Inc, South San Francisco, CA*

MOD pm 03:30 **Where Did the Linker-Payload Go? A Quantitative Investigation on the Destination of Released Linker-Payload from Antibody-Drug-Conjugate with Maleimide-Linker in Plasma**; Cong Wei[1]; Guodong Zhang[2]; Tracey Clark[1]; Frank Barletta[1]; Nathan Tumey[1]; Brian Rago[1]; Steven Hansel[1]; Xiaogang Han[1]; *[1]Pfizer, Groton, CT; [2]Shire, Lexington, MA*

MOD pm 03:50 **Profiling Multiple Post-translational Modifications of Therapeutic Antibodies Circulating in Human Patients**; Yinyin Li[1]; Michael Monine[1]; Yu Huang[1]; Patrick Swann[1]; Yelena Lyubarskaya[1]; *[1]Biogen Inc., Cambridge, MA*

MOD pm 04:10 **Model-Based Algorithms for Intact Mass Analysis of Biotherapeutics**; Marshall W. Bern[1]; Yong J Kil[2]; Eric Carlson[1]; Doron Kletter[1]; Wilfred Tang[1]; Christopher Becker[1]; *[1]Protein Metrics, Palo Alto, CA; [2]Protein Metrics, San Carlos, CA*

2:30-4:30 pm MONDAY
DATA INDEPENDENT ACQUISITION: INNOVATIVE METHODS AND APPLICATIONS
Andrew K. Ottens (Virginia Commonwealth University)
Stars Ballroom 3-4, level 3

MOE pm 02:30 **LC–SWATH-MS/MS Data Acquisition with Deconvolution of High-Resolution MS Data in Metabolomics**; Tomas Cajka[1]; Oliver Fiehn[1]; *[1]UC Davis Genome Center, Davis, CA*

MOE pm 02:50 **A Promising Alternative to SWATH:MS1-based Strategy(IonStar) Enables In-Depth and Reproducible Proteomics Quantification in Large Cohorts with High Accuracy and Extremely-Low-Level-Missing-Data**; Xiaomeng Shen[1, 2]; Jun LI[3]; Shichen Shen[1, 2]; Qiang Hu[4]; Xin Miao[3]; Chengjian Tu[3, 2]; Lei Nie[5]; Xue WANG[4]; Jianmin Wang[4]; William J Jusko[3]; Benjamin C Orsburn[6]; Jun Qu[2, 3]; *[1]Dept. of Biochemistry at SUNY at Buffalo, Buffalo, NY; [2]Center of Excellence in Bioinformatics&Life Sci., Buffalo, NY; [3]Dept. of Pharmaceutical Sci. at SUNY at Buffalo, Buffalo, NY; [4]Rosewell Park Cancer Institute, Buffalo, NY; [5]Shandong University, Jinan, Shandong; [6]Thermo Fisher Scientific, San Jose, CA*

MOE pm 03:10 **Qualitative and Quantitative Characterization of a Novel DIA Method for Omics Analysis and its Application to Biomedical Analyses**; Arthur Moseley[1]; Chris Hughes[2]; Erik J. Soderblom[3]; Keith Richardson[2]; Will Thompson[4]; Jason Wildgoose[2]; James Langridge[2]; *[1]Duke University School of Medicine, Durham , NC; [2]Waters, Wilmslow, United Kingdom; [3]Duke University School of Medicine, Durham, NC; [4]Duke University School of Medicine, Durham, NC*

MOE pm 03:30 **Bidimensional FT-ICR MS: a fully Data Independent Acquisition**; Fabrice Bray[1]; Lionel Chiron[2]; Matthias Witt[3]; Marc-André Delsuc[4]; Christian Rolando[5]; *[1]Univ. de Lille 1, Sciences et Technologies, Villeneuve d'Ascq, France; [2]CASC4DE, Strasbourg, France; [3]Bruker Daltonic GmbH, Bremen, Germany; [4]Université de Strasbourg, Strasbourg, France; [5]Univ. de Lille 1, Sciences et Technologies, Villeneuve d'Ascq*

MOE pm 03:50 **Data Independent Acquisition for the Rapid Screening of *de novo* Protein Designs**; Jason Michael Gilmore[1]; Jorge Fallas[1]; George Ueda[1]; David Baker[1]; Michael J MacCoss[1]; *[1]University of Washington, Seattle, WA*

MOE pm 04:10 **High Content Discovery Proteomics of a Breast Tumor Tissue Microarray using Data Independent Acquisition**; Bin Fang[1]; Douglas C Marchion[1]; Amol Prakash[2]; Scott M Peterman[3]; Michelle Fournier[1]; Zena Sayegh[1]; Joseph J Johnson[1]; Agnieszka Kasprzak[1]; Daryoush Saeed-Vafa[1]; Roohi Ismail-Khan[1]; Steven A Eschrich[1]; Anthony M Magliocco[1]; John Koomen[4]; *[1]Moffitt Cancer Center, Tampa, FL; [2]Optys Tech Corporation, Philadelphia, PA; [3]Thermo Fisher, San Jose, CA; [4]H. Lee Moffitt Cancer Center, Tampa, FL*

2:30-4:30 pm MONDAY
INFORMATICS: METABOLOMICS
Hyung Won Choi (National University of Singapore)
Hemisfair Ballroom 3, level 3

MOF pm 02:30 **Collaborative Human Computing: The Next Generation Paradigm in Metabolomics**; Mingxun Wang[1, 2]; Pieter Dorrestein[3]; Nuno Bandeira[1, 2, 3]; *[1]Center for Computational Mass Spectrometry, University of California San Diego, La Jolla, CA; [2]Computer Science and Engineering, University of California San Diego, La Jolla, CA; [3]Skaggs School of Pharmacy, UC San Diego La Jolla, CA*

MOF pm 02:50 **FDR-controlled Metabolite Annotation for High-Resolution Imaging Mass Spectrometry**; Andrew Palmer[1]; Michael Becker[2]; Ilya Chernyavsky[3]; Dominik Fay[1]; Artem Tarasov[1]; Vitaly Kovalev[1]; Jens Fuchser[2]; Sergey Nikolenko[1]; Theodore Alexandrov[1, 4, 5]; *[1]European Molecular Biology Laboratory, Heidelberg, Germany; [2]Bruker Daltonic GmbH, Bremen, Germany; [3]University of Bremen, Bremen, Germany; [4]Skaggs School of Pharmacy, UC San Diego La Jolla, CA; [5]SCiLS GmbH, Bremen, Germany*

MOF pm 03:10 **Tandem Mass Spectral Libraries of Recurrent Unidentified Spectra for Urine and Plasma: A New Kind of Library for Metabolomics Applications**; Yamil Simon[1]; Ramesh Marupaka[2]; Xinjian Yan[2]; Yuri Mirokhin[2]; Kelly H. Telu[2]; William E Wallace[2]; Stephen E Stein[2]; *[1]NIST, Gaithersburg, MD; [2]NIST, Gaithersburg MD*

MOF pm 03:30 **Hydrogen Rearrangement Rules for Computational MS/MS Fragmentation**; Hiroshi Tsugawa[1]; Wataru Tanaka[2]; Ryo Nakabayashi[1];

Kazuki Saito[1,3]; Masanori Arita[1,4]; *[1]RIKEN Center for Sustainable Resource Science, Yokohama, Japan; [2]SOKENDAI, Mishima, Japan; [3]Chiba University, Inage-ku, Japan; [4]National Institute of Genetics, Mishima, Japan*

MOF pm 03:50 **New in BioCyc: Pathway Collages and Pathway Prediction Algorithm**; Peter Karp; *SRI International, Menlo Park, CA*

MOF pm 04:10 **Normalization and Integration of Large-Scale Mass Spectrometry-based Metabolomics Data Using Support Vector Regression**; Xiaotao Shen[1]; Zhengjiang Zhu[1]; *[1]IRCBC, Chinese Academy of Sciences, Shanghai, China*

2:30-4:30 pm MONDAY
NUCLEIC ACID MS
Silvia Balbo (University of Minnesota)
Hemisfair Ballroom 2, level 3

MOG pm 02:30 **RNA Modification Mapping from Multiple Bacteria in a Single Sample using LC-MS/MS**; Xiaoyu Cao[1]; Patrick A Limbach[2]; *[1]University of Cincinnati, Cincinnati, Ohio; [2]University of Cincinnati, Cincinnati, OH*

MOG pm 02:50 **Exploring the Use of Top-Down Mass Spectrometry for the Identification, Localization, and Relative Quantitation of RNA Nucleobase Methylations**; Heidelinde Glasner[1]; Christian Riml[2]; Christoph Falschlunger[2]; Ronald Micura[2]; Kathrin Breuker[2]; *[1], Innsbruck, Tyrol; [2]University of Innsbruck, Innsbruck, Austria*

MOG pm 03:10 **Cation Binding to Nucleic Acids**; Adrien Marchand[1]; Clémence Rabin[1]; Sandrine Livet[1]; Solenne Delahaye[1]; Valentina D'Atri[1]; Josephine Abi-Ghanem[1]; Frédéric Rosu[2]; Valerie Gabelica[1]; *[1]Univ. Bordeaux / Inserm / CNRS (ARNA Laboratory), IECB Pessac, France; [2]CNRS UMS 3033, IECB Pessac, France*

MOG pm 03:30 **Plasticity in Cancer Nucleotide Metabolism Revealed by Multiplexed MRM Assays**; Thuc Le[1]; Soumya Poddar[1]; Joseph Capri[1]; Evan Abt[1]; Woosuk Kim[1]; Julian P Whitelegge[1]; Kym F Faull[1]; Caius Radu[1]; *[1]UCLA, Los Angeles, CA*

MOG pm 03:50 **Identification and Characterizations of 8,5′-cyclo-2′-deoxypurine Lesion-binding Proteins**; Preston Williams[1]; Pengcheng Wang[1]; Yinsheng Wang[1]; *[1]University of California - Riverside, Riverside, CA*

MOG pm 04:10 **Multi-Class Carcinogenic DNA Adduct Quantification in Formalin-Fixed Paraffin-Embedded Tissues by Ultra-Performance Liquid Chromatography–Tandem Mass Spectrometry**; Jingshu Guo[1]; Byeong Hwa Yun[1]; Pramod Upadhyaya[1]; Lihua Yao[1]; Sesha Krishnamachari[1]; Thomas A. Rosenquist[2]; Arthur P. Grollman[2]; Robert J. Turesky[1]; *[1]University of Minnesota, Minneapolis, MN; [2]Stony Brook University, Stony Brook, NY*

2:30-4:30 pm MONDAY
COVALENT LABELING AND CHEMICAL CROSSLINKING
Juri Rappsilber (University of Edinburgh and TU Berlin)
Hemisfair Ballroom 1, level 3

MOH pm 02:30 **Crosslink-assisted Structure Determination of the Human Spliceosomal Subcomplex, U4/U6.U5 tri-snRNP**; Olexandr Dybkov[1]; Romina V. Hofele[1,2]; Dmitry E. Agafonov[1]; Berthold Kastner[1]; Wen-Ti Liu[1]; Holger Stark[1,3]; Reinhard Luehrmann[1]; Henning Urlaub[1,2]; *[1]Max Planck Institute for Biophysical Chemistry, Goettingen, Germany; [2]University Medical Center (UMG), Goettingen, Germany; [3]Georg-August-Universitaet Goettingen, Goettingen, Germany*

MOH pm 02:50 **Developing a New Quantitative Cross-linking Mass Spectrometry (XL-MS) Strategy to Define *in vivo* Structural Dynamics of Protein Complexes**; Clinton Yu[1]; Xiaorong Wang[1]; Rosa I Viner[2]; Alex Huszagh[1]; Eric Novitsky[1]; Tonya Second[2]; Scott Rychnovsky[1]; Lan Huang[1]; *[1]University of California, Irvine, Irvine, CA; [2]Thermo Fisher Scientific, San Jose, CA*

MOH pm 03:10 **Solving the Tertiary Structure of SalBIII Protein by Chemical Cross-Linking/Mass Spectrometry and Molecular Modeling**; Allan Jhonathan Ramos Ferrari[1]; Hugo Cesar de Jesus[1]; Marcio Vinicius Bertacine Dias[2]; Luciana Gonzaga de Oliveira[1]; Peter Leadlay[3]; Fabio Cesar Gozzo[1]; *[1]University of Campinas, Campinas, Brazil; [2]University of São Paulo, São Paulo, SP; [3]University of Cambridge, Cambridge, UK*

MOH pm 03:30 **Combining Zero-Length Cross-Linking and Label-free Proteomics to Identify Functional Binding Residues in an Ordered-Disordered Heterodimeric Protein Complex**; Michelle Dubuke[1]; Stephanie Maniatis[1]; Mary Munson[1]; Scott A Shaffer[1]; *[1]UMass Medical School Department of Biochemistry and Molecular Pharmacology, Worcester, MA*

MOH pm 03:50 **Charting the Cellular Interactome by Proteome-Wide Cross-Linking Mass Spectrometry**; Fan Liu[1]; Phlip Lossl[1]; Richard Scheltema[1]; Rosa Viner[2]; Albert Heck[1]; *[1]Utrecht University, Utrecht, The Netherlands; [2]Thermo Fisher Scientific, San Jose, CA*

MOH pm 04:10 **Global XL-MS: Proteome-scale Interactomes Unifying Cross-Linked Datasets**; Devin Schweppe[1]; Chunxiang Zheng[1]; Juan Chavez[1]; Arti Navare[1]; Xia Wu[1]; Jimmy K Eng[1]; James Bruce[1]; *[1]University of Washington, Seattle, WA*

4:45 - 5:30 PM, MONDAY AFTERNOON
AWARD LECTURE
Jenny Brodbelt (University of Texas, Austin) presiding
Hall 1, level 1

Award for a Distinguished Contribution in Mass Spectrometry

Scott A. McLuckey
Purdue University

There are light refreshments in common areas.

01 Top-Down Proteomics: Ready for Primetime?
Ying Ge and Paul Thomas presiding
Room 220, level 2

Top Down protein mass spectrometry allows comprehensive analysis of intact, multiply modified proteoforms from complex mixtures. In this workshop, we will provide an update from the Consortium for Top Down Proteomics, discussing new community-wide pilot projects. We will also review and discuss common roadblocks to successful top down proteomics experiments from sample preparation to data acquisition to data analysis in a panel format. A limited number of 5 minute 'lightning talks' will be available for researchers to provide rapid-fire updates on recent achievements and accomplishments of note. Contact workshop chairs if you are interested in presenting.

02 Next Generation LC-MS:
Critical Insights & Future Perspectives
Hongying Gao presiding
Room 221, level 2

Recent advancement in high resolution mass spectrometry has expanded the capabilities of the instrumentation for both qualitative and quantitative analysis. Coupling UPLC with HRMS, samples can be analyzed without authentic standards nor the knowledge of the analytes in the samples, and data can be banked for post-acquisition data processing when the knowledge of the analytes or the authentic standards becomes available. The ideal super LC/MS technology needs to capture the quantitative and qualitative information of the unknown analytes with a variety of physiological properties in a wide range of chemical space. This data banking approach presents new challenges and opportunities for high resolution LC/MS system. In this workshop, a case in industry will be presented to illustrate the need for advancement in LC and mass spectrometry, and then the latest technology advances in high resolution LC/MS and ion mobility will be presented, followed by open discussions on the capabilities and feasibility of the features of next generation LC/MS.

Introduction and Objectives of the Session. Why We Need Super LC/MS System? Hongying Gao, Pfizer Inc.

Challenges and Opportunities in High Resolution LC/MS. Alexander Makarov, Thermo Fisher Scientific.

How the Rise of IMS Will Change the Use of LC/MS. Richard (Dick) D. Smith, Pacific Northwest National Laboratory.

03 Art and Cultural Heritage Mass Spec Applications
Mehdi Moini presiding
Room 225A, level 2

The purpose of this workshop is to discuss the application of MS to art and cultural heritage objects, as well as natural history specimens. This will be an interactive workshop in which various subjects relevant to museums' specimens will be discussed in a casual, dialog format. A preliminary list of topics include: 1) Analysis of paint, coating and binders; textiles; bone and tissue; ink and paper. 2) Mechanism of aging and degradation of art and natural history objects. 3) Dating. 4) Impact of radiation on museums' specimens. 5) Fossilomics and ancient DNA. 6) Forensic archeology. 7) Species identification of proteinaceous materials used in work of art and natural history. 8) Identification of forgery.

04 Bioinformatics: Challenges & Opportunities in Proteogenomics (Bioinformatics for MS)
Sangtae Kim and Meena Choi presiding
Room 225B, level 2

Proteogenomics (integrated proteomics and genomics) has gained lots of popularity in recent years. Traditionally, it was mainly used to improve genome annotation of newly or partially sequenced organisms, but now it is also increasingly applied in cancer studies. In this workshop, we will discuss bioinformatics challenges and opportunitiesin proteogenomics. It will begin with short introductory presentations by researchers who have recently conducted large-scale proteogenomics studies, and be followed by audience driven discussions.

05 Environmental Analysis: Emerging Topics (Environmental Applications Interest Group)
Achille Cappiello, Marc E. Engel, and Christopher G. Gill presiding
Room 225C, level 2

This workshop will feature three or four members of the environmental mass spectrometry community that will informally present a maximum of five slides to generate discussion within the working group. Topic areas for the workshop this year are centered upon emerging contaminants (targeted and non targeted) as well as new analytical approaches for their characterization and measurement.

06 Metal Cationization in MS/MS of Biomolecules (Metal Ion Coordination Chemistry Interest Group)
Alexandre Shvartsburg and Cheng Lin presiding
Room 225D, level 2

A viable alternative to the prevailing paradigm of ionizing biomolecules by protonation (or deprotonation) is the addition of other charged moieties. Metal cationization commonly introduces distinct isotopic patterns, major conformational changes, novel electronic properties, and/or new dissociation chemistry (especially in electron activated mechanisms) that present diverse and still sparsely explored analytical opportunities. In tandem mass spectrometry, metalation has been employed to stabilize labile modifications, promote complementary and more informative fragmentation pathways, and facilitate isomer separation. In another aspect, the native structure of many biomolecules that is often desirable to preserve in MS depends on the metal coordination. This workshop will encourage the adoption of metal cationization in biological mass spectrometry and particularly MS/MS applications.

07 Proteomics Informatics for the Trans-Proteomic Pipeline
Luis Mendoza and Eric Deutsch presiding
Room 301A, level 3

The workshop will begin with a brief overview of the Trans-Proteomic Pipeline (TPP) and its newest features and capabilities. We will then focus on 5 individual topics, fostering a discussion with workshop participants on the current strengths, weaknesses, and future directions for the TPP. The workshop will enable participants to describe challenges in proteomic data analysis and help drive directions in software approaches through needs of the community. The topic leads for discussion are: cross-linking analysis with Kojak, label-free quantitative analysis with StPeter, chimeric spectrum analysis with reSpect, proteomics informatics using cloud computing infrastructure such as Amazon Web Services, and analysis of SWATH-MS data with SWATHProphet. Each topic will be introduced with a brief summary of features and ideas. Then feedback and discussion by the workshop participants will be promoted.

08 Metabolomics: Emerging Technologies for Continued Innovation (Metabolomics Interest Group)
Timothy Garrett and Andrew Patterson presiding
Room 301BC, level 3

This workshop will begin with a brief discussion of the most exciting technological advances in the field of metabolomics over the past year. The moderators will highlight 2-3 noteworthy metabolomic publications that they feel are particularly impressive achievements and survey the audience for their opinions. Three-four invited scientists with expertise in the technologies highlighted will serve as panelists and answer questions posed by the moderators and attendees. The workshop will close with a discussion among the panelists on their perspectives of emerging trends and the role that these technologies are playing in future development. Advances intended to be highlighted are: (i) advances in chromatographic separation of metabolites and its influence on metabolomics data, (ii) innovative experimental designs, and (iii) new tools for metabolite identification.

09 Polymer MS Technology: Advancements and Discussion
(Polymeric Materials Interest Group)
Stephen Rumbelow and Gyorgy Vas presiding
Room 302A, level 3

This workshop will focus on updating the group on recent work and challenges faced in the various fields such as academic, government, and industry. The focus of this group is polymer and material analysis utilizing various mass spectrometric techniques for both characterization and quantitation of oligomeric species. This workshop will explore the various ways that polymers and materials are not only analyzed themselves but also how they interact with other materials such as patients, and different type of products such as packaging and medical devices.

10 MS Analysis of Antibody-Drug Conjugates
(Pharmaceuticals Interest Group)
Christine Gu and Matthew Schenauer presiding
Room 302BC, level 3

Due to the success of pharmaceutical interest group workshops since 2013, and continued interest in MS analysis of antibody drug-conjugates (ADCs), we propose a similar workshop for 2016. After a short informal presentation, less than ten minutes, the majority of the workshop would include an audience driven discussion with the opportunity to ask questions to a panel of experts. The organizers will have backup questions prepared for the panel to start or prompt the discussion if needed. The short presentation will provide an update on current workflows for ADC MS analysis in the industry for the discovery and development. Potential areas of discussion may include the large range of characterization required for ADCs from initial MAb assessment to bioanalytical assay development, with the focus on Mass Spec method development and optimization. To identify potential panelists, gauge the level of interest of the ASMS community, and tailor the discussion we will send out a survey of open ended questions in April.

11 Protocol Repositories for Proteomics and Metabolomics
(Analytical Lab Managers Interest Group)
Allis Chien and Brett Phinney presiding
Room 303A, level 3

Protocols and SOP's are the lifeblood of any analytical core facility. Although finding detailed protocols has gotten easier over the years (Nature Protocols for example), finding protocols that have been validated, via successful use by numerous people, is still challenging and fraught with failure. Often even following a detailed published protocol can fail and the user is left wondering: What happened? In this workshop we will discuss options for finding and using protocol repositories for mass spectrometry-based analytical core facilities (Proteomics and Metabolomics). Specifically, we will discuss the new protocol repository set up by the Association of Biomolecular Resource Facilities (ABRF) along with several other freely available options.

12 Miniaturization of Ion Traps and Related Devices
(Ion Trap Interest Group)
Daniel Austin and Zheng Ouyang presiding
Room 303BC, level 3

Ion traps constitute a major portion of the effort to produce miniaturized mass spectrometers. In addition, the wealth of new ionization techniques have led to many new devices for introduction, transmission, and detection of ions in the context of portable devices. The workshop will start with short (4-minute) snippets from several groups working in this area. Next, a panel-led discussion will address opportunities, applications, and challenges of portable mass spectrometry.

13 MS Career Options: How to Kick-Start your Career
(Young Mass Spectroscopists Interest Group)
Kristin Wildsmith and Violet Lee presiding
Room 304, level 3

The workshop features an interactive panel discussion on professional development (Bring your questions). Topics will be centered around career planning and management, fundamental training, industrial internship, and diversity of career options within the MS field. A panel of representatives from government, industrial (domestic and foreign) and academic organizations, will share their knowledge, experience, and practices on career prospects.

14 System Performance: Tracking through Statistical QC Monitoring (LC/MS & Related Topics Interest Group)
Michael Bereman and Brent Dixon presiding
Room 305, level 3

Liquid chromatography mass spectrometry systems are recognized as highly sensitive and specific tools for metabolomic and proteomic analyses. Ensuring the integrity of data through a system of controls referred to as quality control standards enables a higher level of confidence in the obtained results. Providing intra-laboratory personnel with quality control charts allows for correction when standards exceed acceptability limits. Control charts may be used in an inter-laboratory manner to compare results across labs. By monitoring performance standards, a higher level of commutability of experimental results may be achieved.

The workshop will provide a demonstration of online QC tracking through Skyline; system performance tracking and control charting. The workshop will explore available controls for tryptic digestion to ensure proteolytic cleavage. The content will also include a section related to metabolomic analyses.

Integrating quality control and performance standards in the experimental design is not a new concept. However, the intention to monitor these standards over time and across experiments presents an opportunity. A major limitation in the broader analysis of experimental control performance has been aggregation and visualization. Precious samples may be better utilized by identifying a trend and performing a preventive action to avoid a failed assay. The overall aim is to shift to a prospective action driven review rather than a retrospective control review approach.

AFTER 8:00 PM
CORPORATE HOSPITALITY SUITES
GRAND HYATT HOTEL

8:30-10:30 am TUESDAY
ENERGY, PETROLEUM, AND BIOFUELS: INSTRUMENTATION AND METHOD DEVELOPMENT
Young Jin Lee (Iowa State Unniversity)
Hall 1, level 1

TOA am 08:30 **Petroleomic Characterization using an Ion Mobility-Orbitrap Platform**; Yehia Ibrahim[1]; Roza Wojcik[2]; Spencer A Prost[2]; Sandilya Garimella[2]; Randolph Norheim[2]; Erin Baker[2]; Noor Aly[2]; Hans Ketelslegers[3]; Fabian Grimm[4]; Ivan Rusyn[4]; Richard D Smith[2]; *[1]Pacific Northwest National Laboratory, Richland , WA; [2]Pacific Northwest National Laboratory, Richland, WA; [3]Concawe, Brussels, BELGIUM; [4]Texas A&M, College Station, TX*

TOA am 08:50 **Molecular Composition of Petroleum Interfacially Active Species: Implications in Emulsion Science**; Ryan P. Rodgers[1]; Amy C Clingenpeel[2, 3]; Winston K Robbins[4]; Steven Rowland[4]; Yuri E Corilo[3, 4]; David C Podgorski[4]; *[1]Nat'l High Magnetic Field Lab, Tallahassee, FL; [2]FSU Department of Chemistry and Biochemistry, Tallahassee, FL; [3]National High Magnetic Field Laboratory, Tallahassee, FL; [4]Future Fuels Institute, FSU Tallahassee, FL*

TOA am 09:10 **Gas-phase Hydride Transfer between Carbocations and Analyte Alkanes Provides a Gentle and Controllable Ionization Method with Minimal Fragmentation**; Mingzhe Li[1]; Chunfen Jin[1]; Hanyu Zhu[1]; Mark Romanczyk[1]; Jyrki Viidanoja[2]; Hilkka I Kenttamaa[1]; *[1]Purdue University-Department of Chemistry, West Lafayette, IN; [2]Neste Oil, Keilaranta, Finland*

TOA am 09:30 **Selective Analysis of Complex Crude Oil Mixtures using Chemical and Instrumental Methods**; Wolfgang Schrader[1]; Alessandro Vetere[1]; Xuxiao Wang[1]; *[1]Max-Planck Inst für Kohlenforschung., Mülheim / Ruhr, Germany*

TOA am 09:50 **Gel Permeation Chromatography (GPC) Inductively Coupled Plasma High Resolution Mass Spectrometry (ICP HR MS) Parameters Study in Petroleum Product Analysis**; Sara Gutierrez Sama[1, 2]; Alain Desprez[1, 2, 3]; Gabriel Krier[3]; Charles-Philippe Lienemann[4]; Jérémie Barbier[4]; Ryszard Lobinski[1]; Caroline Barrere-Mangote[2, 5]; Pierre Giusti[2, 5]; Brice Bouyssiere[1, 5]; *[1]CNRS/UPPA, UMR 5254, LCABIE, Pau, France; [2]TOTAL Refining and Chemicals, TRTG Gonfreville l'Orcher, France; [3]UL, LCP-A2MC, Metz, France; [4]IFPEn, Solaize, France; [5]TOTAL RC - CNRS Joint Laboratory C2MC :Complex Matrices Molecular Characterization, -, France*

TOA am 10:10 **Online Photoionization Time-of-Flight Mass Spectrometric Study on the Catalytic Pyrolysis of Bituminous Coal over HUSY and HZSM-5**; Yanan Zhu[1]; Jiuzhong Yang[1]; Fei Qi[2]; Yang Pan[1]; *[1]University of Science and Technology of China/ USTC, Hefei, P.R. China; [2]Shanghai Jiao Tong University, Shanghai, China*

8:30-10:30 am TUESDAY
FUNDAMENTALS: METAL ION CATIONIZATION, METAL-LIGAND INTERACTIONS AND CATALYSIS
Jinhua Ren (University of the Pacific)
Room 221, level 2

TOB am 08:30 **Chemi-ionization Thermochemistry of the Lanthanides: Relevance for Atmospheric Release Studies**; Peter B. Armentrout[1]; Maria Demireva[1]; Cameron Owen[1]; Richard M Cox[2]; *[1]University of Utah, Salt Lake City, UT; [2]Pacific Northwest National Lab, Richland, WA*

TOB am 08:50 **Supermetallization of Peptides and Proteins**; Yury Kostyukevich[1]; Alexey S Kononikhin[2, 3]; Maria Indeykina[4, 3]; Evgeny Kukaev[2, 4]; Igor A Popov[4, 5]; Eugene Nikolaev[1, 2, 3, 4]; *[1]Skolkovo Institute of Science and Technology, Skolkovo, Russian Federation; [2]Moscow Institute of Physics and Technology, Moscow, Russia; [3]Institute for Energy Problems of Chemical Physics, Moscow, Russia; [4]Emanuel Institute of Biochemical Physics, Moscow, Russia; [5]Moscow Institute of Physics and Technology, Dolgoprudny Moscow Oblast, Russia*

TOB am 09:10 **Copper-binding and Redox Activity and of a Series of Alternative Methanobactin Peptides**; Laurence Angel[1]; Yashodharani Vytla[1]; Manogna Deeconda[1]; Sravya Challa[1]; Rajpal Vangala[1]; Jacob W McCabe[1]; *[1]Department of Chemistry, Texas A&M University-Commerce, Commerce, TX*

TOB am 09:30 **Capture of Reactive Monophosphine Ligated Palladium(0) Intermediates by Mass Spectrometry**; Qiuling Zheng[1]; Yong Liu[2]; Qinghao Chen[2]; Meihong Hu[1]; Roy Helmy[2]; Edward Sherer[2]; Christopher Welch[2]; Hao Chen[1]; *[1]Ohio University, Athens, OH; [2]Merck, Darmstadt, Germany*

TOB am 09:50 **Revisiting Organometallic Chemistry by Ion Mobility**; Izabella Czerwinska[1]; Sophie Rappe[1]; Carlos Larriba-Andaluz[2]; Nicolas Smargiasso[1]; Christopher Kune[1]; Albert Demonceau[3]; Johann Far[1]; Lionel Delaude[3]; Edwin A De Pauw[1]; *[1]Mass Spectrometry Laboratory, University of Liege, Liege, Belgium; [2]Department of Mechanical Engineering, Indiana University-Purdue University, Indiana; [3]Laboratory of Catalysis, University of Liege, Belgium*

TOB am 10:10 **Testing Nanoscale Homogeneity with Massive Cluster Secondary Ion Mass Spectrometry**; Michael J Eller[1]; Stanislav V Verkhoturov[1]; Emile A Schweikert[1]; *[1]Texas A&M University, College Station, TX*

8:30-10:30 am TUESDAY
HRMS FOR QUANTITATION IN DRUG DISCOVERY, DEVELOPMENT AND BEYOND
Ashley Ruth (FDA/DPA)
Stars Ballroom 1, level 3

TOC am 08:30 **Analysis of Host Cell Proteins throughout Biopharmaceutical Purification**; Martha Stapels[1]; Michelle Busch[1]; Samantha Cooper[1]; Veena Warikoo[1]; Kate Zhang[1]; *[1]Sanofi Genzyme, Framingham, MA*

TOC am 08:50 **Exploring the Use of HRMS for Circumventing Complex and Lengthy Sample Pre-Treatment for Absolute Quantification of mAbs in Plasma/ Serum Samples**; Ulrik Hvid Mistarz[1, 2]; Tam T. T. N. Nguyen[1]; Amaury Herbet[2]; Narciso Costa[2]; Didier Boquet[2]; Christophe Junot[2]; François Becher[2]; Kasper Dyrberg Rand[1]; *[1]Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark; [2]CEA Saclay, DSV/iBiTec-S/LEMM, Gif sur Yvette, France*

TOC am 09:10 **Evaluation of Ion Mobility and Targeted QTof Acquisition Modes for the Quantitative Analysis of Peptides**; Jayne Kirk[1]; Mark Wrona[2]; Kelly Doering[2]; Russell Mortishire-Smith[1]; Lisa A Vasicek[3]; Kevin P Bateman[3]; *[1]Waters Corporation, Wilmslow, UK; [2]Waters Corporation, Milford, MA; [3]Merck & Co., West Point, PA*

TOC am 09:30 **Bioanalysis and *in vivo* Stability Evaluation of a PEGylated Protein Drug by UHPLC-HRMS using a Disulfide-Containing Surrogate Peptide**; Naiyu Zheng[1]; Jianing Zeng[1]; Amy Manney[1];

Lakenya Williams[1]; Anne-Françoise Aubry[1]; Kimberly Voronin[1]; Adela Buzescu[1]; Yan J Zhang[1]; Alban Allentoff[1]; Carrie Xu[1]; Hongwu Shen[1]; William Warner[1]; Mark E Arnold[1]; *[1]Research and Development, Bristol-Myers Squibb Company, Princeton, NJ*

TOC am 09:50 **High-throughput MALDI TOF Mass Spectrometry for Drug Discovery in the Ubiquitin Pathway**; Virginia De Cesare[1]; Axel Knebel[1]; Matthias Trost[1]; *[1]MRC PPU, University of Dundee, Dundee, United Kingdom*

TOC am 10:10 **Simultaneous Quantitation and Metabolite Profiling of RG-125, a GalNAc-conjugated Oligonucleotide, and Its Five Metabolites using HRAM LC/MS**; Brandon Wilcock[1]; Kai Liu[2]; Daniel J. Mauchley[1]; Min Meng [1]; Troy Voelker[1]; Brian P. Schultz[2]; Tate Owen[2]; John Grundy[2]; *[1]Covance, Salt Lake City, UT; [2]Regulus Therapeutics Inc., San Diego, CA*

8:30-10:30 am TUESDAY
IMAGING: INSTRUMENTATION & METHOD DEVELOPMENT
Wendell P. Griffith (University of Texas at San Antonio)
Stars Ballroom 2-3, level 3

TOD am 08:30 **Design and Optimization of a Fully-controlled Stainless Steel Sublimator for Matrix Deposition in MALDI-IMS Experiments**; Roberto Fernández[1]; Jone Garate[1]; Sergio Lage[1]; Jose A Fernandez[1]; *[1]University of Basque Country, UPV/EHU Leioa Basque Country, Spain*

TOD am 08:50 **Identification of Bio-Molecules at Sub-Micron Lateral Resolution by TOF-SIMS Parallel Imaging MS/MS**; Gregory L FisheR[1]; Nina Ogrinc Potocnik[2]; Anne L Bruinen[2]; John S Hammond[1]; Ron M.A. Heeren[2]; *[1]Physical Electronics, Chanhassen, MN; [2]Maastricht University, M4I, Maastricht, Netherlands*

TOD am 09:10 **Developing a Gas Cluster Ion Beam (GCIB) for Enhanced Ionization and Reduced Matrix Effects in Secondary Ion Mass Spectrometry (SIMS)**; Hua Tian[1]; Andreas Wucher[2]; Nicholas Winograd[1]; *[1]Pennsylvania State University, University Park, PA; [2]University of Duisburg-Essen, Essen, Germany*

TOD am 09:30 **Ultra-High Spatial Resolution AP-SMALDI Mass Spectrometry Imaging of Lipids**; Mario Kompauer[1]; Sven Heiles[1]; Bernhard Spengler[1]; *[1]Justus Liebig University, Giessen, Germany*

TOD am 09:50 **Forensic Analysis of Latent Fingermarks by Silver-Assisted LDI Imaging MS on Non-Conductive Surfaces**; Nidia Lauzon[1]; Martin Dufresne[2]; Alexandre Beaudoin[3]; Pierre Chaurand[2]; *[1]University of Montreal, Montreal, Canada; [2]University of Montreal, Montreal Qc, Canada; [3]Sûreté du Québec, Montreal Qc, Canada*

TOD am 10:10 **Quantitative Imaging of Gold Nanoparticles in Tissues using inkjet-Printed Standards**; Sukru Gokhan Elci[1]; Brian Creran[1]; Bradley Duncan[1]; Alyssa L M Marsico[1]; Vincent M Rotello[1]; Richard W Vachet[1]; *[1]University of Massachusetts, Amherst, MA*

8:30-10:30 am TUESDAY
QUANTITATIVE PROTEOMICS IN SYSTEMS BIOLOGY
Stephanie Cologna (University of Illinois, Chicago)
Stars Ballroom 4, level 3

TOE am 08:30 **Diacylglycerol Metabolism in Regulation of Innate and Adaptive Functions of Dendritic Cells**; Ku-Lung Hsu[1]; Myungsun Shin[1]; *[1]University of Virginia, Charlottesville, VA*

TOE am 08:50 **A Systems Approach to Define the Spatial-Temporal Dynamics of Host Organelles upon Viral Infection**; Pierre Jean Beltran[1]; Rommel Mathias[1]; Ileana M. CristeA[1]; *[1]Princeton University, Princeton, NJ*

TOE am 09:10 **Analysis of Proteomic Variation in the Human Population: The HipSci iPS Cell Project**; Dalila Bensaddek[1]; Alejandro Brenes Murillo[1]; Helena Kilpinen[2]; Angela Goncalves[3]; Mariya Chhatriwala[4]; Rachel Nelson[5]; Chris Kirton[5]; Ludovic Vallier[4]; Daniel Gaffney[3]; Oliver Stegle[2]; Richard Durbin[3]; Angus Iain Lamond[1]; *[1]University of Dundee, Dundee, UK; [2]European Molecular Biology Laboratory, European Bioinformatics Institute (EMBL-EBI), Wellcome Trust Genome Campus, Cambridge, UK; [3]Wellcome Trust Sanger Institute, Wellcome Trust Genome Campus, Cambridge, UK; [4]Pancreatic Genetics, Wellcome Trust Genome Campus, Cambridge, UK; [5]Cellular Generation & Phenotyping, CGaP, Wellcome Trust Sanger Institute, Cambridge, UK*

TOE am 09:30 **Interrogating Oncogenic B-Raf Signaling through microRNAs using Functional Proteomics**; Thomas Lee[1]; Nan Wang[1, 2]; Stephane Houel[1, 3]; Kasey L. Couts[1]; Natalie G. Ahn[1]; *[1]University of Colorado, Boulder, Colorado; [2]University of Alberta, Edmonton, Canada; [3]Thermo Fisher Scientific, San Jose, CA*

TOE am 09:50 **Correlation of KRAS Proteoform Expression Profiles to Cancer Phenotypes via Integrated Proteogenomic Analysis of Colorectal Tumors**; Ioanna Ntai[1]; Josiah E Hutton[2]; Richard D Leduc[1]; Ryan T Fellers[1]; Neil L Kelleher[1]; *[1]Northwestern University, Evanston, IL; [2]Vanderbilt University, Nashville, TN*

TOE am 10:10 **Hunting Biomass Degrading Enzymes and Their Active Proteoforms through an Activity-Correlated Quantitative Proteomics Platform**; Hongyan Ma[1]; Delafield Graham Daniel[1]; Zhe Wang[1]; Si Wu[1]; *[1]University of Oklahoma, Norman, OK*

8:30-10:30 am TUESDAY
INSTRUMENTATION: NON-FT BASED ANALYZERS
Michael Westphall (University of Wisconsin-Madison)
Hemisfair Ballroom 3, level 3

TOF am 08:30 **Application of Multi Frequency Waveforms for Ion Isolation and Enhancement with the MOMA Ion Trap Mass Spectrometer**; Ryan M Danell[1]; Andrej Grubisic[2]; Friso H W Van Amerom[3]; Veronica T Pinnick[4]; Xiang Li[4]; Stephanie Getty[5]; Ricardo Arevalo[5]; William Brinckerhoff[5]; *[1]Danell Consulting, Inc., Winterville, NC; [2]Center for Research and Exploration in Space Science and Technology (CRESST), University of Maryland, College Park, MD; [3]Mini-Mass Consulting, Inc., Hyattsville, MD; [4]Center for Research and Exploration in Space Science and Technology (CRESST), University of Maryland, Baltimore County, MD; [5]NASA Goddard Space Flight Center, Greenbelt, MD*

TOF am 08:50 **Second Order Space and Velocity Focusing Time of Flight Mass Spectrometry using an Accelerator Field Free Region**; Robert E. Haufler[1]; Bill Loyd[2]; *[1]AB Sciex, Concord, ON; [2]SCIEX, Concord, ON*

TOF am 09:10 **Ion-Ion Proton Transfer and Parallel Ion Parking for Top-Down Analysis of Complex Protein Mixtures**; Scott A Ugrin[1]; Michelle A English[1]; Dina L Bai[1]; John E P Syka[2]; Jeffrey Shabanowitz[1]; Donald F Hunt[1]; *[1]University of Virginia, Charlottesville, VA; [2]Thermo Fisher Scientific, San Jose, CA*

TOF am 09:30 **System Architecture for Charge-independent Mass Spectrometry using Nanomechanical Resonators**; Shawn Fostner[1, 2]; Sergio Dominguez Medina[1, 3, 4]; Marc Sansa Perna[1, 2]; Thomas Alava[1, 2]; Ann-Kathrin Stark[1, 3, 4]; Ariel Brenac[5, 6]; Henri Blanc[1,2]; Marc Gely[1, 2]; Sébastien Hentz[1, 2]; Christophe Masselon[1, 3, 4]; *[1]Université Grenoble Alpes, Grenoble, France; [2]CEA, LETI, Grenoble, France; [3]CEA BIG-BGE, Grenoble, France; [4]INSERM U1038, Grenoble, France; [5]Université Grenoble Alpes, INAC-SP2M, Grenoble, France; [6]CEA, INAC-SP2M, Grenoble, France*

TOF am 09:50 **Dual-Polarity Ion Trap Mass Spectrometry: Dynamic Control and Monitoring of Gas-phase Ion-ion Reactions**; Muyi He[1]; Dan Guo[1]; You Jiang[2]; Xiong Xingchuang[2]; Zejian Huang[2]; Xiang Fang[2]; Wei Xu[1]; *[1]Beijing Institute of Technology, Beijing, China; [2]National Institute of Metrology, Beijing, China*

TOF am 10:10 **Quadrupole Wideband Isolation Directed by Ion Mobility Drift Separation for Analyzing Complex Protein Digests**; Bruce Wang[1]; Ruwan T Kurulugama[1]; George Stafford[1]; John Fjeldsted[1]; Joseph Roark[1]; Frank Kuhlmann[1]; Gregor Overney[1]; *[1]Agilent Technologies, Santa Clara, CA*

8:30-10:30 am TUESDAY
LIPIDS AND PROFILING
Ginger Milne (Vanderbilt University)
Hemisfair Ballroom 2, level 3

TOG am 08:30 **Enhanced Discrimination of Healthy Human Brain Tissue and Glioma using Positive and Negative Polarity Desorption Electrospray Ionization with Data Fusion**; Clint Miles Alfaro[1]; Alan K Jarmusch[2]; Valentina Pirro[2]; Eyas M Hattab[3]; Aaron A Cohen-Gadol[3]; Graham R Cooks[4]; *[1]Purdue University, Winston-Salem, NC; [2]Purdue University, West Lafayette, IN; [3]Indiana University School of Medicine, Indianapolis, IN; [4]Purdue University, West Lafayatte, IN*

TOG am 08:50 **A Novel Post-column Derivatization Method for Profiling "Diolome" using LC/MS/MS**; Jun Yang[1]; Debin Wan[1]; Chang Wang[1]; Bruce D Hammock[1]; *[1]University of California, Davis, Davis, CA*

TOG am 09:10 **Separation and Characterisation of Human Meibum Lipids by Differential Ion Mobility Mass Spectrometry**; Sarah E Hancock[1]; Peta Snikeris[1]; Stephen J Blanksby[2]; Todd W Mitchell[1]; *[1]University of Wollongong, Wollongong, Australia; [2]Queensland University of Technology, Brisbane, Australia*

TOG am 09:30 **Nitrated Fatty Acids: Biomarkers of Inflammation and Regulators of Redox Homeostasis**; Stacy Gelhaus Wendell[1]; Bruce A Freeman[1]; Franca Golin-Bisello[1]; Gregory Buchan[1]; Sonia Salvatore[1]; Soma Jobbagy[1]; Kara Hughan[1]; Mark Gladwin[1]; *[1]University of Pittsburgh, Pittsburgh, PA*

TOG am 09:50 **Structure Elucidation of Omega-3 Fatty Acid Fish Oil Glycerolipid Dietary Supplements by Supercritical Fluid Chromatography Q-TOF-MS**; Sheher Mohsin[1]; Gene S Hall[2]; Joe Hedrick[3]; *[1]Agilent Technologies, Schaumburg, IL; [2]Department of Chemistry and Chemical Biology, Rutgers, The State University of New Jersey, Piscataway, NJ 08854, Piscataway, NJ; [3]Agilent Technologies, Wilmington, DE*

TOG am 10:10 **Characterizing the Natural History of Acute Radiation Syndrome of the Gastrointestinal Tract: Combining High Mass and Spatial Resolution using MALDI-FTICR-MSI**; Claire Louise Carter[1]; Jace W Jones[1]; Kim Hankey[2]; Ann M Farese[3]; Thomas J MacVittie[2]; Maureen A Kane[1]; *[1]University of Maryland, School of Pharmacy Baltimore, MD; [2]University of Maryland School of Medicine, Baltimore, MD; [3]University of Maryland Baltimore, Baltimore, USA*

8:30-10:30 am TUESDAY
NATIVE MS IN STRUCTURAL BIOLOGY
Alison E. Ashcroft (University of Leeds)
Hemisfair Ballroom 1, level 3

TOH am 08:30 **Accurate Determination of the Carbohydrate Content of Highly Heterogeneous Glycoproteins by Native Mass Spectrometry**; Guanbo Wang[1, 2]; Albert J. R. Heck[1, 2]; *[1]Biomolecular Mass Spectrometry and Proteomics, Utrecht University, Utrecht, The Netherlands; [2]Netherlands Proteomics Center, Utrecht, The Netherlands*

TOH am 08:50 **High-Confidence Models of Multiprotein Complexes from Ion Mobility-Mass Spectrometry Datasets: Frontiers in Model Generation and Assessment**; Joseph D Eschweiler[1]; Aaron T. Frank[1]; Brandon T Ruotolo[1]; *[1]University of Michigan, Ann Arbor, MI*

TOH am 09:10 **Structural Characterization of Missense Mutations using High Resolution Mass Spectrometry: The Parkinson's Related Protein DJ-1 Case Study**; Gili Ben-Nissan[1]; Almog Chotiner[2]; Michal Sharon[2]; *[1]Weizmann Institute of Science, Rehovot, Rehovot; [2]Weizmann Institute of Science, Rehovot, Israel*

TOH am 09:30 **Characterization of a Nitrogenase Complex from Azotobacter Vinelandii in Gas Phase using Native Mass Spectrometry And Ion Mobility.**; Monika Tokmina-Lukaszewska[1]; Natasha Pence[1]; Rhesa Ledbetter[2]; Stephen Keable[1]; Sudipta Shaw[2]; Zhiyong Yang[2]; John Peters[1]; Lance Seefeldt[2]; Brian Bothner[1]; *[1]MSU, Bozeman, MT, Bozeman, MT; [2]Utah State University, Logan, UT*

TOH am 09:50 **Top Down Proteomics and Native Ion Mobility-MS Reveals Phosphorylation-Mediated Effects on NF-kB Conformation and Interactions**; Matthias Vonderach[1]; Manohar Dange[1]; Claire Eyers[1]; *[1]University of Liverpool, Liverpool, United Kingdom*

TOH am 10:10 **Charge Detection Mass Spectrometry Monitors Virus Assembly from Single Subunit to Complete Capsid**; Corinne Lutomski[1]; Kevin Zhao[2]; Adam Zlotnick[2]; Martin F Jarrold[2]; *[1]Indiana University, Bloomington , IN; [2]Indiana University, Bloomington, IN*

10:30 AM – 2:30 PM, TUESDAY
TUESDAY POSTER SESSION
Poster/Exhibit Hall
Lunch concessions are open 11:00 am – 2:00 pm
Odd-number posters present 10:30 am - 1:00 pm
Even-number posters present 12:00 - 2:30 pm

2:30-4:30 pm TUESDAY
ENVIRONMENTAL: NEW INSTRUMENTATION AND APPROACHES
Alla Zelenyuk (Pacific Northwest National Laboratory)
Hall 1, level 1

TOA pm 02:30 **Comparison of Soft Ionisation Techniques for the High Resolution Mass Spectrometry Analysis of Environmental Samples with Complex Matrices**; Ivan Kourtchev[1]; Pak Yiu Paddy Szeto[1]; Duncan Scott[1]; Ian P O'Connor[2]; Olalekan Popoola[1]; Arthur Zielinski[1]; John C Wenger[2]; Markus Kalberer[1]; *[1]University of Cambridge, Cambridge, UK; [2]University College Cork, Cork, Ireland*

TOA pm 02:50 **Laser Diode Thermal Desorption (LDTD)-MS and Machine Learning: a Novel Approach for Ultra Fast Environmental Analysis**; Pier-Luc Plante[1, 2]; Prudencio Tossou[1]; Alexandre Drouin[1]; Francis Brochu[1]; François Laviolette[1]; Mario Marchand[1]; Jacques Corbeil[1, 2]; *[1]Université Laval, Québec, Canada; [2]Centre de recherche du CHU de Québec, Québec, QC*

TOA pm 03:10 **Measurement of Protonated Ions as Sensitive Indicator for Neutral Polycyclic Aromatic Hydrocarbon Chemistry in Combustion by Time-of-Flight Mass Spectrometry**; Yasin Karakaya[1]; Thomas Bierkandt[1]; Tina Kasper[1]; *[1]Thermodynamics, University of Duisburg-Essen, Duisburg, Germany*

TOA pm 03:30 **Ultrafast Quantitative Analysis of Pesticides in Food and Environmental Matrices by SPME-Transmission Mode and Direct Analysis in Real Time**; Emanuela Gionfriddo[1]; German Augusto Gomez-Rios[1]; Justen Poole[1]; Janusz Pawliszyn[1]; *[1]University of Waterloo, Waterloo ON, Canada*

TOA pm 03:50 **Multivariate Statistics Applied to MALDI-TOF MS Data of Pollen Samples**; Franziska Lauer[1, 2]; Stephan Seifert[1, 2]; Janina Kneipp[1, 2]; Steffen M. Weidner[3]; *[1]Federal Institute f. Material Research and Testing, Berlin, Germany; [2]Humboldt University, Berlin, Germany; [3]Fed.Inst.f.Mat.Research, Berlin, Berlin*

TOA pm 04:10 **On the Application of Electrochemistry-Mass Spectrometry to Study the Biotransformation of UV Blockers in the Environment**; Pedro A. Segura[1]; Delphine Canion[1]; Emmanuel Eysseric[1]; *[1]Université de Sherbrooke, Sherbrooke, QC*

2:30-4:30 pm TUESDAY
NEW DEVELOPMENTS IN ION DETECTION
Martin F. Jarrold (Indiana University)
Room 221, level 2

TOB pm 02:30 **The Dynamics of Superconducting Tunnel Junction Cryodetector Energy Response as it Relates to Ion Structure, Surface Area and Density**; Logan D. Plath[1]; David M Sipe[1]; Jonathan Feldman[1]; Chenjie Zeng[1]; Yuxiang Chen[1]; Rongchao Jin[1]; Mark E. Bier[1]; *[1]Carnegie Mellon University, Pittsburgh, PA*

TOB pm 02:50 **A Novel Charge Detection Rectilinear Ion Trap Mass Spectrometer (CD-RIT MS) for Detection of High Mass Proteins**; Avinash Adhikrao Patil[1]; Szu-Wei Chou[1]; Chen-Wei Lee[1]; Wen-Ping Peng[1]; *[1]National Dong Hwa University, Shoufeng Hualien, Taiwan*

TOB pm 03:10 **Neutralization Charge Detection Method Facilitating Fast and Sensitive Hetero-Phase Ion Detection**; Ko-Keng Chang[1, 2]; Yi-Hong Cai[1]; YI-Sheng Wang[1]; *[1]Genomics Research Center, Academia Sinica Taipei, Taiwan; [2]Chemistry Department, National Taiwan University, Taipei, Taiwan*

TOB pm 03:30 **Maximising Ion Detection Efficiency using Cycloidal Transport Of Secondary Electrons In Crossed Electric and Magnetic Fields**; Dick Stresau[1]; Scott Morgan[1]; Toby Shanley[1]; *[1]ETP Ion Detect, Clyde, Australia*

TOB pm 03:50 **A Novel Wide Dynamic Range oa-ToF Detection System Based on Dual 10-bit ADCs and FPGA Processing**; Martin Green[1]; Garry Scott[1]; Stephen Platt[1]; Peter Spreadbury[1]; Darrell Williams[1]; Frank Buckley[1]; Witold Niklewski[1]; Stephen Hinde[1]; Martin Palmer[1]; John Chipperfield[1]; *[1]Waters, Wilmslow, United Kingdom*

TOB pm 04:10 **Multiple Frequency Resonance Methods in Quadrupole Ion Trap Mass Spectrometry: Expanding Capabilities and Improving Performance**; Dalton Snyder[1]; Christopher Pulliam[1]; Joshua S Wiley[2]; Jason Duncan[3]; R Graham Cooks[1]; *[1]Purdue University-Department of Chemistry, West Lafayette, IN; [2]California Institute of Technology, Pasadena, CA; [3]Acuity Brands Lighting Inc, Crawfordsville, IN*

2:30-4:30 pm TUESDAY
QUANTITATIVE ANALYSIS IN DRUG DISCOVERY AND DEVELOPMENT
Jian Wang (Bristol-Myers Squibb)
Stars Ballroom 1, level 3

TOC pm 02:30 **The Potential of Micro Sampling in Regulated Bioanalysis using LC-MSMS**; Martijn Hilhorst[1]; Roderik Prins[2]; Frank Schalken[2]; *[1]PRA Health Sciences, Assen, Drenthe; [2]PRA Health Sciences, Assen, The Netherlands*

TOC pm 02:50 **Universal LBA/LCMS Workflow for Protein Biotherapeutics PK Analysis in Preclinical Assay**; Bruce Aungst[1]; Caroline Becker[1]; Xun Wang[1]; Lei Xiong[2]; Witold Woroniecki[2]; Yihan Li[2]; Suma Ramagiri[2]; Hua-fen Liu[2]; Zamas Lam[1]; *[1]QPS, Newark, DE; [2]SCIEX, Redwood City, CA*

TOC pm 03:10 **A Trapping micro-LC/MS for Ultra-sensitive, Robust and High-Throughput Quantification of Biotherapeutics and Biomarkers in Complex Matrices**; Bo An[1]; Ming Zhang[1]; Yang Qu[1]; Jun Qu; *[1]SUNY at Buffalo, Buffalo, NY*

TOC pm 03:30 **Measuring Drug-Target Engagement in Tissue Biopsies Using Affinity Extraction LC-MS/MS**; Eugene F. Ciccimaro[1]; Yongxin Zhu[2]; Dmitry Ostanin[2]; Suzanne Suchard[2]; Jamus MacGuire[2]; Qing Xiao[2]; Ashok R Dongre[2]; Petia A Shipkova[2]; Timothy Olah[2]; *[1]Bristol-Myers Squibb, Princeton , NJ; [2]Bristol-Myers Squibb, Princeton, NJ*

TOC pm 03:50 **A Label-free, Mass Spectrometry-based High Throughput Candidate Drug Screening Assay: Application to Smith-Lemli-Opitz Syndrome**; Jaqueline A Picache[1]; Stephanie M Cologna[2, 1]; Alfred L Yergey[1]; Pierre Picard[3]; Catherine Chen[1]; Kathryn R Burkert[1]; Christopher A Wassif[1]; Wei Zheng[1]; Forbes D Porter[1]; *[1]National Institutes of Health, Bethesda, MD; [2]University of Illinois at Chicago, Chicago, IL; [3]Phytronix Technologies, Quebec, Canada*

TOC pm 04:10 **Cleavable Antibody Drug Conjugate (ADC) Assay Support Enables ADC ADME and Discovery Programs**; Brian Rago[1]; Fengping Li[1]; Cong Wei[1]; Xiaogang Han[1]; Tracey Clark[1]; Lindsay King[1]; Nathan Tumey[1]; Frank Barletta[1]; Mauricio Leal[1]; Steven Hansel[1]; *[1]Pfizer, Groton, CT*

2:30-4:30 pm TUESDAY
ION MOBILITY, FAIMS & DMS: NEW DEVELOPMENTS & APPLICATIONS
George Stafford (Agilent Technologies)
Stars Ballroom 2-3, level 3

TOD pm 02:30 **Moving beyond Collision Cross Sections: Using Cryogenic Infrared Spectroscopy to Determine the Structures of the Mobility-Selected Neuropeptide CabTRP1a (APSGFLGMR-NH2)**; Michael Kamrath[1]; Matthew Glover[2]; Marta A. S. Perez[1]; Ursula Rothlisberger[1]; David E Clemmer[2]; Thomas R Rizzo[1]; *[1]Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland; [2]Indiana University Dept. Chemistry, Bloomington, IN*

TOD pm 02:50 **Integration of High-field Asymmetric Waveform Ion Mobility and Ambient Ionization Mass Spectrometry for Biological Tissue Imaging**; Clara Feider[1]; Livia S. Eberlin[2]; *[1]University of Texas at Austin, Austin, Texas; [2]University of Texas at Austin, Austin, TX*

TOD pm 03:10 **A Theoretical and Empirical Approach to Separating Isomer Classes in Uniform Field Ion Mobility**; James Dodds[1]; Jody C May[1]; John A McLean[1]; *[1]Vanderbilt University, Nashville, TN*

TOD pm 03:30 **Separation and Identification of Isomeric Lipids using a Combination of Differential Mobility Spectrometry and Ozone-induced Dissociation**; Stephen J Blanksby[1]; Berwyck L. J. Poad[2]; Alan T. Maccarone[3]; Todd W Mitchell[3]; *[1]Queensland University of Technology, Brisbane, QLD; [2]Queensland University of Technology, Brisbane, Australia; [3]University of Wollongong, Wollongong, Australia*

TOD pm 03:50 **Gas Phase Epitope Mapping - A Mass Spectrometric Method for Accurate, Facile, and Rapid Identification of Specific Antibody-Peptide Reactivities**; Yelena Yefremova[1]; Frimpong-Manso Kwabena Opuni[1]; Hans-Juergen Thiesen[2]; Michael O Glocker[1]; *[1]Proteome Center Rostock, Rostock, Germany; [2]Institute of Immunology, Rostock, Germany*

TOD pm 04:10 **Ultrahigh IMS Resolution using Novel Traveling Wave Approaches and Long Serpentine Path Length SLIM Modules**; Richard D. Smith[1]; Liulin Deng[1]; Ahmed Hamid[1]; Ian K Webb[1]; Sandilya V.B. Garimella[1]; Erin S Baker[1]; Yehia M Ibrahim[1]; *[1]PNNL, Richland, WA*

2:30-4:30 pm TUESDAY
QUALITATIVE AND QUANTITATIVE ANALYSIS OF POST-TRANSLATIONAL MODIFICATIONS
Amber L. Mosley (Indiana University School of Medicine)
Stars Ballroom 4, level 3

TOE pm 02:30 **Disease-specific Post-translational Modifications in Cystic Fibrosis**; Sandra Pankow[1]; Casimir Bamberger[1]; John Yates[1]; *[1]The Scripps Research Institute, La Jolla, CA*

TOE pm 02:50 **PTM'omics: What Do We Learn from Surveying Many Modifications Simultaneously in Non-Enriched Proteomes? A Study of Lysine Acylations**; Hong Nguyen[1]; Michael McInerney[2]; Robert Gunsalus[1]; Joseph A Loo[1]; Rachel Ogorzalek Loo[1]; *[1]UCLA, Los Angeles, CA; [2]University of Oklahoma, Norman, OK*

TOE pm 03:10 **Redox Proteomics to Study Cysteine Status in Alzheimer's Disease**; Renã A. S. Robinson[1]; Liqing Gu[1]; *[1]University of Pittsburgh, Pittsburgh, PA*

TOE pm 03:30 **The Phosphoproteome of the NCI-60 Cell Line Panel Reveals Markers of Drug Sensitivity**; Benjamin Ruprecht[1]; Chen Meng[2]; Martin Frejno[3]; Alexander Hogrebe[1]; Dominic Helm[2]; Bernhard Kuster[2]; *[1]TU Muenchen, Freising, Germany; [2]TU Muenchen, Freising, Germany; [3]Oxford University, Oxford, United Kingdom*

TOE pm 03:50 **Identification of Histone ADP-Ribosylation Sites using High Resolution Mass Spectrometry**; Kelly Karch[1]; Benjamin A. Garcia[1]; Ben E. Black[1]; *[1]University of Pennsylvania, Philadelphia, PA*

TOE pm 04:10 **Comparative Ubiquitylome Analysis of Major Proteasome Inhibitors**; Tanya Rocio Porras-Yakushi[1]; Michael Sweredoski[1]; Sonja Hess[1]; *[1]Caltech, Pasadena, CA*

2:30-4:30 pm TUESDAY
IMAGING: COMPUTATIONAL METHODS AND ANALYSIS
Theodore Alexandrov (EMBL / UCSD / SCiLS)
Hemisfair Ballroom 3, level 3

TOF pm 02:30 **Absorption Mode Processing of MALDI-FT-ICR Imaging Data Improves Mapping of Gram-Negative Bacterial Virulence Factors on-Tissue**; Alison Scott[1]; David P A Kilgour[2]; Robert K Ernst[1]; David R Goodlett[1]; *[1]University of Maryland, Baltimore, MD; [2]Nottingham Trent University, Nottingham, UK*

TOF pm 02:50 **Deep Autoencoders for Dimensionality Reduction of 3D Mass Spectrometry Imaging Data-Sets for Tumour Classification and Novel Subtypes Identification**; Paolo Inglese[1]; James McKenzie[1]; Anna Mróz[1]; James Kinross[1]; Elaine Holmes[1]; Zoltan Takats[1]; Jeremy K Nicholson[1]; Robert C Glen[1, 2]; Kirill Veselkov[1]; *[1]Imperial College London, South Kensington Campus London, United Kingdom; [2]University of Cambridge, Cambridge, UK*

TOF pm 03:10 **Dimensionality Reduction of MALDI Imaging Datasets using Non-Linear Redundant Wavelet Transform-based Representations**; Luis Mancera[1]; Lyna Sellami[2]; Jamie Cunliffe[2]; Luis González[1]; Omar Belgacem[2]; *[1]Clover Bioanalytical Software, Granada, SPAIN; [2]Shimadzu, Kratos Manchester, United Kingdom*

TOF pm 03:30 **Current Status and Applications of the Open Data Format imzML**; Nicolas Desbenoit[1]; Amol Fatangare[1]; Andreas Roempp[2]; *[1]Bioanalytical Sciences and Food Analysis, University of Bayreuth, Bayreuth, Germany; [2]Bioanalytical Sciences and Food Analysis, University of Bayreuth, Bayreuth*

TOF pm 03:50 **Generation of Realistic Synthetic Mass Spectrometry Imaging (MSI) Data for the Validation of Multivariate Analysis Methods**; Alexander Dexter[1, 2]; Alan Race[2]; Iain B Styles[1]; Helen J Cooper[1]; Josephine Bunch[2, 3]; *[1]University of Birmingham, Birmingham, UK; [2]National Physical Laboratory, Teddington, United Kingdom; [3]University of Nottingham, Nottingham, UK*

TOF pm 04:10 **Characterisation of Molecular Signatures in the Xenograft Microenvironment using Novel Tools to Combine Histopathology and Mass Spectrometry Imaging Data**; Jo Cappell[1]; Gert B Eijkel[1]; Martha Ingola[1]; Richard J A Goodwin[2]; Peter Webborn[2]; Ron M A Heeren[1]; *[1]M4I Institute - Maastricht University, Maastricht, The Netherlands; [2]AstraZeneca, Cambridge, UK*

2:30-4:30 pm TUESDAY
METABOLOMICS: NEW TECHNOLOGIES AND APPLICATIONS
Nichole Reisdorph
(University of Colorado Anschutz Medical Campus)
Hemisfair Ballroom 2, level 3

TOG pm 02:30 **Symbiotic Interaction between Legumes and Rhizobia Explored by Laser Ablation Electrospray Ionization Mass Spectrometry with Ion Mobility Separation**; Sylwia Stopka[1]; Beverly Agtuca[2]; Christopher Anderton[3]; David W Koppenaal[3]; Ljiljana Pasa-Tolic[3]; Gary Stacey[2]; Akos Vertes[1]; *[1]George Washington University, Washington, District of Columbia; [2]University of Missouri, Columbia, MO; [3]Pacific Northwest National Laboratory, Richland, WA*

TOG pm 02:50 **Temporal Analysis of Living Human Bronchial Epithelial Cell Signaling and Drug Transportation using nano-DESI MS**; Ingela Lanekoff[1]; Erik Lundin[1]; Jan-Christer Ulvinge[2]; Mark Nicholas[2]; *[1]Uppsala University, Uppsala, Sweden; [2]AstraZeneca R&D, Gothenburg, Sweden*

TOG pm 03:10 **Solid Phase Microextraction as a Sample Preparation Tool for Untargeted Analysis of Brain Tissue**; Nathaly Reyes-Garces[1]; Ezel Boyaci[1]; German Augusto Gomez-Rios[1]; Barbara Bojko[1]; Janusz Pawliszyn[1]; *[1]University of Waterloo, Waterloo ON, Canada*

TOG pm 03:30 **An Integrated Platform for Quantitative Full-Scan Polar LC/MS Metabolomics Reveals Structured Environmental Stress Response in the Yeast Saccharomyces Cerevisiae**; Amy Anne Caudy[1]; Julia A Hanchard[1]; Kaitlin U Laverty[1]; Anton Lunyov[1]; Olga Zaslaver[1]; Soumaya Zlitni[1]; Adam Rosebrock[1]; *[1]University of Toronto, Toronto ON, Canada*

TOG pm 03:50 **High-throughput Targeted Metabolomics of CoA Metabolites for Modulation of Antibiotic Influx and Efflux in Gram Negative Bacteria**; Christopher M. Rath[1]; Bret Benton[1]; Javier De Vicente[2]; Cindy Li[1]; Bob Moreau[1]; Xiaoyu Shen[1]; Lisha Wang[1]; Brian Feng[1]; *[1]Novartis Institutes for Biomedical Research, Emeryville, CA - California; [2]Denali Therapeutics, South San Francisco, CA - California*

TOG pm 04:10 **Higher-throughput Annotation of Plant Metabolomes using Spectral Matching, Computational Identification Tools and Empirical UHPLC-MS-SPE-NMR**; Lloyd W. Sumner[1, 2]; Feng Qiu[1, 2]; Dennis Fine[2]; Daniel Wherritt[3]; Zhentian Lei[1, 2]; Aiko Barsch[4]; *[1]University of Missouri, Columbia, MO; [2]The Samuel Roberts Noble Foundation, Ardmore, OK; [3]University of Texas, San Antonio, TX; [4]Bruker Daltonic GmbH, Bremen, Germany*

2:30-4:30 pm TUESDAY
PROTEIN-LIGAND INTERACTIONS
John S. Klassen (University of Alberta)
Hemisfair Ballroom 1, level 3

TOH pm 02:30 **An Integrated HDX-MS-Based Platform Characterizes the Interaction between apoE3 and a ligand: High-Resolution Kinetics, PLIMSTEX, and SUPREX**; Hanliu Wang[1]; Don L Rempel[1]; Tridib Mondal[2]; Carl Frieden[2]; Michael L Gross[1]; *[1]Center for Biomedical and Bioorganic Mass Spectrometry, Washington University in St. Louis, St. Louis, MO; [2]Department of Biochemistry and Molecular Biophysics, Washington University in St. Louis, St. Louis, MO*

TOH pm 02:50 **Ligand-Induced Disorder-to-Order Transitions Characterized by Structural Proteomics**; Nicholas I Brodie[1]; Geoff M Gudavicius[2]; Christopher J Nelson[2]; Evgeniy V Petrotchenko[1]; Christoph H. Borchers[3, 2]; *[1]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [2]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada; [3]University of Victoria - Genome BC Proteomics Centre, Victoria, BC*

TOH pm 03:10 **Targeted MS-based Approach for Protein Ligand Binding Analysis in Complex Biological Mixtures using a Phenacylbromide Modification Strategy**; Lorrain Jin[1]; Carol H Ball[2]; Michael C Fitzgerald[1]; *[1]Duke University, Durham, NC; [2]Agilent Technologies, Santa Clara, CA*

TOH pm 03:30 **Unveiling the Heterogeneity of an Uncharacterized Manganese Oxidizing Multicopper Oxidase Using High Resolution Native Mass Spectrometry and Surface Induced Dissociation**; Mowei Zhou[1]; Jing Yan[2]; Christine Romano[3]; Yang Song[2]; Jeremy J Wolff[4]; Joshua Gilbert[2]; Randall E Pedder[5]; Bradley Tebo[3]; Vicki H Wysocki[2]; Ljiljana Pasa-Tolic[1]; *[1]Pacific Northwest National Laboratory - PNNL, Richland, WA; [2]Ohio State University, Columbus, OH; [3]Oregon Health & Science University, Portland, OR; [4]Bruker Daltonic, Billerica, MA; [5]Ardara Technologies L.P., Ardara, PA*

TOH pm 03:50 **Probing KIX:Peptide Allosteric Interactions by Ion Mobility-Mass Spectrometry**; Jessica Rabuck-Gibbons[1]; Jean M Lodge[1]; Anna K Mapp[1]; Brandon T Ruotolo[1]; *[1]University of Michigan, Ann Arbor, MI*

TOH pm 04:10 **Tetrameric BanLec Neutralises HIV through Bidentate Binding to Specific Viral Glycan Structures**; Jonathan Hopper[1]; Oliver Grant[2]; Stephen Ambrose[1]; Stefanie Krumm[3]; Timothy Allison[1]; Mark Tully[4]; Laura Pritchard[1]; Gabriel Ozorowski[5]; Andrew Ward[5]; Max Crispin[1]; Katie Doores[3]; Robert J Woods[2]; Justin Benesch[1]; Carol V Robinson[1]; Weston Struwe[1]; *[1]University of Oxford, Oxford, UK; [2]University of Georgia, Athens, GA; [3]King's College London, London, UK; [4]Diamond Light Source, Didcot, UK; [5]The Scripps Research Inst., La Jolla, CA*

4:45 – 5:30 PM, TUESDAY AFTERNOON
AWARD LECTURE
Jenny Brodbelt (University of Texas, Austin) presiding
Hall 1, level 1

Presentation of the 2016 Research Awards

Biemann Medal

Kristina "Kicki" Håkansson
University of Michigan

There are light refreshments in common areas.

01 Glycoproteomics: Site Specific Glycan Analysis
Ron Orlando presiding
Room 220, level 2

Modulating the activities and functions of proteins is a significant role of post-translational modifications (PTMs), with glycosylation being an excellent example. Glycan moieties of glycoproteins affect protein folding, stability, and localization and thus play a role in numerous biological functions, including cell signaling, adhesion, and communication. The analysis of released glycans has been a primary focus of glyco-analytical development over the past several years. However, these glycan centric analyses do not provide information on the glycans present at each glycosylation sites. Often the site occupancy is critical for biological activity. This behavior is clearly shown with therapeutic antibodies, where glycans located in the variable domain influence the serum clearance rate while glycans in constant domain affect the activity. The comprehensive characterization of protein glycosylation microheterogeneity entails the identification and quantitation of isomeric glycan occupancy of potentially all glycosylation sites on a protein, which is a significantly more difficult challenge than glycomic profiling. This workshop critical evaluation of state-of-the-art methods currently employed for enrichment and analysis at a glycoproteomic level.

02 Ion Mobility: How to Interpret the Data
(Ion Mobility MS Interest Group)
Erin Baker, Valerie Gabelica, and Stephen Valentine presiding
Room 221, level 2

Over the past decade, MS instrumentation featuring various forms of mobility-based separations have proliferated. One hurdle to intra- and inter-instrumental platform data comparison is, however, the lack of common interpretation schemes and practical tools. In part this results from gaps in knowledge related to correct data interpretation. This workshop will discuss the tools currently available for ion mobility data analyses, and participants will be invited to show tricky cases where data analysis can lead to ambiguous or erroneous interpretations. The workshop discussion will help make progress toward finding common ground and sound fundamental principles for the correct interpretation of ion mobility data.

03 H/D Exchange, Covalent Labeling & Cross-Linking
(H/D Exchange, Covalent Labeling & Cross-Linking Interest Group)
Joshua Sharp and David Weis presiding
Room 225A, level 2

This workshop will provide a forum for discussing hydrogen exchange, covalent labeling, and cross-linking approaches for protein analysis (structure, function, folding, dynamics). There will be a several brief presentations introducing late-breaking advances in MS-based methods, experiments, data analysis, and applications to the attendees. The goal of these abbreviated presentations will be to stimulate discussion. There will be ample time for questions and answers including an opportunity for novices/students to contribute anonymous questions on fundamentals.

04 Food Safety & Security: HRMS Applications
(Flavor, Fragrance & Foodstuff Interest Group)
Walter Hammack and David Schroeder presiding
Room 225B, level 2

A continued discussion of applications and developments in the use of High Resolution Mass Spectrometry (HRMS) in food safety and food security. A focus on new developments and applications in pesticide residue analysis, non-target screening, and natural product authenticity.

05 Microcontrollers and Microcomputers: Emerging Technologies
Vincent Sica and Bindesh Shrestha presiding
Room 225C, level 2

Smaller is becoming better - computers as smart phones, nanotechnology, miniature mass spectrometers, even tiny homes! The latest trend in "do-it-yourself" (DIY) electronics is microcontrollers (i.e. Arduino) and microcomputers (i.e. Raspberry Pi). These small, yet powerful devices have put electronic innovation right into our hands. Sensors, displays, and detectors can all be added at a whim without requiring the knowledge of advanced computer circuitry.

This year's discussion will focus on the implementation and use of microcontrollers and microcomputers to support advancements in the field of mass spectrometry. Short presentations showcasing applications of this technology will be followed by the discussion of the following topics:
1) Hardware (microcontrollers and microcomputers)
2) Software/code
3) Where to begin/which microelectronic is right for you?
3) Utility of DIY-microelectronics in mass spectrometry
4) Add-ons of the future (what type of sensors, displays, and detectors could really help push advancement in MS?)
5) Ideas (Active audience participation is encouraged to discuss new ideas/concepts/suggestions)

These discussions aim to not only educate others on how they can improve their research with microcontrollers and microcomputers, but also to spark ideas on what the future may bring to the growing technologies of both microelectronics and mass spectrometry.

06 DNA/RNA Adducts: Assay Development in Detection and Quantification
(Oligonucleotides and Nucleic Acids Interest Group)
Patrick Limbach and Laixin Wang presiding
Room 225D, level 2

Recent mass spectrometry developments now enable high sensitivity detection of DNA or RNA adducts (or modifications). This workshop will focus on the practical issues involved in developing MS-friendly assays to measure these adducts. Selected presentations will illustrate assay development with a focus on sample prep, HPLC conditions, and data analysis. An emphasis in these informal discussions will be on pitfalls and "what did not work" to freely share strengths and weaknesses of assay development. The remaining time will be spent discussing challenges facing MS assays, especially given the advantages now being presented by high-throughput genome-based technologies.

07 Petroleum and Biofuels: Handling the Data (Energy,
Petroleum & Biofuels Interest Group)
Mark Barrow and Lateefah Stanford presiding
Room 301A, level 3

Petroleum-related mass spectra, often acquired using ultrahigh resolution instruments, are well-known for their complexity. With coupling of ion mobility and chromatography becoming more widespread, the level of complexity will be expected to significantly increase. Accompanying this, issues such as data size, data analysis, usage of chemometrics, software development, and comparisons of results from different analytical techniques will become progressively important. The workshop will highlight some of the existing approaches and will focus upon an active discussion of the current and emerging challenges.

08 Metabolism of Biotherapeutics: When, Why and How?
(DMPK Interest Group)
Kevin Bateman and Philip Tiller presiding
Room 301BC, level 3

Biotherapeutics are a steadily growing proportion of the pharmaceutical research and development landscape. Molecules are evolving beyond traditional monoclonal antibodies and antibody-drug conjugates

to include bispecifics, truncated mAbs, nanobodies, cyclic and stapled peptides, Ig fragments, Non-Ig based scaffolds and so on. Understanding the metabolism of these new modalities is an expanding opportunity for mass spectrometry and requires that traditional small molecule scientists adapt to these new large(r) molecules. The goal of this workshop is to stimulate a discussion on the when, why and how for the metabolism of biotherapeutics in the discovery, pre-clinical and clinical arena. A panel will offer opening comments on the current state and provide thoughts on where the field is going. Questions from the audience will be strongly encouraged to stimulate robust discus

09 Modification of Commercial Instruments for Fundamental Research (Fundamentals Interest Group)
Alessandra Ferzoco and Michael Van Stipdonk presiding
Room 302A, level 3

It was once the case that building instruments from scratch was essential for fundamental gas phase ion chemistry research. More recently it seems that the rather astounding performance of commercial instruments and increasing pressure for short project time frames has sparked a trend of modifying commercial instruments and working within academic/industrial collaborations. The purpose of the workshop is to explore the elements of effective instrument design within such collaborations. A variety of instruments that range in purpose and invasiveness of the modification will be presented, and both the researchers and company representatives will be present for discussion. We hope the workshop will provide guidance for researchers designing experiments and deciding where to be on the continuum between building from scratch and near-in-tact commercial instruments.

10 Lipidomics in the Era of Systems Biology: The Big Fat Challenges (Lipids and Lipidomics Interest Group)
Christer Ejsing and Todd Mitchell presiding
Room 302BC, level 3

There is a growing interest in using lipidomics for systems biology studies for understanding the molecular underpinnings of cellular processes and mechanisms of diseases. This workshop will focus on key challenges in integrating lipidomics with other -omics technologies, and how computational strategies can be designed to support meaningful insights into (patho)physiological processes. The discussion will be led by a panel of experts who will invite opinion from participants on current solutions and challenges in using lipidomics for systems biology studies of lipid function in both basic and clinical sciences.

11 Undergraduate Research in Mass Spectrometry (Undergraduate Research in MS Interest Group)
Elaine Marzluff and Megan Gessel presiding
Room 303A, level 3

This panel discussion, aimed at undergraduate students and their mentors, will focus on helping undergraduate students leverage their undergraduate research experiences into successful scientific careers. Panelists will discuss their experiences applying to graduate school and transitioning to a graduate school research environment, as well as working in industrial labs.

12 The Chorus Project: Sustainable Cloud Solution for MS Data
Michael MacCoss, Andrey Bondarenko, Christine Wu, and Nathan Yates presiding
Room 303BC, level 3

The storage, sharing, analysis, and public dissemination of mass spectrometry data is a major challenge for our community. The lack of permanent infrastructure and sustainability is clearly exemplified by the discontinuation of noted resources such as Tranche, NCBI Peptidome, and more recently, the NHGRI's announcement that the funding for many key data resources are in jeopardy. Chorus provides the framework to facilitate a community supported solution to big data generated by the mass spectrometry field. Chorus is a professionally developed application that has a graphical user interface targeted towards the organization and visualization of mass spectrometry data stored on the Amazon cloud. Uploaded data can be exclusive and private, shared with a specified group of collaborators, or made entirely public. Software tools can be added through a software developer's kit. These tools provide analytical workflows and can be made accessible to the community. Our recent focus has been the integration of analytical workflows such as Byonic, Comet, MaxQuant, PeakExplorer, Pecan, and Skyline.

13 Data Independent Acquisition (Data Independent Acquisition Interest Group)
Ludovic Gillet and Jarrett Egertson presiding
Room 304, level 3

Data independent acquisition (DIA) is a versatile mass spectrometry approach that aims to comprehensively record time-resolved fragment ion (MS/MS) signals for all detectable analytes in a sample. To identify and quantify analytes from those complex time- and mass-continuous MS/MS data structures, a diverse panel of analysis strategies is now available. These include leveraging spectral libraries, adapting DIA data for traditional database search engines, redesigning search engines to handle highly chimeric spectra, and detecting peptides/analytes based on extracted chromatograms. Notably, some strategies begin with a collection of features derived from the data (e.g. individual spectra, groups of spectra, or co-eluting peaks) and aim to interpret those features to generate identifications. Other strategies begin with a collection of analytes (e.g. a list of peptides) and query the data for evidence of detection. Each strategy can also differ in the modeling of a decoy scoring distribution and ultimately the assessment of false discovery rate. This workshop aims to disentangle the wealth of DIA analysis strategies available, to discuss the advantages and disadvantages of each approach, and to propose the adoption of a consensus nomenclature to meaningfully refer to them in future DIA studies.

14 Good Manufacturing Practice (GMP); Mass Spectrometric Instrument Qualification
Gyorgy Vas presiding
Room 305, level 3

This workshop will focus on initiating a discussion between the instrument users regulators and the instrument vendors, to discuss issues relating to regulatory compliance. More rigorous regulatory expectations are requiring higher instrument qualification standards and more involved calibration processes. This workshop is intended to discuss best practice approaches and potential qualification issues.

AFTER 8:00 PM
CORPORATE HOSPITALITY SUITES
GRAND HYATT HOTEL

8:30-10:30 am WEDNESDAY
ENERGY, PETROLEUM AND BIOFUELS: STRUCTURE, QUANTIFICATION, AND DATA ANALYSIS
Patrick G. Hatcher (Old Dominion University)
Hall 1, level 1

WOA am 08:30 **In ESI-source H/D Exchange Facilitated a Structural Characterization of Individual Compound in Complex Mixtures by FTICR MS**; Alexey S Kononikhin[1, 2]; Yury Kostyukevich[1, 3]; Alexander Zherebker[4]; Igor A Popov[1, 5]; Oleg N Kharybin[2, 6]; Evgeny Kukaev[1, 5]; Andrey Konstantinov[4]; Irina V Perminova[4]; Eugene Nikolaev[1, 2, 5, 6, 7]; *[1]Moscow Institute of Physics and Technology, Moscow, Russia; [2]Institute for Energy Problems of Chemical Physics, Moscow, Russia; [3]Skolkovo Institute of Science and Technology, Skolkovo, Russia; [4]Lomonosov Moscow State University, Moscow, Russia; [5]Emanuel Institute of Biochemical Physics, Moscow, Russia; [6]Institute of Biomedical Problems RAS, Moscow, Russia; [7]Skolkovo Institute of Technology, Moscow, Russia*

WOA am 08:50 **Characterization of Organic Indicator Compounds of Petroleum Biosouring using Novel Soft Ionization and Fourier Transform Ion Cyclotron Resonance Mass Spectrometry**; Jeremy Nowak[1]; Robin Weber[1]; Pravin Shrestha[1]; Dana Loutey[1]; Amy McKenna[2]; John Coates[1]; Allen Goldstein[1]; *[1]UC Berkeley, Berkeley, California; [2]National High Magnetic Field Laboratory, Tallahassee, FL*

WOA am 09:10 **High-resolution Broad Mass Range Collision-Energy Scanning Tandem Mass Spectrometry for Structural Characterization of Asphaltene Molecular Ions**; Xueming Dong[1]; Xin Lu[2]; Yuyang Zhang[1]; Weijuan Tang[3, 1]; Hilkka Kenttamaa[1]; *[1]Purdue University, West Lafayette, IN; [2]Harbin Institute of Technology, Harbin, China; [3]Dow AgroSciences, Indianapolis, IN*

WOA am 09:30 **Multidimensional Comprehensive Gas Chromatography with High Resolution-TOFMS/photo Ionization-TOFMS: Combining Ultra-high Chromatographic Resolution, Accurate Mass-information and Soft Photoionisation for Petrochemical Samples**; Thomas Groeger[1]; Maximilian Jennerwein[2]; Benedikt Weggler[1]; Mohammad Saraji-Bozorgzad[3]; Juergen Wendt[4]; Ralf Zimmermann[5]; *[1]Helmholtz Zentrum Muenchen, Oberschleissheim, Germany; [2]ASG GmbH, Augsburg, Germany; [3]Photonion GmbH, Schwerin, Germany; [4]LECO Instrumente GmbH, Moenchengladbach, Germany; [5]University of Rostock, Rostock*

WOA am 09:50 **Reaction Pathway Analysis using Isotopically-Labeled Glucose in Real-Time Monitoring of Thin-Film Fast Pyrolysis**; Carolyn Hutchinson[1]; Kristen O'Connor[1]; Young Jin Lee[1]; *[1]Iowa State University, Ames, IA*

WOA am 10:10 **UPLC-MS and MS/MS of Grass Lignins: Evidence for New Structural Units and Cross-Linkers**; Afrand Kamali Sarvestani[1, 2]; Leonardo Da Costa Sousa[3, 4]; Venkatesh Balan[3, 4]; Xiaoxiao Liu[1]; Bruce Dale[3, 4]; A Daniel Jones III[1, 2, 5]; *[1]Department of Chemistry, Michigan State University, East Lansing, MI; [2]DOE Great Lakes Bioenergy Research Center, Michigan State University, East Lansing, MI; [3]Department of Chemical Engineering and Material Science, Michigan State University, East Lansing, MI; [4]DOE Great Lake Bioenergy Research Center, Michigan State University, East Lansing, MI; [5]Department of Biochemistry and Molecular Biology, Michigan State University, East Lansing, MI*

8:30-10:30 am WEDNESDAY
FUNDAMENTALS: ENERGETICS AND MECHANISMS OF UNI AND BIMOLECULAR REACTIONS
John R. Stutzman (The Dow Chemical Company)
Room 221, level 2

WOB am 08:30 **Mechanistic Study of Gas Phase In-source Hofmann Elimination of Doubly Quaternized Cinchona-Alkaloid Based Phase-Transfer Catalysts by (+)-ESI/Tandem Mass Spectrometry**; Huaming Sheng[1]; Rong-Sheng Yang[1]; Katrina M Lexa[1]; Edward Sherer[1]; Li-Kang Zhang[1]; Bangping Xiang[1]; Roy Helmy[1]; *[1]Merck, Darmstadt, Germany*

WOB am 08:50 **Probing the Effect of Charge on the Energetics and Reactivity of Distonic Peroxyl Radical Ions in the Gas Phase**; Peggy Williams[1]; Nadia Skeljo[1]; David Marshall[1]; Benjamin Kirk[2]; Berwyck Poad[1, 3]; Stephen Blanksby[1]; *[1]Queensland University of Technology, Brisbane, Australia; [2]Lawrence Berkeley Nat'l Lab, Berkeley, CA; [3]University of Wollongong, Wollongong, Australia*

WOB am 09:10 **Computational and Experimental Investigation of Gas Phase Ion/Ion Reactions between Nucleophiles and HOAt/HOBt Reagents**; Jiexun Bu[1]; Feifei Zhao[1]; Scott A McLuckey[1]; *[1]Purdue University, West Lafayette, IN*

WOB am 09:30 **Photo-Electron Transfer Dissociation Pathways Reveal Zwitterion Locations in Peptides**; Ryan R. Julian; *University of California, Riverside, Riverside, CA*

WOB am 09:50 **Reactions of Hydroxyl Radicals and Cysteine Disulfide Derivatives (CySSR) – Mechanism and Reactivity Studies**; Sarju Adhikari[1]; M. Anglada Josep[2]; Joseph S. Francisco[3]; Yu Xia[4]; *[1]Purdue University, West Lafayette, IN; [2]Institute of Advanced Chemistry of Catalonia, Barcelona, Spain; [3]University of Nebraska-Lincoln, Lincoln, NE; [4]Purdue University-Department of Chemistry, West Lafayette, IN*

WOB am 10:10 **Radical-Mediated Peptide Tyrosine Nitration In Vacuo: Experimental Evidence and Theoretical Examination**; Ivan K. Chu[1]; Cheuk Kuen Lai[2]; Wai Kit Tang[3]; Chi-Kit Siu[3]; *[1]University of Hong Kong, Hong Kong; [2]The University of Hong Kong, Hong Kong, China; [3]City University, Hong Kong, Hong Kong*

8:30-10:30 am WEDNESDAY
IMAGING: PHARMACEUTICALS AND METABOLITES
Livia D. Eberlin (University of Texas at Austin)
Stars Ballroom 1, level 3

WOC am 08:30 **C60-SIMS Imaging of Pharmaceutical Compounds within Mammalian Cells**; Anna N Bloom[1]; Hua Tian[1]; Nicholas Winograd[1]; *[1]Pennsylvania State University, University Park, PA*

WOC am 08:50 **Spatio-temporal Metabolomics of Tumor Organoids Treated with Chloroquine**; Andrew Palmer[1]; Eric Weaver[2]; Katherine A Kellersberger[3]; Amanda B Hummon[2]; Theodore Alexandrov[1]; *[1]EMBL Heidelberg, Heidelberg, Germany; [2]University of Notre Dame, Notre Dame, Indiana; [3]Bruker Daltonic, Billerica, MA*

WOC am 09:10 **Mass Spectrometry Imaging for Characterizing Parasite Host Interactions in Malaria Research**; Saleh Mahmud Khalil[1]; Andreas Römpp[1]; Jette Pretzel[2]; Katja Becker[2]; Bernhard Spengler[1]; *[1]Institute of Inorganic and Analytical Chemistry, Justus Liebig University, Giessen, Hessen,Germany; [2]Biochemistry and Molecular Biology, Institute of Nutritional Sciences, Justus Liebig University, Giessen, Hessen,Germany*

WOC am 09:30 **Simultaneous Desorption Electrospray Ionization Mass Spectrometry Imaging of Multiple Neurotransmitters and Neuroactive Substances**; Mohammadreza Shariatgorji[1]; Nicole Strittmatter[2]; Anna Nilsson[3]; Theodosia Vallianatou[1]; Per Svenningsson[4]; Richard J A Goodwin[2]; Per E Andren[1]; *[1]Uppsala University, Uppsala, Sweden; [2]AstraZeneca, Cambridge, UK; [3]Uppsala University, Uppsala; [4]Karolinska Institute, Stockholm, Sweden*

WOC am 09:50 **Visualizing Tumors in Three Dimensions: a First Look at Drug Distribution in Brain Tumors using 3D MSI**; David Calligaris[1]; Armen Changelian[1]; Katherine A Kellersberger[2]; Yonatan Morocz[1]; Forest White[3]; Jeffrey N Agar[4]; Jann N Sarkaria[5]; Nathalie Y. R. Agar[1]; *[1]Department of Neurosurgery, and Department of Radiology, BWH, and Department of Cancer Biology, Dana-Farber Cancer Institute, Harvard Medical School, Boston, MA; [2]Bruker Daltonics, Billerica, MA; [3]Massachusetts Institute of Technology, Boston, MA; [4]Department of Chemistry and Pharmaceutical Sciences, Northeastern University, Boston, MA; [5]Department of Radiation Oncology, Mayo Clinic, Rochester, MN*

WOC am 10:10 **Growth, Metabolism, and Antibiotic Susceptibility of Bacterial Colonies Imaged by Laser Ablation Electrospray Ionization Mass Spectrometry**; Hang Li[1]; Pranav Balan[2]; Akos Vertes[1]; *[1]George Washington University, Washington, DC; [2]Thomas Jefferson High School for Science and Technology, Alexandria, VA*

8:30-10:30 am WEDNESDAY
INSTRUMENTATION: MINIATURIZATION OF MS
Christopher C. Mulligan (Illinois State University)
Stars Ballroom 2-3, level 3

WOD am 08:30 **Development of a Point-of-Care (POC) Miniature Mass Spectrometry System**; Xiao Wang[1]; Yue Ren[1]; Li Linfan[1]; Xinwei Liu[2]; Zheng Ouyang[1, 2]; *[1]Purdue University, West Lafayette, IN; [2]Tsinghua University, Beijing, China*

WOD am 08:50 **LITMS: Dual Ion Source Switchable Polarity Linear Ion Trap Mass Spectrometer for Space Flight Applications**; Andrej Grubisic[1, 2]; William B Brinckerhoff[2]; Friso Van Amerom[3]; Ryan Danell[4]; Veronica T Pinnick[5]; Ricardo Arevalo[2]; Xiang Li[5]; Stephanie Getty[2]; Daniel Glavin[2]; Lars Hovmand[6]; Phil Chu[7]; Kris Zacny[7]; Steve Rogacki[8]; Timothy J Cornish[9]; Paul Mahaffy[2]; *[1]University of Maryland, College Park, MD; [2]NASA GSFC, Greenbelt, MD; [3]Mini-Mass Consulting, Inc., Hyattsville, MD; [4]Danell Consulting, Inc. Winterville, NC; [5]University of Maryland, Baltimore County Greenbelt, MD; [6]Linear Labs LLC, Washington DC, DC; [7]Honeybee Robotics, Pasadena, CA; [8]University of Michigan, Ann Arbor, MI; [9]C&E Research, Inc. Columbia, MD*

WOD am 09:10 **Reverse Gas Stack Model for Localization of Chemical Interests Utilizing Mobile Mass Spectrometry**; Phillip Mach[1]; Kenneth C Wright[2]; Guido F Verbeck[1]; *[1]University of North Texas, Denton, TX; [2]Inficon, Syracuse, NY*

WOD am 09:30 **miniSPLAT:A Miniaturized Aircraft-CompatibleSingle Particle Mass Spectrometer for *in-situ* Quantitative Multidimensional Single Particle Characterization**; Alla Zelenyuk[1]; Dan Imre[2]; Jacqueline Wilson[1]; David Bell[1]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]Imre Consulting, Richland, WA*

WOD am 09:50 **Development and Applications of Microchip Capillary Electrophoresis Coupled with High Pressure Mass Spectrometry**; William McKay Gilliland[1]; John Michael Ramsey[1]; *[1]University of North Carolina at Chapel Hill, Chapel Hill, NC*

WOD am 10:10 **Multi-sample Reaction Monitoring: a Miniature Process Analytical Tool using a Miniature Ion Trap**; Christopher J Pulliam[1]; Ryan M Bain[1]; Heather I. Osswald[1]; Dalton T Snyder[1]; Stephen Ayrton[1]; Shannon Raab[1]; R. Graham Cooks[1]; *[1]Purdue University, West Lafayette, IN*

8:30-10:30 am WEDNESDAY
BIOMARKERS: QUALITATIVE ANALYSIS
Jennifer Van Eyk (Cedars-Sinai Medical Center)
Stars Ballroom 4, level 3

WOE am 08:30 **Organismal Level Dynamic Molecular Map of Mouse Proteome**; Bingyun Sun[1]; Shizhen Qin[2]; Cynthia Lorang[2]; Gray Li[2]; Zhiyuan Hu[2]; Ken Liu[3]; Leory Hood[2]; *[1]Simon Fraser University, Burnaby, BC; [2]Institute for Systems Biology, Seattle, WA; [3]Simon Fraser University, Burnaby, BC, Canada*

WOE am 08:50 **Intact Metabolome Analysis of Mice Biological Tissues by Probe Electrospray Ionization-Tandem Mass Spectrometry and Its Preliminary Application to Real-Time Analysis**; Kei Zaitsu[1]; Yumi Hayashi[1]; Tasuku Murata[2]; Hiroki Nakajima[2]; Tetsuya Ishikawa[1]; Maiko Kusano[1]; Hitoshi Tsuchihashi[1]; Akira Ishii[1]; *[1]Nagoya University Graduate School of Medicine, Nagoya, Japan; [2]Global Application Development Center, Shimadzu Corporation, Kyoto, Japan*

WOE am 09:10 **Imaging Mass Spectrometry Identifies New Markers in Prostate Cancer Pathology**; Kristina Schwamborn[1]; Peter Wild[2]; Jeremy L Norris[3]; Richard M Caprioli[3]; *[1]Technical University Munich, Munich; [2]Institute of Surgical Pathology, University Hospital Zurich, Zurich, Switzerland; [3]Department of Biochemistry and the Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN*

WOE am 09:30 **Top-down Proteomics Identified Novel Biomarkers for Hypertrophic Cardiomyopathy**; Wenxuan Cai[1]; Zachery Gregorich[1]; Andrew Messer[2]; Ziqing Lin[1]; Zachary Hite[1]; Steve Marston[2]; Takushi Kohmoto[1]; Ying Ge[1]; *[1]University of Wisconsin-Madison, Madison, WI; [2]Imperial College London, London, UK*

WOE am 09:50 **Profiling of Intact Proteins in the CSF of Alzheimer's Disease Patients using Top Down Proteomics: Revealing Specific Isoform Biomarker Candidates**; Jerôme Vialaret[1]; Schmit Pierre-Olivier[2]; Audrey Gabelle[3]; Christophe Hirtz[1]; Sylvain Lehmann[1]; *[1]LBPC-IRB, CHU de Montpellier Montpellier, France; [2]Bruker Daltonique S.A., Wissembourg, bas-rhin; [3]Centre Mémoire Ressources Recherche, Montpellier, france*

WOE am 10:10 **A Mass Spectrometry Approach to Discover Naturally-occurring Oxidation-specific Malondialdehyde Adducts**; Juliane Weißer[1]; Christoph J Binder[1, 2]; Keiryn L Bennett[1]; *[1]CeMM Research Center for Molecular Medicine, Vienna, Austria; [2]Medical University of Vienna, Vienna, Austria*

8:30-10:30 am WEDNESDAY
INFORMATICS: MULTIOMICS INTEGRATION AND APPLICATION
Catherine Minogue (Hartwick College)
Hemisfair Ballroom 3, level 3

WOF am 08:30 **Integrating and Mining Spatial Omics through Imaging Mass Spectrometry and Anatomical Atlases**; Nico Verbeeck[1]; Jeffrey Spraggins[2]; Junhai Yang[2]; Etienne Waelkens[3, 4]; Richard M. Caprioli[2]; Raf Van de Plas[1]; *[1]Delft University of Technology, Delft, The Netherlands; [2]Vanderbilt University, Nashville, TN; [3]KU Leuven, Leuven, Belgium; [4]Sybioma, Leuven, Belgium*

WOF am 08:50 **Mitochondrial Protein Functions Revealed by Global Mass Spectrometry Profiling**; Jonathan A Stefely[1, 2]; Nicholas W Kwiecien[1]; Alexander S Hebert[1]; Alicia L Richards[1]; Elyse C Freiberger[1]; Matthew J P Rush[1]; Arne Ulbrich[1]; Adam Jochem[1]; Michael T Veling[1]; Paul D Hutchins[1]; Harald Marx[1]; Michael S Westphall[1]; David J Pagliarini[1, 2]; Joshua J Coon[1]; *[1]University of Wisconsin Madison, Madison, Wisconsin; [2]Morgridge Institute for Research, Madison, Wisconsin*

WOF am 09:10 **Incorporating Multiple Information Layers to Understand Viral Antigen Presentation: Stepping Away from the Streetlamp**; Kavya Swaminathan[1]; Peder J Lund[1]; Caleb D Marceau[1]; Niclas E Olsson[1]; Mark M Davis[1]; Jan Carette[1]; Joshua E Elias[1]; *[1]Stanford University, Stanford, CA*

WOF am 09:30 **Quantitative Proteogenomics for Personalised Molecular Profiling**; Christoph Schlaffner[1, 2]; Theodoros Roumeliotis[1]; Hendrik Weisser[1]; James Wright[1]; Jonathan Mudge[3]; Sergio Santos[4]; Graham Ritchie[4, 5, 6, 7]; Julia Steinberg[5]; Andreas Bender[2]; Alvis Brazma[4]; Jennifer Harrow[3]; Christine Le Maitre[8]; Mark Wilkinson[9]; Eleftheria Zeggini[5]; Jyoti Choudhary[1]; *[1]Proteomic Mass Spectrometry, Wellcome Trust Sanger Institute, Cambridge, UK; [2]Department of Chemistry, University of Cambridge, Cambridge, UK; [3]Human and Vertebrate Analysis and Annotation Team, Wellcome Trust Sanger Institute, Cambridge, UK; [4]European Bioinformatics Institute, European Molecular Biology Laboratory, Cambridge, UK; [5]Department of Human Genetics, Wellcome Trust Sanger Institute, Cambridge, UK; [6]Usher Institute of Population Health Sciences & Informatics, University of Edinburgh, Edinburgh, UK; [7]MRC Institute of Genetics & Molecular Medicine, University of Edinburgh, Edinburgh, UK; [8]Biomolecular Sciences Research Centre, Sheffield Hallam University, Sheffield, UK; [9]Department of Human Metabolism, University of Sheffield, Sheffield, UK*

WOF am 09:50 **Integrated Analysis of Human Tissues with a Multi-Omics Approach**; Hannes Hahne[1, 2]; Dongxue Wang[2]; Björn Hallström[3]; Lihua Li[2]; Anna Asplund[4]; Mathias Wilhelm[1, 2]; Harald Marx[5]; Frederik Ponten[4]; Mathias Uhlen[3]; Bernhard Kuster[2]; *[1]OmicScouts GmbH, Freising, Germany; [2]Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; [3]KTH Royal Institute of Technology, Stockholm, Sweden; [4]Uppsala University, Uppsala, Sweden; [5]University Wisconsin-Madison, Madison*

WOF am 10:10 **Integration of Multiple 'Omics' Data Sets via Application of OnPLS Methodology**; Johan Trygg[1]; Izabella Surowiec[1]; *[1]Computational Life Science Cluster (CLiC), Umeå University, Umeå, Sweden*

8:30-10:30 am WEDNESDAY
MS IN THE QC LAB
Da Ren (Amgen)
Hemisfair Ballroom 2, level 3

WOG am 08:30 **Application of Mass Spectrometry in the Quality Control Related Investigations During Protein Therapeutics Manufacturing and Stability Studies**; Li Tao; *Bristol-Myers Squibb Co., New Hope, PA*

WOG am 08:50 **Monitoring Product Attributes in Biopharmaceutical Development and QC with LC/HRMS**; Scott Berger[1]; Liuxi Chen[1]; Min Du[1]; Henry Y Shion[1]; Ying-Qing Yu[1]; *[1]Waters Corporation, Milford, MA*

WOG am 09:10 **Extending the Capabilities of a MS Based Multi Attribute Characterization Method to Promote Quality by Design In Biotherapeutic Drugs**; Michael Blank[1]; Jonathan L Josephs[1]; Richard Rogers[2]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Just Biotherapeutics, Seattle, WA*

WOG am 09:30 **Development of QC-Friendly Mass Spec Assay for Monitoring Antibody Oxidation**; Izabela Sokolowska[1]; Jingjie Mo[1]; Jia Dong[1]; Michael J Lewis[1]; Ping Hu[1]; *[1]Janssen Research & Development, Malvern, PA*

WOG am 09:50 **O-linked Glycosylation for a Fc Fusion Protein: Characterization and Understanding of Biological Relevance**; Le Zhang[1]; Wael Hamouda[1]; Joshua Pearson[1]; Xiaoyan Guan[1]; Hyo Chung[1]; Jette Wypych[1]; *[1]Amgen, Inc., Thousand Oaks, CA*

WOG am 10:10 **Practical Applications of Mass Spectrometry in a Quality Control Laboratory**; Patrick Bulau; *Roche Diagnostics GmbH, Penzberg, Germany*

8:30-10:30 am WEDNESDAY
MACROMOLECULAR COMPLEXES
Mowei Zhou (Pacific Northwest National Laboratory)
Hemisfair Ballroom 1, level 3

WOH am 08:30 **A Native Proteomics Platform for Untargeted Identification and Characterization of Protein Complexes**; Owen Skinner[1]; Rafael Melani[1]; Luca Fornelli[1]; Nicole Haverland[1]; Luis Henrique Ferrer Do Vale[1]; Henrique Seckler[1]; Peter Doubleday[1]; Luis Schachner[1]; Neil L Kelleher[1]; Compton Philip[1]; *[1]Northwestern University, Evanston, IL*

WOH am 08:50 **Towards Routine Native Mass Spectrometric Analysis of Affinity-Isolated Endogenous Protein Complexes**; Paul Dominic B. Olinares[1]; Amelia D Dunn[1]; Julio C Padovan[1]; Javier Fernandez-Martinez[1]; Michael P Rout[1]; Brian T Chait[1]; *[1]The Rockefeller University, New York, NY*

WOH am 09:10 **Integrating Native MS, Crosslinking-MS and HDX-MS with High-Resolution Cryo-Electron Microscopy Reveals the Molecular Architecture of the Sub-Megadalton Circadian Oscillator KaiCBA**; Philip Lössl[1]; Joost Snijder[1, 2, 3]; Jan Michael Schuller[4]; Anika Wiegard[5]; Ilka M Axmann[5]; Jürgen M Plitzko[4]; Friedrich Förster[4]; Albert J R Heck[1, 2]; *[1]Utrecht University, Utrecht, The Netherlands; [2]Netherlands Proteomics Center, Utrecht, The Netherlands; [3]University of Washington, Seattle, WA; [4]Max Planck Institute for Biochemistry, Martinsried, Germany; [5]Heinrich Heine University, Dusseldorf, Germany*

WOH am 09:30 **Mobile-Proton MD Simulations for Modeling the Dissociation of Electrosprayed Protein Complexes**; Vlad Popa[1]; Danielle Trecroce[1]; Robert G McAllister[1]; Lars Konermann[1]; *[1]University of Western Ontario, London, Canada*

WOH am 09:50 **Confirmation of Subunit-Subunit Connectivity and Topology of Computationally Designed Protein Complexes using Surface Induced Dissociation/Ion Mobility**; Aniruddha Sahasrabuddhe[1]; Yang Hsia[2]; Florian Busch[1]; David Baker[2]; Vicki Wysocki[1]; *[1]The Ohio State University, Columbus, OH; [2]University of Washington, Seattle, WA*

WOH am 10:10 **Native Top-Down IRMPD of Macromolecular Protein Complexes — Game Over or Game Changing?**; Huilin Li[1]; Shirin Jamshidi[2]; Hong Hanh Nguyen[1]; Iain Campuzano[3]; Rachel O Loo[1]; Joseph A Loo[1]; *[1]UCLA, Los Angeles, CA; [2]University of Warwick, Coventry, United Kingdom; [3]Amgen, Inc., Thousand Oaks, CA*

10:30 AM – 2:30 PM, WEDNESDAY
WEDNESDAY POSTER SESSION
Poster/Exhibit Hall
Lunch concessions are open 11:00 am – 2:00 pm
Odd-number posters present 10:30 am - 1:00 pm
Even-number posters present 12:00 - 2:30 pm

WEDNESDAY AFTERNOON ORAL SESSIONS

2:30-4:30 pm WEDNESDAY
EXPOSOMICS: TARGETED, UNTARGETED AND BIOINFORMATICS METHODOLOGIES
David M. Balshaw (National Institute of Environmental Health Sciences, National Institutes of Health)
Hall 1, level 1

WOA pm 02:30 **Causal Biomarker Discovery of Childhood Leukemia by Untargeted Metabolomics of Neonatal Dried Blood Spots**; Lauren Petrick[1]; William MB Edmands[1]; Courtney L Schiffman[1]; Alan Hubbard[1]; Stephen M Rappaport[1]; *[1]UC Berkeley, Berkeley, CA*

WOA pm 02:50 **High-coverage Metabolomic Analysis of Microliter Blood Using Isotope Labeling and High-resolution LC-MS**; Wei Han[1]; Liang Li[1]; *[1]Department of Chemistry, University of Alberta, Edmonton, AB, Canada*

WOA pm 03:10 **Improving Detection and Coverage of Microbially-derived Metabolites using GC-MS Based Strategies for Targeted and Untargeted Profiling**; Bhavapriya Vaitheesvaran[1]; Vladimir Yong[1]; Anthony Macherone[2]; Justin R Cross[1]; *[1]Memorial Sloan Kettering Cancer Center, New York, NY; [2]Agilent Technologies, Little Falls, DE*

WOA pm 03:30 **Novel Metabolites Revealed by High Resolution Orbitrap Mass Spectrometry and Their Implications in Quantitation of Urinary Exposure Markers**; Jen-Yi Hsu[1]; Jing-Fang Hsu[1]; Yi-Jen Chen[1]; Pao-Chi Liao[1]; *[1]National Cheng Kung University, Tainan, Taiwan*

WOA pm 03:50 **An Exposomic Study of Health Assessment of Children with Autism and Control Children Using New Mass Spectrometry Methods for Quantitation**; H M Skip Kingston[1]; Scott Faber[2]; Patrick benecewicz[1]; *[1]Duquesne University, Pittsburgh, PA; [2]The children Institute, Pittsburgh, PA*

WOA pm 04:10 **Detection and Identification of Generally Unknown Toxins and Altered Endogenous Components in Poisoned Patients using Data-Independent Acquisition and Untargeted Metabolomics**; Cheng Chen[1]; Ziquan Fan[2]; Xiaojie Tan[2]; Hui Xu[3]; Hongliang Jiang[1]; Mingshe Zhu[4]; *[1]Huazhong University of Science and Technology, Wuhan, China; [2]Waters Technology (Shanghai) Co., Ltd, Shanghai, China; [3]Maternal and Child Health Hospital of Hubei Province, Wuhan, China; [4]Bristol-Myers Squibb, Princeton , NJ*

2:30-4:30 pm WEDNESDAY
FUNDAMENTALS: MOLECULAR MODELING AND QUANTUM MECHANICAL CALCULATIONS IN IM AND MS
Iain D. G. Campuzano (Amgen)
Room 221, level 2

WOB pm 02:30 **Molecular Dynamics/Kinetic Theory Algorithm for Numerical Determination of Electrical Mobility**; Carlos Larriba Andaluz; *Indiana University-Purdue University Indianapolis, Indianapolis, IN*

WOB pm 02:50 **Using Molecular Dynamics Simulations to Uncover the Mechanism of Supercharging in Protein ESI**; Lars Konermann[1]; Haidy Metwally[2]; Robert G McAllister[2]; Vlad Popa[2]; *[1]Univ. of Western Ontario, London, ON; [2]Univ. of Western Ontario, London, Canada*

WOB pm 03:10 **Multi-scale Simulations Coupled with Ion Mobility Experiments Reveal the Fate of nucleic Acids in the Gas Phase**; Massimiliano Porrini[1, 2, 3]; Clémence Rabin[1, 2, 3]; Josephine Abi-Ghanem[1, 2, 3]; Frédéric Rosu[4]; Valerie Gabelica[1, 2, 3]; *[1]INSERM-U1212, ARNA laboratory, Bordeaux, France; [2]CNRS-UMR5320, ARNA laboratory, Bordeaux, France; [3]Université de Bordeaux, IECB, ARNA laboratory, Pessac, France; [4]CNRS UMS 3033, IECB, University of Bordeaux, Pessac, France*

WOB pm 03:30 **How Important is the Charge Distribution in Ion Mobility Experiments, and Can We Predict It?**; Jasper Boschmans[1]; Filip Lemiere[2]; Frank Sobott[3]; *[1]Owlstone, Cambridge, UK; [2]University of Antwerp, Antwerp, Belgium; [3]University of Antwerp, CGB V4, Antwerp, Belgium*

WOB pm 03:50 **Polyproline Fragmentation in Negative Mode. What We Can Learn from Chemical Dynamics Simulations**; Ana Martin-Somer[1]; William L. Hase[2]; Riccardo Spezia[3]; *[1]Université d'Evry-val-d'Essonne, Evry, France; [2]Texas Tech University, Lubbock, TX; [3]CNRS, Evry, Île-de-France*

WOB pm 04:10 **Computations for the Gas-Phase Study of Macromolecular Structure**; Erik G Marklund[1, 2]; Matteo T Degiacomi[1]; Carol V Robinson[1]; Michael Landreh[1]; Mathieu Moog[2]; David Drew[3]; Carl Caleman[2, 4]; Andrew Baldwin[1]; Justin L P Benesch[1]; *[1]University of Oxford, Oxford, UK; [2]Uppsala University, Uppsala, SE; [3]Stockholm University, Stockholm, Sweden; [4]Center for Free-Electron Laser Science, Hamburg, Germany*

2:30-4:30 pm WEDNESDAY
ENVIRONMENTAL: EMERGING CONTAMINANTS
Marc E. Engel (FDACS, Food Safety Laboratories)
Stars Ballroom 1, level 3

WOC pm 02:30 **Hydraulic Fracturing Impacts on Drinking Water: High Resolution-MS Uncovers New Chemical By-Products**; Susan Richardson[1]; Hannah K. Liberatore[2]; Jeanne M. VanBriesen[3]; Plewa J. Michael[4]; Leslie H. Cizmas[5]; *[1]University of South Carolina, Department of Chemistry and Biochemistry, Columbia, SC; [2]University of South Carolina, Columbia, SC; [3]Carnegie Mellon University, Pittsburgh, PA; [4]University of Illinois, Urbana, IL; [5]Texas A&M, College Station, TX*

WOC pm 02:50 **Heterogeneous Atmospheric Reactions: Identification of the Oxidation Products of Polycyclic Aromatic Hydrocarbons**; Richard E. Cochran[1, 2]; Shokouh Haddadi[1, 3]; Rebeka Fisseha

Derseh[1]; Alena Kubatova[1]; *[1]University of North Dakota, Grand Forks, ND; [2]University of California San Diego, San Diego, CA; [3]SUNY Oswego, Oswego, NY*

WOC pm 03:10 **Data-independent Mass Spectrometry for Development of Occupational Nanomaterial Exposure Biomarkers**; Andrew K. Ottens[1]; Pretal P. Muldoon[1]; Aleksandar Vucetic[1]; Demetrius R. Carter[1]; Stefan Tenzer[2]; Matthew J. Campen[3]; Aaron D. Erdely[4]; *[1]Dept Anatomy and Neurobiology, Virginia Commonwealth University, Richmond, VA; [2]Institute of Immunology, University of Mainz, Mainz, Germany; [3]Dept Pharmaceutical Sciences, University of New Mexico, Albuquerque, NM; [4]National Institute for Occupational Safety and Health, Centers for Disease Control and Provention, Morgantown, WV*

WOC pm 03:30 **Tracing Gadolinium-based Contrast Agents from Surface Water to Drinking Water by means of Speciation Analysis**; Uwe Karst[1]; Marvin Birka[2]; Oliver Hachmöller[2]; Michael Sperling[2]; Christoph Alexander Wehe[2]; *[1]University of Münster, Münster; [2]University of Münster, Münster, DE*

WOC pm 03:50 **Determination of Unknown Dichlorophenols from the Oxidation of Triclosan Using Hydrogen Peroxide**; Matthew Reichert[1]; Paul M Chiarelli[1]; *[1]Loyola University, Chicago, IL*

WOC pm 04:10 **Identification of Emerging Contaminants from a Waste Water Influenced Water Body Using High Resolution Accurate Mass LC/MS and Statistical Analysis**; Jerry Zweigenbaum[1]; Tarun Anumol[1]; Linda Kennedy[2]; *[1]Agilent Technologies, Wilmington, DE; [2]Mansfield University of Pennsylvania, Mansfield, PA*

2:30-4:30 pm WEDNESDAY
IMAGING: BIOMEDICAL APPLICATIONS
Bindesh Shrestha (Waters Corporation)
Stars Ballroom 2-3, level 3

WOD pm 02:30 **Guided DESI-MS Imaging Allows Accelerated Mapping of Heterogeneity in Breast Cancer**; Alessandra Tata[1]; Michael Woolman[1]; Milan Ganguly[1]; Manuela Ventura[1]; Nicholas Bernards[1]; Adam Gribble[2]; Alex Vitkin[2]; Howard Ginsberg[3]; Arash Zarrine-Afsar[2]; *[1]University of Health Network, Toronto, Canada; [2]University of Toronto, Toronto ON, Canada; [3]St.Michael Hospital, Toronto, Canada*

WOD pm 02:50 **Three-dimensional MALDI Imaging to Understand Metastasis in Pediatric Medulloblastomas**; Martin R L Paine[1]; Jingbo Liu[2]; Danning Huang[1]; Shane R Ellis[3]; Ron M A Heeren[3]; Facundo M Fernández[1]; *[1]Georgia Institute of Technology, Atlanta, GA; [2]Emory University School of Medicine, Atlanta, GA; [3]Maastricht University, Maastricht, NL*

WOD pm 03:10 **Formalin-Fixed Paraffin Embedded Tissue Analysis by DESI-MSI and its Potential Use in Diagnostics**; Renata Soares[1]; James McKenzie[1]; Anna Mróz[1]; Francesca Rosini[1]; James L Alexander[1]; Robert Goldin[1]; Zoltan Takats[1]; *[1]Imperial College London, London, United Kingdom*

WOD pm 03:30 **Redefining the Pathogen-host Interaction: Imaging Mass Spectrometry Reveals Staphylococcus Aureus Proteins within Host Tissues**; Jessica Moore[1]; Neal D. Hammer[2]; Kristie M Lindsey Rose[1]; Jeffrey M Spraggins[1]; James Cassat[3]; Eric P Skaar[3]; Richard M Caprioli[4, 1, 5]; *[1]Vanderbilt University MSRC, Nashville, TN; [2]Michigan State University, East Lansing, MI; [3]Vanderbilt University School of Medicine, Nashville, TN; [4]Vanderbilt University, Nashville, TN; [5]Vanderbilt Dept. of Biochemistry, Nashville, TN*

WOD pm 03:50 **Integrating Mass Spectrometry Imaging with Multiple Microscopy Modalities for Enhanced Spatiochemical Characterization of Dynamic Microbial Communities**; Sage J. B. Dunham[1]; Kyungwon Ko[1]; Nameera Baig[2]; Nydia Morales-Soto[2]; Troy J Comi[1]; Bin Li[1]; Joseph F Ellis[1]; Joshua Shrout[2]; Paul W Bohn[2]; Jonathan V Sweedler[1]; *[1]University of Illinois at Urbana-Champaign, Urbana-Champaign, IL; [2]University of Notre Dame, Notre Dame, IN*

WOD pm 04:10 **Biomedical Applications of Cardinal: a Mass Spectrometry Imaging Toolbox for Statistical Analysis.**; April Harry[1]; Kyle D Bemis[1]; David Calligaris[2]; Nathalie Agar[2, 3]; Olga Vitek[4]; *[1]Purdue University, West Lafayette, IN; [2]Brigham and Women's Hospital, Boston, MA; [3]Harvard Medical School, Boston, MA; [4]Northeastern University, Boston, MA*

2:30-4:30 pm WEDNESDAY
TOP DOWN PROTEIN ANALYSIS
Si Wu (University of Oklahoma)
Stars Ballroom 4, level 3

WOE pm 02:30 **Comparing Electron Ionization Dissociation and Ultraviolet Photodissociation for Top-Down Native MS of Proteins and Protein Complexes**; Huilin Li[1]; Yuewei Sheng[1]; Jennifer S Brodbelt[2]; Joseph A. Loo[1]; *[1]UCLA, Los Angeles, CA; [2]University of Texas at Austin, Austin, TX*

WOE pm 02:50 **Elucidating Proteoform Families from Proteoform Intact Mass and Lysine Count Measurements**; Michael R. Shortreed[1]; Brian L Frey[1]; Mark Scalf[1]; Rachel Knoener[1]; Anthony J Cesnik[1]; Lloyd M Smith[1]; *[1]University of Wisconsin Madison, Madison, WI*

WOE pm 03:10 **A Novel Approach to Sequencing Native Protein Complexes with an Orbitrap**; Mikhail Belov[1, 2]; Philip D Compton[3]; Neil L Kelleher[3]; Stevan Horning[4]; Alexander A Makarov[4]; *[1]Thermo Fisher Scientific (Bremen), Bremen, Germany; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [3]Northwestern University, Evanston, IL; [4]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

WOE pm 03:30 **Chemical Modification as a Path to Improved Top-down Sequencing and Structural Analysis of Proteins and Protein Complexes**; Daniel A. Polasky[1]; Philip C Andrews[2, 1]; Brandon T. Ruotolo[1]; *[1]Department of Chemistry, University of Michigan, Ann Arbor, MI; [2]Department of Biological Chemistry, University of Michigan, Ann Arbor, MI*

WOE pm 03:50 **A Novel Top Down Proteomics Pipeline Utilizing Capillary Electrophoresis Separation and Ultraviolet Photodissociation**; Jolene K Diedrich[1,2]; Mathieu Lavallée-Adam[1]; Qian Chu[2]; Bryan Fonslow[3, 1]; James J Moresco[1, 2]; Alan Saghatelian[2]; John R Yates III[1, 2]; *[1]The Scripps Research Institute, La Jolla, CA; [2]The Salk Institute, La Jolla, CA; [3]SCIEX, Brea, CA*

WOE pm 04:10 **Novel Strategies for Top-down Phosphoproteomics**; Bifan Chen[1]; Leekyoung Hwang[1]; Tania Guardado[1]; William Ochowicz[1]; Albert Chen[1]; Cyrus Colah[1]; Kunal Dani[1]; Song Jin[2]; Ying Ge[2]; *[1]University of Wisconsin-Madison, Madison, WI; [2]University of Wisconsin Madison, Madison, Wisconsin*

2:30-4:30 pm WEDNESDAY
MS IN THE REGULATORY ENVIRONMENT
Jennifer Liu (Amgen)
Hemisfair Ballroom 3, level 3

WOF pm 02:30 **The Use of Mass Spectrometry in FDA Applications for Biotherapeutics: A Retrospective Review**; Sarah Rogstad[1]; Anneliese Faustino[1]; David Keire[2]; Michael T Boyne[3]; Jun Park[1]; *[1]FDA, Silver Spring, MD; [2]Food and Drug Administration, St. Louis, MO; [3]Biotechlogic, Chicago, IL*

WOF pm 02:50 **The Roles and Opportunities for Mass Spectrometry in Regulatory CMC Submissions**; Heidi Zhang; *Genentech, SSF, CA*

WOF pm 03:10 **Quantitative Analysis of Influenza Vaccine Antigens: How Does the Hi3 Method Compare to Methods Requiring Labeled Isotopes?**; Daryl G S Smith[1]; Lisa Walrond[1]; Marybeth Creskey[1]; Genevieve Gingras[1]; Yves Aubin[1]; Caroline Gravel[1]; Sean Li[1]; Terry D Cyr[1]; *[1]Health Canada, Ottawa, Canada*

WOF pm 03:30 **Development of a LC-SRM Method Based on Anion Attachment Mass Spectrometry for Improved Detection of Neutral Anabolic Androgenic Steroids**; Quentin Dumont[1]; Mariana Barcenas[1]; Isabelle Bailloux[2]; Corinne Buisson[2]; Nathalie Mechin[2]; Richard B. Cole[1]; *[1]Sorbonne Universités, UPMC Univ Paris 06, Paris, France; [2]Agence Française de Lutte Contre le Dopage, Châtenay-Malabry, France*

WOF pm 03:50 **NISTmAb Reference Material 8671: A Tool for Advancing Biopharmaceutical Mass Spectrometry**; John SchieL[1]; Trina Formolo[2]; Abigail Turner[2]; Katharina Yandrofski[2]; *[1]NIST, Gaithersburg, MD; [2]NIST, Rockville, MD*

WOF pm 04:10 **The Challenges in Quantifying Tree Nut Residues of Phosphonic Acid and its Salts with LC-MSMS and CESI-MSMS**; Wiley Hall[1]; Bill Beckham[2]; Spencer Walse[3]; Thomas Michael Jones[2]; Leonel Jimenez[3]; Alan Stone[4]; *[1]DFA of California, Fresno, CA; [2]DFA of California, Fresno, CA - California; [3]USDA-ARS-CPQ, Parlier, CA - California; [4]Johns Hopkins University, Baltimore, MD*

2:30-4:30 pm WEDNESDAY
CARBOHYDRATES
John Froehlich (Boston Children's Hospital & Harvard Medical School)
Hemisfair Ballroom 2, level 3

WOG pm 02:30 **Relative Quantification of Glycans using Multiplexed Carbonyl-Reactive Tandem Mass Tags and MultiNotch MS3**; Bingming Chen[1]; Xuefei Zhong[1]; Sergei Snovida[2]; John Rogers[2]; Lingjun Li[1]; *[1]University of Wisconsin-Madison, Madison, WI; [2]Thermo Fisher Scientific, Rockford, IL*

WOG pm 02:50 **Highly Sensitive N-and O-glycomics From Archived Formalin-Fixed Paraffin-Embedded (FFPE) Tissue Sections Using Porous Graphitized Carbon (PGC)-nanoLC-ESI-MS/MS**; Hannes Hinneburg[1, 2]; Petra Korac[3]; Slavko Gasparov[4, 5]; Peter H Seeberger[1, 2]; Vlatka Zoldos[3]; Daniel Kolarich[1]; *[1]Department of Biomolecular Systems, Max Planck Institute of Colloids and Interfaces, Potsdam, Germany; [2]Department of Biology, Chemistry, Pharmacy, Freie Universität Berlin, Berlin, Germany; [3]Faculty of Science, Department of Biology, Division of Molecular Biology, University of Zagreb, Zagreb, Croatia; [4]Institute for Pathology and Cytology, University Hospital Merkur, Zagreb, Croatia; [5]Department of Pathology, Medical School Zagreb, University of Zagreb, Zagreb, Croatia*

WOG pm 03:10 **Measuring Variability of Glycosylation Analysis Methods for Monoclonal Antibodies: A NIST Interlaboratory Study**; M. Lorna A De Leoz[1]; David Lee Duewer[1]; Stephen E Stein[1]; *[1]National Institute of Standards and Technology, Gaithersburg, MD*

WOG pm 03:30 **Strategies to Improve the Accuracy of De Novo Glycan Topology Analysis**; Cheng Lin[1]; Pengyu Hong[2]; Yi Pu[3]; Catherine E. Costello[1, 3]; *[1]Boston University School of Medicine, Boston, MA; [2]Brandeis University, Waltham, MA; [3]Boston University, Boston, MA*

WOG pm 03:50 **Oligosaccharide Isomer Discrimination by Ion Mobility Spectrometry and Tandem Mass Spectrometry: Roles of Metal Ion Adduction and Gas-Phase Ion Chemistry**; Eric D. Dodds[1]; Yuting Huang[1]; Katherine N. Schumacher[1]; Abby S. Gelb[1]; Lauren Petrosh[1]; *[1]University of Nebraska - Lincoln, Lincoln, NE*

WOG pm 04:10 **Temporal Glycan Analysis of IgG and Paraprotein from Multiple Myeloma Reveals Strong Pathological Associations with Altered Glycosylation**; Stefan Mittermayr[1]; Giao Le[1, 2]; Peter O'Gorman[3]; Jonathan Bones[1]; *[1]The National Institute for Bioprocessing Research & Training, Dublin, Ireland; [2]Department of Haematology, Mater Misericordiae University Hospital, Dublin, Ireland; [3]Department of Haematology, Mater Misericordiae University Hospital, Dublin 7, Ireland, Dublin, Ireland*

2:30-4:30 pm WEDNESDAY
NEW SEPARATIONS APPROACHES COUPLED TO MS
Michael L. Heien (University of Arizona)
Hemisfair Ballroom 1, level 3

WOH pm 02:30 **Fundamentals of Ion Dynamics in Structures for Lossless Ion Manipulations (SLIM)**; Sandilya V B Garimella[1]; Yehia M Ibrahim[1]; Ian K Webb[1]; Ahmed M Hamid[1]; Liulin Deng[1]; Erin S Baker[1]; Xueyun Zheng[1]; Richard D Smith[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

WOH pm 02:50 **Capillary Zone Electrophoresis-Tandem Mass Spectrometry with the Third-Generation Electro-Kinetically Pumped Sheath Flow Interface for Large-Scale Proteomics**; Liangliang Sun[1]; Katelyn R Ludwig[2]; Guijie Zhu[2]; Amanda B. Hummon[2]; Norman J Dovichi[2]; *[1]University of Notre Dame, South Bend, IN; [2]University of Notre Dame, Notre Dame, IN*

WOH pm 03:10 **A Novel Sensitive Sheathless CE-MS Device for Peptide and Protein Analysis**; Tam T. T. N. Nguyen[1]; Nickolaj J. Petersen[1]; Kasper D. Rand[1]; *[1]University of Copenhagen, Copenhagen, Denmark*

WOH pm 03:30 **Developing an Ultra UltraHigh Pressure Liquid Chromatography (UUHPLC) system for LC-MS Based Metabolomics**; Beixi Wang[1]; Jeremy Felton[1]; Paige Malec[1]; Stephanie Moore[2]; James Treadway[2]; Dan Lunn[2]; James Jorgenson[2]; Robert Kennedy[1]; *[1]University of Michigan, Ann Arbor, MI; [2]University of North Carolina at Chapel Hill, Chapel Hill, NC*

WOH pm 03:50 **Characterization of the Sarcomeric Proteome by Multidimensional Liquid Chromatography Fractionation and Top-down High-Resolution Mass Spectrometry**; Trisha Tucholski[1]; Wenxuan Cai[2, 3]; Andrew J Alpert[2, 4]; Bifan Chen[5]; Yutong Jin[5]; Ying Ge[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]Molecular and*

Cellular Pharmacology Training Program, University of Wisconsin - Madison, Madison, WI; [4]PolyLC Inc., Columbia, MD; [5]Department of Chemistry, University of Wisconsin-Madison, Madison, WI

WOH pm 04:10 **Liquid Chromatography High Resolution Tandem Mass Spectrometry of Laser Ablation Sampled Tissue**; Fabrizio Donnarumma[1]; Michael E Pettit[2]; Touradj Solouki[2]; Kermit K Murray[1]; *[1]Louisiana State University, Baton Rouge, LA; [2]Baylor University, Waco, TX*

4:45 – 5:30 PM, WEDNESDAY AFTERNOON
ASMS MEETING
Jenny Brodbelt, ASMS President, presiding
Enjoy a beverage and hear the latest ASMS news.
Stars Ballroom 1, level 3

5:45 - 7:00 PM WEDNESDAY WORKSHOPS

There are light refreshments in common areas.

01 Bioanalysis: Current Status of Strategy and Practice of a Tiered Approach (Regulated Bioanalysis Interest Group)
Fabio Garofolo and Jian Wang presiding
Room 220, level 2

The workshop will review the recent development and current status of strategy and practice of tiered approach in bioanalysis. The recommendations from various bioanalytical societies and organizations such as Global Bioanalytical Consortium (GBC) and European Bioanalytical Forum (EBF) and from Crystal City Conferences will be discussed. A pre-workshop survey will be conducted among ASMS members on the tiered approach in bioanalysis. The workshop will provide an opportunity for attendees to exchange opinions, experiences, and practices with the ultimate goal of having a better understanding of how to apply a tiered approach as part of the bioanalytical strategy.

02 Large-Scale Analysis of MS Big Data: From Data to Knowledge and Back
Nuno Bandeira presiding
Room 221, level 2

Advances in mass spectrometry instrumentation, integration with genomics/transcriptomics data and the public availability of hundreds of Terabytes of mass spectrometry data have created significant challenges for the analysis of proteomics and metabolomics data. This workshop will focus on publicly available algorithms and resources illustrating how distributed computing and mass spectrometry data repositories can be used to assist with the analysis of newly acquired data. Furthermore, we will also discuss ways to productively engage the mass spectrometry community in aggregating their contributions into a community-wide knowledge base reusable for both experimental design and continuous reanalysis towards complete annotation of public mass spectrometry data.

03 FTMS: Day-to-Day Concerns for High Resolution Mass Analysis (FTMS Interest Group)
David Kilgour and Don Smith presiding
Room 225A, level 2

This year's workshop will be a round-table discussion focusing on day-to-day considerations for optimum FTMS operation and data collection. A poll will be taken prior to the workshop to determine the most popular discussion points. In addition, there will be an open discussion on any other points of interest. What are the major opportunities to make the next generation of FTMS instruments better than the current ones? What are the most common day-to-day struggles that FTMS users encounter? Worried about mass calibration or mass errors? Bad or variable sensitivity? Instrument maintenance? Data processing and confidence in results? There are many more besides these. But, which are the most important to us as a community and can we use this information to shape our own future? Our aim will be to identify those key priority areas which might inform future programs for improving the capabilities offered by FTMS instrumentation.

04 Novel Mass Spectrometry Instrumentation: Moving into the Hands of Practitioners (Forensics & Homeland Security Interest Group)
Guido Verbeck presiding
Room 225B, level 2

Researchers are pushing the limits on trace forensic analysis and novel sampling techniques. They are also making mass spectrometry (MS) portable and durable for direct field applications; not just gas inlet, but liquid and solid sampling also. Recent developments in portable mass spectrometry present several interesting questions for workshop attendees to discuss. Questions for discussion include; Is it possible to create a reliable analytical tool that is "red light - green light"? Can portable MS become a tool that first responders can use without the need for extensive training? Will portable MS be considered a screening or a confirmatory method of analysis (e.g. by SWGDRUG) or will the error rates be measured (e.g. to meet Daubert requirements). How readily will portable MS be admissible in court? Could on-site measurements influence the way the criminal justice system operates and thereby save money?

Here we will explore these issues, and have a series of presentations that include portable MS developers and representatives from the practitioner/law enforcement perspectives. We will explore the courtroom, and what burden-of-proof is laid at the feet of the tool developer. A discussion will be moderated about moving portable MS forward as the presumptive test, as well as the prosecutorial final test.

05 Photoionization: New Developments (Photoionization MS Interest Group)
Jack Syage and Ralf Zimmermann presiding
Room 225C, level 2

This will be the fourth year for a Photoionization (PI) workshop. Previous ones were very successful with strong turnout and varied and vigorous discussions. There are two flavors of photoionization currently being practiced today: (1) atmospheric pressure photoionization (APPI) is a commercial technology and practiced mostly on LC/MS instrumentation though there are vibrant growing new applications in direct ambient analysis, GC/MS and direct vapor (or vaporized) sample analysis. (2) Vacuum photoionization more commonly referred to as single-photon ionization (SPI) involves VUV light sources including lasers that ionize sample inside the vacuum chamber and is more of a research tool for studying spectroscopic properties of molecules, but also finding powerful applications in air monitoring particularly pollutant monitoring such as vehicle or flue exhaust.

In this fourth year we will focus on new applications. APPI and PI are finding unique uses in high volume applications, most specifically explosives detection in security environments for its unique benefits that are not provided by competing ionization methods.

06 The NIH Review and Funding Process
Charles Edmonds, Salvatore Sechi, and Douglas Sheeley presiding
Room 225D, level 2

A major source of financial support for many ASMS members and participants is the National Institutes of Health. During this workshop the general funding and review process of grant proposals will be presented. Issues like identifying the best NIH contact, writing an effective application, and responding to the reviewers' criticisms will be discussed. Speakers will explore these issues from the perspectives of the applicant, reviewer, and administrator, with some emphasis on new investigators and training opportunities. A "mock" NIH study section presentation will provide additional insight into the review process and opportunity for discussion with NIH staff. Substantial time will be allotted for discussion and questions.

07 Entrepreneurship: Creating a Job in Mass Spectrometry
Alexandre Shvartsburg presiding
Room 301A, level 3

Much of the employment growth and technological advance in North America has lately come from start-ups. While spectacular successes of young companies in the IT and new media arena are widely covered and acclaimed, the entrepreneurial opportunities in other hi-tech areas are much less known. In mass spectrometry, start-ups have hugely contributed to the maturation of novel instrumentation and methods that define the frontline of our field and provided exciting and gainful employment for many analytical chemists including recent graduates.

This new ASMS workshop will focus on the key strategies and processes to create successful businesses leveraging the rapid development of MS technology and associated expansion of bioanalytical and environmental applications, and raise the awareness in broad ASMS community about entrepreneurship as a viable career path. The program would feature brief presentations by a diverse group of academic and industrial scientists who have launched prosperous ventures involving MS within the last two decades. Speakers will focus on key aspects of establishing a start-up in the field, such as funding, marketing, securing and protecting the intellectual property, licensing, staff hiring, manufacturing options, and relationships with major vendors. The workshop will conclude in a panel discussion with questions from the audience.

08 Protein Quantitation (Absolute) by LC-MS: Biomarker and Biotherapeutic
Dawn Dufield and Nalini Sadagopan presiding
Room 301BC, level 3

With increase in focus on biologic/biotherapeutic drugs by the pharmaceutical industry and also an increase in need for biomarkers (efficacy and safety) the deployment of LC-MS based techniques is on the rise primarily due to the speed in method development, and specificity of the technique. Scientists are finding new ways of doing sample prep to increase sensitivity/specificity, address reproducibility issues associated with enzymatic digestion and mass spectrometric methods to address specificity. The forum will provide a platform to share common themes, issues on these fronts and perhaps to surface newer needs in software, mass spec design, and automation.

09 Isomeric Glycans: Characterization & Quantitation
Yehia Mechref presiding
Room 302A, level 3

Glycosylation of proteins is one of the most common protein posttranslational modifications (PTM). A correlation between changes in the glycan moieties of glycoproteins and many mammalian diseases, including hereditary disorders, immune deficiencies, cardiovascular disease, and cancer has been suggested. The diverse biological roles of glycans and their implications in diseases have created a demand for reliable glycomic strategies, permitting sensitive monitoring of isomeric glycans in biological systems. These strategies are needed to better understand the roles and attributes of glycan in biological systems. In this workshop, the use of different MS/MS and LC-MS/MS strategies for the compressive characterization of glycan isomers will be critically described and discussed. These strategies employ several separation and mass spectrometric techniques, including liquid chromatography (different modes), matrix-assisted laser desorption ionization-mass spectrometry (MALDI-MS), and electrospray ionization-mass spectrometry (ESI-MS).

10 Protein Therapeutics: Characterization using MS (Biotherapeutics Interest Group)
Damian Houde and Ashley Ruth presiding
Room 302BC, level 3

This workshop will be a forum to discuss the current technical challenges and solutions for the characterization of protein therapeutics by mass spectrometry. Mass spectrometry is now used for protein characterization from discovery through product development. The workshop will begin with a discussion of hot topics identified at this year's Sanibel Conference on Protein Therapeutic Characterization. This may include a variety of topics, ranging from protein modifications, higher-order structure characterization, protein batch comparability and biosimilarity, or protein production lot release to initiate a discussion. Recent advancements in instrumentation and software for data analysis and reporting may also be discussed.

11 The Exposome: MS-based Metabolomic Workflows to Characterize the Exposome (Exposomics Interest Group)
Anthony Macherone presiding
Room 303A, level 3

The exposome compliments the genome and integrates genetic information with non-genetic exposures and the associated biological response pathways in the search for causative factors of chronic human disease. Within the exposome paradigm, the internal environment is composed of all bio-active chemicals circulating in the body regardless of their origin e.g. genetically derived or exposure derived. Examples include dietary chemicals, drugs, persistent organic pollutants, bio-transformation products (metabolites), foreign DNA, reactive electrophiles adducted to human serum albumin and other sources of exposure (e.g., noise pollution, place of residence, lifestyle choices, etc.) that stimulate biochemical responses.

Exposomics is the application of omics-based tools such as NMR, mass spectrometry and bioinformatics to characterize and measure the exposome and applies the tools of systems biology in a truly multi-platform, multi-omics approach. Mass spectrometric workflows in metabolomics and the bioinformatics software required to interpret the resulting data, provide an excellent model for the characterization of the exposome. This workshop will define how metabolomic procedures and workflows can be used to characterize human exposure profiles and will provide examples used to characterize the exposome.

12 Biomarker Translation: Quality Control & Quality Assurance (Clinical Chemistry Interest Group)
Timothy Garrett and Brian Rappold presiding
Room 303BC, level 3

Quality control and quality assurance (QC/QA) procedures for translating discovery assays to clinical use are poorly, if at all, defined. This workshop will offer brief topic introductions regarding the expectations of QC/QA in clinical diagnostics for multimarker assays, including algorithm based assessments. A similar dearth of QC/QA procedures is found in technologies which are highly naive to the industry, such as high resolution MS and tissue/imaging. As such, speakers from the field will introduce concepts related to QC/QA in such methodologies to enable discussion amongst the group. Hopefully, such discussion will introduce new approaches to ensuring quality in translational workflows for all attendees.

13 Imaging MS: Present and Future of Multimodal Studies (Imaging MS Interest Group)
Vilmos Kertesz and Raf Van de Plas presiding
Room 304, level 3

It is increasingly common for Imaging MS to make up part of multimodal imaging studies in which a set of different image types are brought to bear on the same or related samples. Analytical approaches that characterize a sample using different principles, measuring for example functional, chemical, as well as biological information within a single experiment, can often provide insights not available from a single modality alone. While multimodal imaging that includes a mass spectral modality has greatly advanced, different research groups have gone about such studies with widely-varying workflows and approaches. In this workshop, we want to discuss how challenges can be tackled at the sample preparation, at the instrumental, as well as at the computational level. Furthermore, we want to see whether an overall direction for the field and a set of best practices can be distilled, complemented by a list of major challenges that yet need to be tackled. The central topic of the workshop will therefore be "Imaging by Mass Spectrometry as part of Multimodal Imaging Studies".

The workshop proposes to examine three different aspects of multimodal imaging MS experiments:

1. Experimental design - How to design a good multimodal imaging MS experiment? (e.g. What modalities to acquire? How to make the collected image types synergistic and not just a simple combination?)

2. Measurement - How to acquire the different image types? (e.g. How do you properly prepare the sample for multimodal measurements? Is it better to integrate mass spectrometry and other image type measurements into a single device? Or are we better off keeping separate instruments?

3. Data analysis - How can multimodal data be brought together, and what are the advantages and disadvantages of the different approaches? (e.g. What are the different strategies to handle/visualize multimodal data sets?

14 Galaxy for Proteomics Data Analysis: An Interactive Demonstration
Tim Griffin presiding
Room 305, level 3

The Galaxy framework has emerged as a useful and powerful tool for MS-based proteomics data analysis and also multi-omic application (for example see recent publications such as Nat Biotechnol. 2015, 33:137-9; Mol Cell Proteomics. 2015, 14:3087-93; Mol Cell Proteomics. 2012, 11:M111.015974). The Galaxy operating environment offers an informatics workbench where disparate software can be deployed and integrated into complex workflows. Galaxy also offers the ability to share complete workflows and data with other users, promoting reproducibility and dissemination of even complex data analysis schemes.

This workshop will provide attendees the opportunity to take Galaxy for a "test drive" in analyzing MS-based protoemics data. Attendees will have the opportunity to access a Galaxy instance and walk through the basic steps of setting up an analysis of representative MS data from a proteomics experiment. The hands-on tutorial will include steps such as pre-processing of mass spectral data, sequence database searching, and filtering and visualizing outputs.

Attendees will also be introduced to basic operations and concepts of the Galaxy operating environment, such as the creation of histories and workflows, and functionalities for sharing tools and workflows with others. An overview of the current state of software available in Galaxy for proteomics and multi-omics applications will also be provided.

The workshop will be led by both developers and users well-versed in the use of Galaxy for multi-omics data analysis.

Attendees are encouraged to bring a laptop computer to participate.

AFTER 8:00 PM
CORPORATE HOSPITALITY SUITES
GRAND HYATT HOTEL

THURSDAY MORNING ORAL SESSIONS

8:30-10:30 am THURSDAY
NEW CONCEPTS FOR FORENSIC MS
Candice Bridge (National Center for Forensic Science)
Hall 1, level 1

ThOA am 08:30 **Paper Spray Mass Spectrometry for Screening of Illicit Drugs from Blood Samples**; Rachel Potter[1]; Nicholas Manicke[1]; *[1]IUPUI, Indianapolis, IN*

ThOA am 08:50 **Comparative Study for the Authentication of Marijuana Varieties by Conventional and High-Resolution Mass Spectrometric Profiling**; Xinyi Wang[1]; Peter B Harrington[1]; Steven F Baugh[2]; *[1]Ohio University, Athens, OH; [2]Cannaprint, LLC, Broomfield, CO*

ThOA am 09:10 **Coupling Ambient Ionization and In-source Collision Induced Dissociation for the Detection and Chemical Imaging of Organic and Inorganic Forensic Compounds**; Thomas P. Forbes[1]; Edward Sisco[1]; *[1]National Institute of Standards and Technology, Gaithersburg, MD*

ThOA am 09:30 **Classification of Blow Fly Eggs for Determination of Post-Mortem Interval**; Justine E. Giffen[1]; Jennifer Y. Rosati[2]; Rabi A. Musah[3]; *[1]University at Albany - SUNY, Albany, NY; [2]John Jay College of Criminal Justice, NY, NY; [3]University at Albany-SUNY, Albany, NY*

ThOA am 09:50 **Proteomics and Ancient History - Identification of Proteins from Skin and Muscle Tissue from Ancient Egyptian Mummies**; Prathiba Ravishankar[1]; Dylan Xavier[2]; Fallen Kai Yik Teoh[1]; David C.L. Handler[1]; Mads Moeller Foged[1]; Mehdi Mirzaei[1]; Dong Hoon Shin[3]; Raffaella Bianucci[4]; Jana Jones[1]; Paul A Haynes[5]; *[1]Macquarie University, Sydney, Australia; [2]Australian Proteome Analysis Facility, Sydney, Australia; [3]Seoul National University, Seoul, South Korea; [4]University of Turin, Torino, Italy; [5]Macquarie University, North Ryde, Sydney, NSW*

ThOA am 10:10 **Illuminating Lifestyles of People by Metabolomics of Personal Objects**; Amina Bouslimani[1]; Alexey V Melnik[1]; Zhenjiang Zech Xu[1]; Amnon Amir[1]; Ricardo Silva[1, 2]; Mingxun Wang[1]; Nuno Bandeira[1]; Theodore Alexandrov[3, 4]; Rob Knight[1]; Pieter Dorrestein[1]; *[1]UCSD, San Diego, CA; [2]Universidade de São Paulo - USP, Sao Paulo, Brazil; [3]EMBL Heidelberg, Heidelberg, Germany; [4]SCiLS GmbH, Bremen, Germany*

8:30-10:30 am THURSDAY
FUNDAMENTALS: PHOTODISSOCIATION
John P. O'Brien (The Dow Chemical Company)
Room 221, level 2

ThOB am 08:30 **Diazirine Enabled Gas Phase Coupling of Pepitdes Utilizing Newly Developed Photo-Lysine Amino Acid**; Robert Pepin[1]; Christopher L Shaffer[1]; Frantisek Turecek[1]; *[1]University of Washington, Seattle, WA*

ThOB am 08:50 **Conformational Specific Infrared and Ultraviolet Spectroscopy of Cold YA(D-Pro)AA·H+Ions: A Stereochemical "Twist" on the Proline Effect**; Christopher Harrilal[1]; Andrew DeBlase[1]; Nicole Burke[1]; Timothy Zwier[1]; Scott A McLuckey[1]; *[1]Purdue University-Department of Chemistry, West Lafayette, IN*

ThOB am 09:10 **Examination of the Asymmetric and Symmetric Dissociation Pathways of Tetrameric Protein Complexes using 193 nm UVPD**; Lindsay Morrison[1]; Jennifer S Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX*

ThOB am 09:30 **UVPD on the Benchtop Q Exactive Orbitrap Applied to Peptides, Proteins, and Protein Complexes**; Kyle Fort[1]; Sam Tamara[1]; Andrey Dyachenko[1]; Alexander A Makarov[2, 1]; Richard Scheltema[1]; Albert J R Heck[1]; *[1]Utrecht University, Utrecht, The Netherlands; [2]Thermo Fisher Scientific, Bremen, DE*

ThOB am 09:50 **From the Top to the Bottom and Back: hvPD on Conformer Selected Ions Probing the Role of Co-factors of Structure**; Alina Theisen[1]; Bin Yan[1]; Rodger Kutta[1]; Alex Jones[1]; Bruno Bellina[1]; Perdita E Barran[2]; *[1]The University of Manchester, Manchester, United Kingdom; [2]The University of Manchester, Manchester, Greater Manchester*

ThOB am 10:10 **Performance Considerations for Ultraviolet Photo-Dissociation using the Nd:YAG 5th Harmonic (213nm)**; Chad Weisbrod[1]; Eugene Zhuk[1]; Jean-Jacques Dunyach[1]; Jae Schwartz[1]; *[1]ThermoFisher Scientific, San Jose, CA*

8:30-10:30 am THURSDAY
NEW DEVELOPMENTS IN IONIZATION AND SAMPLING FOR DMPK
Naidong Weng (Johnson & Johnson)
Stars Ballroom 1, level 3

ThOC am 08:30 **Coated Blade Spray-Mass Spectrometry (CBS-MS) as a Versatile Approach for Quantitative Analysis in Small and Large Sample Volumes of Biofluids**; German Augusto Gomez-Rios[1]; Nathaly Reyes-Garces[1]; Ezel Boyacı[1]; Justen Poole[1]; Janusz Pawliszyn[1]; *[1]University of Waterloo, Waterloo ON, Canada*

ThOC am 08:50 **Functionalized Sampling Probe for Direct Mass Spectrometry Analysis of Lipids in Blood Samples**; Wenpeng Zhang[1]; Zheng Ouyang[1]; *[1]Biomedical Engineering, Purdue University West Lafayette, IN*

ThOC am 09:10 **Microfluidic Electrochemical Cell for Studying the Adduct Formation of Reactive Metabolites by ESI-MS**; Tina Wigger[1, 2]; Floris T.G. van den Brink[3]; Mathieu Odijk[3]; Wouter Olthuis[3]; Albert van den Berg[3]; Uwe Karst[1, 2]; *[1]University of Münster, Institute of Inorganic and Analytical Chemistry, Münster, Germany; [2]NRW Graduate School of Chemistry, Münster, Germany; [3]University of Twente, MESA+ Institute for Nanotechnology and MIRA Institute for Biomedical Technology and Technical Medicine, BIOS – Lab on a Chip group, Enschede, The Netherlands*

ThOC am 09:30 **Effective Coupling of CE with nanoESI MS via a True Sheathless Metal-coated Emitter Interface for Robust and Sensitive Sample Quantification**; Keqi Tang[1]; Xuejiang Guo[2]; Thomas Fillmore[1]; Yuqian Gao[1]; *[1]Pacific NW National Laboratory, Richland, WA; [2]Nanjing University, Nanjing, China*

ThOC am 09:50 **Novel Acoustic Interface for Ultra-High-Throughput Mass Spectrometry Utilizing Multiple Ambient Ionization Techniques**; Ian Sinclair[1]; Jonathan Wingfield[2]; Martin Bachman[1]; Steven D Pringle[3]; Luke Ghislain[4]; Eric Hall[4]; Rick Stearns[4]; Sammy Datwani[4]; Lars Majlof[4]; Michael Morris[3]; *[1]AstraZeneca, Macclesfield, UK; [2]AstraZeneca, Cambridge, UK; [3]Waters, Wilmslow, United Kingdom; [4]Labcyte Inc, Sunnyvale, CA - California*

ThOC am 10:10 **Sub Second Quantitative Mass Spectrometry Analysis No Longer a Fiction with Acoustic Sample Deposition and Fiber Coupled LDTD-MS/MS**; Pierre Picard[1]; Jean Lacoursière[1]; Alex Birsan[1]; Serge Auger[1]; *[1]Phytronix Technologies, Inc. Quebec, Canada*

8:30-10:30 am THURSDAY
TRANSLATIONAL SUCCESS WITH MS
Ashok R. Dongre (Bristol-Myers Squibb R&D)
Stars Ballroom 2-3, level 3

ThOD am 08:30 **Pathology-driven Comprehensive Proteomic Profiling of the Prostate Cancer Tumor Microenvironment**; Lisa Staunton[1]; Claire Tonry[1]; Espina Virginia[2]; Lance Liotta[2]; John O'Leary[3]; Rosina Lis[4]; Michaela Bowden[4]; Finn Stephen[3]; Massimo Loda[4]; Stephen Pennington[5]; *[1]University College Dublin, Dublin, Ireland; [2]George Mason University, Manassas, Virginia; [3]Trinity College Dublin, Dublin, Ireland; [4]Dana Farber Cancer Institute, Boston, MA; [5]UCD Conway Institute, Dublin, Europe*

ThOD am 08:50 **Development of a Novel Rapid Evaporative Ionisation Mass Spectrometry (REIMS) Platform 'iEndoscope' for *in vivo* Chemical Histology during Colonoscopy.**; James Alexander[1]; Louise Gildea[1]; Julia Balog[2]; Abigail Speller[1]; Anna Mroz[1]; Alasdair Scott[1]; James McKenzie[1]; Kirill Veselkov[1]; Robert Goldin[1]; James Kinross[1]; Jonathan Hoare[1]; Julian P Teare[1]; Zoltan Takats[1]; *[1]Imperial College, London, United Kingdom; [2]Waters, Manchester, United Kingdom*

ThOD am 09:10 **Rapid Identification of Carbapenem-resistant Klebsiella Pneumoniae using High-Resolution Tandem Mass Spectrometry**; Raja Sekhar Nirujogi[1]; Sreelakshmi K Sreenivasamurthy[1]; Santosh Renuse[1]; Pranita J Tamma[1]; Patricia J Simner[1]; Akhilesh Pandey[1]; *[1]Johns Hopkins University School of Medicine, Baltimore, MD*

ThOD am 09:30 **Ultrafast Detection of Amino-Acid Substitutions in DNA Gyrase A Related to Fluoroquinolone Resistant Typhoidal Salmonella Isolates using PRM**; Robert-Jan Hassing[1]; Wil Goessens[1]; Lona Zeneyedpour[1]; Sadaf Sultan[1]; Jeroen van Kampen[1]; Annelies Verbon[1]; Perry van Genderen[2]; John Hayes[1]; Theo Luider[1]; Lennard Dekker[1]; *[1]Erasmus Medical Center, Rotterdam, The Netherlands; [2]Havenziekenhuis, Rotterdam, The Netherlands*

ThOD am 09:50 **A Physical and Genetic Interaction between the Cardiac Transcription Factor Tbx5 and Chromatin Remodeling Complexes is Essential for Cardiac Septation**; Todd M. Greco[1]; Lauren Waldron[2]; Jeffrey D. Steimle[3]; Nicholas C. Gomez[4]; Kerry M. Dorr[2]; Junghun Kweon[3]; Brenda Temple[5]; Xinan Holly Yang[3]; Caralynn M. Wilczewski[2]; Ian J. Davis[6]; Ivan P. Moskowitz[3]; Frank L. Conlon[2]; Ileana M. Cristea[1]; *[1]Princeton University, Princeton,*

NJ; [2]University of North Carolina Heart Institute, UNC-Chapel Hill, Chapel Hill, NC; [3]Departments of Pediatrics, Pathology, and Human Genetics, The University of Chicago, Chicago, IL; [4]Integrative Program for Biological and Genome Science, UNC-Chapel Hill, Chapel Hill, NC; [5]R.L. Juliano Structural Bioinformatics Core, Department of Biochemistry and Biophysics, UNC-Chapel Hill, Chapel Hill, NC; [6]Department of Genetics, UNC-Chapel Hill, Chapel Hill, NC

ThOD am 10:10 **Discovery and Mechanistic Investigation of Novel Metabolic Features of Lung Cancer and Their Potentials of Clinical Applications**; Hyuntae Yoo[1]; Tzu-Fang Lou[1]; Deepa Sethuraman[1]; Pallevi Srivastva[1]; John Minna[2]; *[1]University of Texas at Dallas, Richardson, TX; [2]University of Texas Southwestern Medical Center, Dallas, Texas*

8:30-10:30 am THURSDAY
GLYCOPEPTIDES AND GLYCOPROTEINS
Franklin E. Leach III (Photochem Technologies)
Stars Ballroom 4, level 3

ThOE am 08:30 **Dopant Enriched Nitrogen Gas Enhances Sensitivity and Repeatability,Opening New Possibilities for Glyco(proteo)mics Analysis with Sheathless CE-ESI-MS**; Guinevere S.M. Kammeijer[1]; Isabelle Kohler[1]; Bas C. Jansen[1]; Gerda C.M. Vreeker[1]; Paul J. Hensbergen[1]; Oleg A. Mayboroda[1]; David Falck[1]; Manfred Wuhrer[1]; *[1]Leiden University Medical Center (LUMC), Leiden, Zuid-Holland*

ThOE am 08:50 **Comprehensive Glycoproteomics of Glioblastoma Biospecimens**; Chun Shao[1]; Joshua Klein[1]; Joanna Phillips[2]; Joseph Zaia[1]; *[1]Department of Biochemistry, School of Medicine, Boston University, Boston, MA; [2]Department of Neurological Surgery and Pathology, University of California, San Francisco, San Francisco, CA*

ThOE am 09:10 **Quantification of Human Cell Surface N-Glycoprotein Dynamics**; Haopeng Xiao[1]; Ronghu Wu[1]; *[1]Georgia Institute of Technology, Atlanta, USA*

ThOE am 09:30 **Isomeric Separation of Glycopeptides using Aporous Graphitic Carbon (PGC) LC-MS Platform**; Rui Zhu[1]; Jingfu Zhao[1]; Aiying Yu[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, Texas*

ThOE am 09:50 **Site-directed Analysis of Unnatural Glycopeptide Variants and the Associated Glycan Structures by Semi-Targeted LC/MS and MRM Analysis**; Dayoung Park[1]; Gege Xu[1]; Carlito B Lebrilla[1]; *[1]UC Davis, Davis, CA - California*

ThOE am 10:10 **Quantitative Profiling of O-GlcNAc Glycosites in Human T Cells during Activation**; Christina Woo[1]; Peder J Lund[2]; Sharon J Pitteri[2]; Mark M Davis[2, 3]; Carolyn R Bertozzi[1, 3]; *[1]Stanford University, Stanford, CA; [2]Stanford University School of Medicine, Palo Alto CA, USA; [3]Howard Hughes Medical Institute, Chevy Chase, MD*

8:30-10:30 am THURSDAY
INFORMATICS: TARGETED PROTEOMICS AND DIA
Hannes L. Röst (IMSB, ETH Zurich & Stanford University)
Hemisfair Ballroom 3, level 3

ThOF am 08:30 **EncyclopeDIA: a New Algorithmic Approach to Detect, Site-Localize, And Quantify Phosphopeptide Positional Isomers from DIA Experiments**; Brian C. Searle[1, 2]; Robert T Lawrence[1]; Michael J MacCoss[1]; Judit Villén[1]; *[1]University of Washington, Seattle, WA; [2]Proteome Software, Portland, OR*

ThOF am 08:50 **A Novel Framework for Spectral Assay Library Construction and Targeted Quantitative Data Extraction in Metabolomics with Data Independent Acquisition**; Gengbo Chen[1]; Scott Walmsley[2]; Lei Zhou[1, 3, 4]; Liyan Chen[3]; Ching-Yu Cheng[3, 4]; Roger W Beuerman[3, 4]; Tien-Yin Wong[1,3,4]; Gemmy C.M. Cheung[3, 4]; Hyungwon Choi[1]; *[1]National University of Singapore, Singapore, Singapore; [2]University of Colorado Denver-Anschutz In Aurora, CO, Denver, USA; [3]Singapore Eye Research Institute, Singapore, Singapore; [4]Duke-NUS Graduate Medical School, Singapore, Singapore*

ThOF am 09:10 **Targeted Analysis of MS1 Data for Quantitative Studies**; Roland M. Bruderer[1]; Yue Xuan[2]; Ian Lienert[1]; Oliver M. Bernhardt[1]; Tejas Gandhi[1]; Lukas Reiter[1]; *[1]Biognosys AG, Schlieren, Switzerland; [2]Thermo Fisher Scientific, Bremen, DE*

ThOF am 09:30 **Benchmarking SWATH by LFQBench: a Multi-Centered Study Evaluates and Improves Data-Independent-Acquisition-Based Label Free Quantification Tools**; Pedro Navarro[1]; Joerg Kuharev[1]; Ludovic C Gillet[2]; Oliver M Bernhardt[3]; Brendan MacLean[4]; Stephen Tate[5]; Chih-Chiang Tsou[6]; Lukas Reiter[3]; George Rosenberger[2]; Yasset Perez-Riverol[7]; Alexey I Nesvizhskii[6]; Ruedi Aebersold[2]; Stefan Tenzer[1]; *[1]University Medical Center of the Johannes Gutenbe, Mainz, Rheinland-Pfalz; [2]ETH Zurich, Zürich, Switzerland; [3]Biognosys AG, Schlieren, Switzerland; [4]University of Washington, Seattle, WA; [5]SCIEX, Concord, ON; [6]University of Michigan, Ann Arbor, MI; [7]EMBL-EBI, Hinxton, UK*

ThOF am 09:50 **Advanced Workflows and Concepts for the Analysis of High Throughput Targeted Proteomics Experiments of Large Heterogeneous Datasets**; Isabell Bludau[1]; George Rosenberger[1]; Ben Collins[1]; Uwe Schmidt[2]; Patrick Pedrioli[1]; Ruedi Aebersold[1]; *[1]Institute of Molecular Systems Biology, ETH Zurich, Zurich, CH; [2]ID Scientific IT Services, ETH Zurich, Zurich, CH*

ThOF am 10:10 **Detection and Quantification of Proteins in SWATH-MS Analysis without using Spectral Libraries**; Stephen A Tate[1]; Jamie Sherman[1]; Pradeep Narayanaswamy[1]; *[1]SCIEX, Concord ON, Canada*

8:30-10:30 am THURSDAY
APPLICATION OF STABLE ISOTOPE LABELING IN MS
Jim Edwards (Saint Louis University)
Hemisfair Ballroom 2, level 3

ThOG am 08:30 **Quantity: An Isobaric Tag for Quantitative Glycomics**; Shuwei Li[1]; Shuang Yang[2]; Meiyao Wang[3]; Lijun Chen[2]; Bojiao Yin[2]; Karen W Phinney[4]; Illarion V Turko[4]; Michael Betenbaugh[2]; Guoqiang Song[5]; Chung Cheng-yu[6]; Hui Zhang[2]; *[1]Center for Advanced Research, Rockville, MD; [2]Johns Hopkins School of Medicine, Baltimore, MD; [3]Center for Disease Control and Prevention, Atlanta, GA; [4]National Institute of Standards and Technology, Gaithersburg, MD; [5]Changzhou University, Changzhou, China; [6]Johns Hopkins University School of Medicine, Baltimore, MD*

ThOG am 08:50 **A Novel Quantitative Mass Spectrometry Platform for Determining Protein O-GlcNAcylation Dynamics through Specific O-GlcNAc Isotopic Labeling**; Xiaoshi Wang[1]; Zuo-Fei Yuan[1]; Jing Fan[2]; Kelly R Karch[1]; Lauren E Ball[3]; John M Denu[2]; Benjamin A Garcia[4]; *[1]University of Pennsylvania School Of Medicine, Philadelphia, PA; [2]University of Wisconsin Madison, Madison,*

Wisconsin; [3]Medical Univ of S Carolina, Charleston, SC; [4]University of Pennsylvania School of Medicine, Philadelphia, PA

ThOG am 09:10 **High-Performance Chemical Isotope Labeling LC-MS for Tracking Disease Progression: Metabolomic Study of Alzheimer's Disease in a Mouse Model**; Liang Li[1]; Wei Han[1]; Kevin Hooton[1]; Dorothea Mung[1]; Keding Cheng[2]; Sharon Simon[2]; David Knox[2]; *[1]University of Alberta, Edmonton, Canada; [2]Public Health Agency of Canada, Winnipeg, Canada*

ThOG am 09:30 **An Integrated Workflow for Qualitative Flux Analysis by Accurate Mass LC/MS**; Stephen Madden[1]; Alex Apffel[1]; Xinning Jiang[2]; Ed Darland[2]; Yinghang Yang[2]; Xiangdong Li[2]; Crystal Cody[2]; Norton Kitagawa[2]; *[1]Agilent Technologies, Inc., Santa Clara, CA; [2]Agilent Technologies, Santa Clara, CA*

ThOG am 09:50 **HAHA: A Novel Strategy for Quantification of Newly Synthesized Proteins**; Yuanhui Ma[1]; Daniel B Mcclatchy[1]; John Yates[1]; *[1]The Scripps Research Institute, La Jolla, CA*

ThOG am 10:10 **Just Add Water and Resolving Power: Metabolic Labeling and MS Techniques for Lipid and Intact Protein Quantitation in Any Organism**; Nicholas D Schmitt[1]; Jeniffer Quijada[1]; Christopher Thompson[2]; Michael L Easterling[2]; Jeffrey Agar[1]; *[1]Northeastern University, Boston, MA; [2]Bruker Daltonic, Billerica, MA*

8:30-10:30 am THURSDAY
ION MOBILITY: STRUCTURE
Kevin Pagel (Freie Universitaet Berlin)
Hemisfair Ballroom 1, level 3

ThOH am 08:30 **An Ion Mobility, Molecular Dynamics, Top-Down and H/DX Study of Monoclonal Antibody Structural Collapse in the Gas-phase**; Iain D G Campuzano[1]; Morgan Lawrenz[1]; Carlos Larriba-Andaluz[2]; Huilin Li[3]; Ulrik H Mistarz[4]; Kasper Rand[4]; Joseph Loo[3]; *[1]Amgen, Inc., Thousand Oaks, CA; [2]Indiana University-Purdue University, Indianapolis, IN; [3]UCLA, Los Angeles, CA; [4]University of Copenhagen, Copenhagen, Denmark*

ThOH am 08:50 **Analysis of Protein Structural Changes with High Resolution Structures for Lossless Ion Manipulations (SLIM) Ion Mobility-Mass Spectrometry**; Ian K. Webb[1]; Liulin Deng[2]; Ahmed M Hamid[1]; Gordon A Anderson[1, 3]; Randolph V Norheim[1]; Spencer A Prost[1]; Sandilya V. B. Garimella[1]; Erin S Baker[1]; Yehia M Ibrahim[1]; Richard D Smith[1]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]Pacific Northwest National Laboratory, Richland, wa; [3]GAA Custom Engineering, Benton City, WA*

ThOH am 09:10 **Ubiquitin Ion Structures from the Solid State using Nothing More than a Small Molecule and Vacuum of an IMS-MS Instrument**; Ellen D. Inutan[1,2]; Tarick J. El-Baba[3]; Casey D. Foley[2]; David E. Clemmer[3]; Sarah Trimpin[2,4];[1] Mindanao State University-Iligan Institute of the Technology, Iligan City, Philippines; [2] Department of Chemistry, Wayne State University, Detroit, MI; [3] Department of Chemistry, Indiana University, Bloomington, IN; [4]Cardiovascular Research Institute, Wayne State University School of Medicine, Detroit, MI

ThOH am 09:30 **Combining Ion Mobility with Cryogenic Ion Spectroscopy for Studying Peptide Structure on the Way from Solution to the Gas Phase**; Liudmila Voronina[1]; Antoine Masson[2]; Michael Kamrath[1]; David E Clemmer[3]; Carsten Baldauf[4]; Thomas R Rizzo[1]; *[1]Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland; [2]UC Berkeley, Berkeley, California; [3]Indiana University Dept. Chemistry, Bloomington, IN; [4]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany*

ThOH am 09:50 **Insights from TIMS-MS, IR Spectroscopy and Molecular Dynamics on Nicotinamide Adenine Dinucleotide Structural Dynamics: NAD+vs NADH**; Juan Camilo Molano[1]; Walter Gonzalez[1]; Jaroslava Miksovska[1]; Philippe Maitre[2]; Francisco Fernandez Lima[1]; *[1]Florida International University, Miami, FL; [2]Laboratoire de Chimie Physique, Orsay, Orsay, France*

ThOH am 10:10 **Polymers as Model Systems to Understand Ion Mobility Mass Spectrometry Structures in Gas Phase**; Jean R. N. Haler[1]; Denis Morsa[1]; Johann Far[1]; Christine Jérôme[2]; Edwin De Pauw[1]; *[1]Mass Spectrometry Laboratory, University of Liege, Liege, Belgium; [2]CERM, University of Liege, Liege, Belgium*

10:30 AM – 2:30 PM, THURSDAY
THURSDAY POSTER SESSION
Poster/Exhibit Hall
Lunch concessions are open 11:00 am – 2:00 pm
Odd-number posters present 10:30 am - 1:00 pm
Even-number posters present 12:00 - 2:30 pm

THURSDAY AFTERNOON ORAL SESSIONS

2:30-4:30 pm THURSDAY
FOOD SAFETY AND CHEMISTRY: NON-TARGETED SCREENING
Juan F. García-Reyes (University of Jaen)
Hall 1, level 1

ThOA pm 02:30 **Comprehensive Pesticide Screening in Complex Matrices by Collision Cross Section using a Novel Geometry Travelling-Wave IMS-QTof Mass Spectrometer**; Olivier Saperas[1]; Brigitte Ogundeji[1]; Jennifer Unsworth[2]; Nick Tomczyk[2]; Martin Palmer[2]; Darren Hewitt[2]; Christophe Siroit[2]; Davy Petit[2]; Daniel J. Weston[2]; *[1]Lacapa, Toulouges, France; [2]Waters, Wilmslow, United Kingdom*

ThOA pm 02:50 **Main Challenges in LC-HRAMS Method Development for Pesticide Residue Analysis**; Łukasz Rajski[1]; María del Mar Gómez Ramos[1]; Amadeo R Fernández-Alba[1]; Maciej P Bromirski[2]; *[1]European Union Reference Laboratory for Pesticide Residues in Fruit & Vegetables. University of Almeria, Agrifood Campus of International Excellence (ceiA3)., Almeria, Spain; [2]Thermo Fisher Scientific, San Jose CA, CA - California*

ThOA pm 03:10 **Characterization of Iodine Containing Disinfection By-Products in Water using Gas Chromatography Orbitrap-based Mass Spectrometry.**; Cristina Postigo[1]; Cristian Cojocariu[2]; Susan D Richardson[3]; Damia Barcelo[4]; Paul Silcock[2]; *[1]Institute for Environmental Assessment and Water Research - Spanish National Research Council (IDAEA-CSIC), Barcelona, Spain; [2]Thermo Fisher Scientific, Runcorn, UK, Runcorn, UK; [3]University of South Carolina, Columbia, SC; [4]ICRA, Girona, Spain*

ThOA pm 03:30 **GC x GC x Q-TOF-MS Survey of Essential Oils**; Edward Ledford[1]; Zhanpin Wu[2]; Sofia Nieto[3]; Stephen E Reichenbach[4]; Qingping Tao[5]; *[1]Zoex Corporation, Houston, TX; [2]Zoex Corporation, Lincoln, NE; [3]Agilent Technologies, Santa Clara, CA; [4]Dep. of Computer Science and Engineering, University of Nebraska at Lincoln, Lincoln, NE; [5]GC Image, LLC Lincoln, NE*

ThOA pm 03:50 **Instantaneous Determination of Cocoa Content and Cocoa Bean origin of Commercial Products with Rapid Evaporative Ionization Mass Spectrometry**; Julia Balog[1, 2]; Richard Schäffer[1]; Tamas Juhasz[1]; Tamas Karancsi[1]; Steven D Pringle[3]; Zoltan Takats[2]; *[1]Waters Research Centre, Budapest, Hungary; [2]Imperial College London, London, United Kingdom; [3]Waters, Wilmslow, United Kingdom*

ThOA pm 04:10 **Classification of Olive Oils using Direct Analysis Atmospheric Pressure Chemical Ionization-Mass Spectrometry**; Pilar Perez-Hurtado[1]; Amy Giles[1]; Mark Allen[2]; Lourdes Arce[3]; Matthew Turner[1]; Jim Reynolds[4]; *[1]Loughborough University, Loughborough, United Kingdom; [2]Advion UK Ltd, Essex, United Kingdom; [3]Universidad de Cordoba, Cordoba, SPAIN; [4]Loughborough University, Loughborough, Leicestershire*

2:30-4:30 pm THURSDAY
FUNDAMENTALS: ION ACTIVATION AND DISSOCIATION
Arpad Somogyi (The Ohio State University)
Room 221, level 2

ThOB pm 02:30 **Charge Transfer Dissociation (CTD): High Energy Radical Fragmentation of Glycans, Peptides and Lipids**; Glen Paul Jackson[1]; Iris Kreft[1]; Pengfei Li[1]; David Ropartz[2]; Hélène Rogniaux[2]; *[1]West Virginia University, Morgantown, WV; [2]INRA, UR1268 Biopolymers Interactions Assemblies Nantes, France*

ThOB pm 02:50 **Improvement of Hydrogen Attachment/ Abstraction Dissociation (HAD) Efficiency for Low-Charged Peptides using Supplemental Activation**; Hidenori TakahashI[1]; Sadanori Sekiya[1]; Takashi Nishikaze[1]; Shosei Yamauchi[1]; Shinichi Iwamoto[1]; Motoi Wada[2]; Koichi Tanaka[1]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]Doshisha University, Kyotanabe, Japan*

ThOB pm 03:10 **Conformational Effects on the Dissociation Kinetics of Proton-Bound Heterodimer Ions: Applications to Gas-Phase Acidities of Alkanols**; Kent M. Ervin[1]; Jerry G Lanorio[1]; Surja B Ghale[2]; Alex A Nickel[2]; *[1]University of Nevada, Reno, Reno, NV; [2]University of Nevada, Reno Reno, NV*

ThOB pm 03:30 **Mobile C-H Protons in a Proton Deficient Peptide**; Damodar Koirala[1]; Paul G Wenthold[2]; *[1]Purdue University, West lafayette, IN; [2]Purdue University, West Lafayette, IN*

ThOB pm 03:50 **Tandem MS of Synthetic Nanoparticles through Analysis of Metastable Fragments using MALDI-TOF MS with Superconducting Tunnel Junction Cryodetection**; Logan D Plath[1]; Chenjie Zeng[1]; Yuxiang Chen[1]; Rongchao Jin[1]; Mark E Bier[1]; *[1]Carnegie Mellon University, Pittsburgh, PA*

ThOB pm 04:10 **Ultraviolet Photodissociation in a Full-Featured Proteomics Search Engine**; Christopher Becker[1]; Yong J Kil[1]; Marshall W. Bern[1]; Sylvester M Greer[2]; Jennifer S Brodbelt[2]; *[1]Protein Metrics, San Carlos, CA; [2]University of Texas at Austin, Austin, TX*

2:30-4:30 pm THURSDAY
MS SOLUTIONS FOR DRUG METABOLISM CHALLENGES
Yang Yuan (Dupont Crop Protection)
Stars Ballroom 1, level 3

ThOC pm 02:30 **Direct and Accurate Quantitation of Labeled and Un-labeled Ion Species from High Resolution LC/MS Data**; Peter L Wang[1]; Dawei Zhou[1]; Xinping Fang[1]; MING GU[2]; Yongdong Wang[3]; Jeff S. Andrews[3]; *[1]XenoBiotic Laboratories, Inc. WuXi AppTec Inc Plainsboro, NJ; [2]Cerno Bioscience, Yardley, PA; [3]Cerno Bioscience, Norwalk, CT*

ThOC pm 02:50 **Understanding the Metabolism of Protein and Peptide Therapeutics by Developing a Top-Down Protein Metabolite Identification Platform**; Xiang Yu[1]; Arthur Fridman[1]; Kristen A Kwasnjuk[1]; Ping Lu[1]; Zhiling Li[1]; Sherrie Xu[1]; Ansu Bagchi[1]; Mark T Cancilla[1]; *[1]Merck & Co., West Point, PA*

ThOC pm 03:10 **Utilizing Tandem Mass Spectrometry for the Identification of Primary and Secondary Sulfonamide Functionalities in Protonated Analytes via Ion/Molecule Reactions**; John Kong[1]; Ravikiran Yerabolu[1]; Huaming Sheng[1]; Weijuan Tang[1]; Raghavendhar Kotha[1]; Chungang Gu[2]; Hilkka Kenttämaa[1]; *[1]Purdue University, West Lafayette, IN; [2]AstraZeneca, Boston, MA*

ThOC pm 03:30 **Software Aided Integrated Workflow for Identification of Metabolic "Soft-spots" of Macromolecular Peptides in Drug Discovery**; Asoka Ranasinghe[1]; Serhiy Hnatyshyn[1]; Eugene Ciccimaro[1]; Celia D'Arienzo[1]; Timothy Olah[1]; Marshall M Siegel[2]; Gary Walker[2]; *[1]Bristol-Myers Squibb Company, Princeton, NJ; [2]MS Mass Spec Consultants, Fair Lawn, NJ*

ThOC pm 03:50 **Toward Intact Protein Mass Spectrometry for Metabolism, Pharmacokinetic, and Toxicokinetic Study Support: Immunocapture LC-MS Methods for AlbudAb and mAb Biotherapeutics**; John Kellie; *GSK, King of Prussia, PA*

ThOC pm 04:10 **Novel and Widely-Applicable Platform to Uncover Pharmacologically Active Metabolites Using Metabolic Biotransformation, Affinity Selection-Mass Spectrometry, and 2D NMR Technique**; Xianshu Yang[1]; Ian W Knemeyer[1]; Chad Chamberlin[1]; Peter J Dandliker[1]; Ting Zhang[2]; Yong Liu[2]; Gary E Martin[2]; Huifang Yao[2]; Jackie Shang[3]; Randal M Bugianesi[3]; Kenneth P Ellsworth[3]; Lisa M Sonatore[3]; Peter Nizner[3]; Edward C Sherer[2]; Susan E Hill[1]; Wayne M Geissler[3]; Roy Helmy[2]; Harold B Wood[2]; *[1]Merck & Co., Boston, MA; [2]Merck, Darmstadt, Germany; [3]Merck & Co, Kenilworth, NJ*

2:30-4:30 pm THURSDAY
AMBIENT IONIZATION: INSTRUMENTATION & APPLICATIONS
Nicholas Brunelli (The Ohio State University)
Stars Ballroom 2-3, level 3

ThOD pm 02:30 **Coupling Electrochemistry with Probe Electrospray Ionization Mass Spectrometry (PESI-MS)**; Yi Cai[1]; Hao Chen[1]; *[1]Ohio University, Athens, OH*

ThOD pm 02:50 **Fundamental Studies of Inlet Ionization with Sample Introduction at Atmospheric Pressure**; Sarah Trimpin[1]; Stephan Rauschenbach[2]; I-Chung Lu[3]; Casey Foley[3]; *[1]Wayne State University , Detroit, MI; [2]Max-Planck-Institute for Solid State Research, Stuttgart, Germany; [3]Wayne State University, Detroit, MI*

ThOD pm 03:10 **Successful Direct SPME-DBDI Coupling for Rapid, Ultrasensitive and Non-Chromatographic Analysis of Pesticides and Illicit Drugs in Complex Matrices**; Mario Francesco Mirabelli[1]; Emanuela Gionfriddo[2]; Janusz Pawliszyn[2]; Renato Zenobi[1]; *[1]ETH Zurich, Zürich, Switzerland; [2]University of Waterloo, Waterloo ON, Canada*

ThOD pm 03:30 **Direct Biofluid Analysis using Hydrophobic Paper Spray Mass Spectrometry**; Deidre Damon[1]; Abraham Badu-Tawiah[2]; *[1]The Ohio State University, Columbus, OH; [2]The Ohio State University, Columbus, Ohio*

ThOD pm 03:50 **Back to Basics - Redesigning the DESI Sprayer for Optimal Performance in Biological Tissue Imaging**; Jocelyn Tillner[1]; James McKenzie[1]; Emrys A Jones[2, 1]; Steven D Pringle[2]; Tamas Karancsi[2]; Anna Mroz[1]; Dipa Gurung[1]; Josephine Bunch[3]; Ian Gilmore[3]; Zoltan Takats[1]; *[1]Imperial College, London, United Kingdom; [2]Waters, Manchester, United Kingdom; [3]National Physical Laboratory, Teddington, United Kingdom*

ThOD pm 04:10 **Fast SAWN MS Assay for Art Restoration and Conservationstudies**; Garry Corthals[1]; Alina Astefanei[2]; Petra J Jansen[2]; Maarten R van Bommel[2]; Erik Nilsson[3]; Gloria Yen[3]; *[1]University of Amsterdam, Amsterdam, ZH; [2]University of Amsterdam, Amsterdam, The Netherlands; [3]Deurion LLC, Seattle, WA*

2:30-4:30 pm THURSDAY
BIOMARKERS: QUANTITATIVE ANALYSIS
Matthew M. Champion (University of Notre Dame)
Stars Ballroom 4, level 3

ThOE pm 02:30 **Disrupted Stoichiometric Relationships as Biomarkers of Altered Cellular States**; Marija Buljan[1]; Tiannan Guo[1]; Qing Zhong[2]; Ulrich Wagner[2]; Li Li[3]; Andreas Beyer[3]; Peter Wild[2]; Ruedi Aebersold[1]; *[1]Institute of Molecular Systems Biology ETH Zurich, Zurich, Switzerland; [2]Institute of Surgical Pathology, University Hospital Zurich, Zurich, Switzerland; [3]University of Cologne, Cologne, Germany*

ThOE pm 02:50 **Understanding Biological Heterogeneity through Mass Cytometry**; Jennifer Frahm[1]; Christina Loh[2]; Tad George[2]; Mark Konrad[1]; Olga Ornastsky[2]; Daniel Majonis[2]; Andrei Terekidi[2]; Gary Impey[2]; *[1]Fluidigm Corporation, South San Francisco, CA USA; [2]Fluidigm Canada Inc., Markham, CANADA*

ThOE pm 03:10 **Antibody-Independent, Deep-Dive Targeted Quantification of Proteins at Ten Picogram per Milliliter Levels in Non-Depleted Human Serum/Plasma**; Song Nie[1]; Tujin Shi[1]; Thomas Fillmore[1]; Yuqian Gao[1]; Athena A Shepmoes[1]; Heather Brewer[1]; Wei-jun Qian[1]; Karin D Rodland[1]; Richard D Smith[1]; Tao Liu[1]; *[1]Biological Sciences Division and Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA*

ThOE pm 03:30 **Mass Spectrometry Based Identification and Quantitation of Maturation Stage Specific Surface Markers of Human Stem Cell Derived Cardiomyocytes**; Matthew Waas[1]; Erin Kropp[1]; Alyssa Nycz[1]; Chelsea Fujinaka[1]; Rebekah Gundry[1]; *[1]Medical College of Wisconsin, Milwaukee, WI*

ThOE pm 03:50 **Discovery and Quantitative Metabolomics to Characterize Metabolites of Bacterial Origin as Biomarkers for Cystic Fibrosis**; Jace W Jones[1]; Angela Nguyen[1]; Bennett Giardina[1]; Luke Brewer[1]; Angela Wilks[1]; Amanda Oglesby-Sherrouse[1]; Maureen Kane[1]; *[1]University of Maryland, School of Pharmacy Baltimore, MD*

ThOE pm 04:10 **Quantifying Concentrations of Molecules in Live Single Cells using the Single-probe MS Technique**; Ning Pan[1]; Wei Rao[1]; Haiqing Yu[1]; Naga Rama Kothapalli[1]; Mei Sun[1]; Anthony Burgett[1]; Zhibo Yang[1]; *[1]University of Oklahoma, Dept. of Chem & Biochem Norman, OK*

2:30-4:30 pm THURSDAY
INFORMATICS: PEPTIDE AND PROTEIN IDENTIFICATION
Natalie Castellana (Digital Proteomics LLC)
Hemisfair Ballroom 3, level 3

ThOF pm 02:30 **A Graph-based Method for Proteoform Identification and Quantification by Top-down Multiplexed Tandem Mass Spectra**; Zhu Kaiyuan[1]; Xiaowen Liu[2]; *[1]Indiana University, Bloomington, IN; [2]Indianapolis, IN*

ThOF pm 02:50 **High Quality Estimation of False Discovery Rate for Proteoform Identification with Top Down Proteomics**; Richard Leduc[1]; Daniel Shams[2, 3]; Ryan T Fellers[1]; Bryan Early[1]; Joseph Greer[1]; David Schwab[3]; Neil L Kelleher[1, 4, 5, 6]; *[1]Proteomics Center of Excellence, Northwestern University, Evanston, IL; [2]Interdisciplinary Biological Sciences, Northwestern University, Evanston, IL; [3]Department of Physics and Astronomy, Northwestern University, Evanston, IL; [4]Chemistry of Life Processes Institute, Northwestern University, Evanston, IL; [5]Department of Chemistry, Northwestern University, Evanston, IL; [6]Department of Molecular Biosciences, Northwestern University, Evanston, IL*

ThOF pm 03:10 **Open-pNovo: *de novo* Peptide Sequencing with Thousands Types of Protein Modifications**; Hao Yang[1]; Hao Chi[1]; Wen-Jing Zhou[1]; Wen-Feng Zeng[1]; Kun He[1]; Chao Liu[1]; Rui-Xiang Sun[1]; Si-Min He[1]; *[1]Institute of Computing Technology, CAS, Beijing, China*

ThOF pm 03:30 **Optimized Open Modification Spectral Library Searching using Approximate Nearest Neighbor Techniques**; Wout Bittremieux[1]; Dirk Valkenborg[2]; Kris Laukens[3]; *[1]University of Antwerp, Antwerp; [2]VITO, Mol, Belgium; [3]University of Antwerp, Antwerp, Belgium*

ThOF pm 03:50 **Sifting through Swarms of Spectra: Lessons Learned Identifying Proteins across 11,782 Affinity-Purification Mass Spectrometry Analyses**; Edward L. Huttlin[1]; Joao A Paulo[1]; Raphael J. Bruckner[1]; Lily Ting[1]; Wade Harper[1]; Steven P Gygi[1]; *[1]Harvard Medical School, Boston, MA*

ThOF pm 04:10 **Building Comprehensive Peptide Spectral Libraries at Repository Scale**; Mingxun Wang[1]; Jian Wang[1]; Anne-Claude Gingras[2]; Nuno Bandeira[1]; *[1]UCSD, San Diego, CA; [2]Lunenfeld Tanenbaum Research Institute, Toronto, Canada*

2:30-4:30 pm THURSDAY
LIPIDOMICS: NEW MS TECHNOLOGIES AND APPLICATIONS
Daniel Amador-Noguez (University of Wisconsin-Madison)
Hemisfair Ballroom 2, level 3

ThOG pm 02:30 **A Quantitative Positive/Negative Ion Switching Method for Shotgun Lipidomics via High Resolution LC-MS/MS from any Biological Source**; Min Yuan[1]; Ying Xu[1]; Susanne Breitkopf[1]; Stephane Ricoult[2]; John M Asara[1]; *[1]Beth Israel Deaconess Medical Center, Boston, MA; [2]Harvard School of Public Health, Boston, MA*

ThOG pm 02:50 **Lipidomic Imaging with a New Hybrid 3D SIMS Molecular Imaging Instrument**; Melissa K Passarelli[1]; Alexander Pirkl[2]; Rudolf Moellers[2]; Ewald Niehuis[2]; Alexander A Makarov[3]; Henrik Arlinghaus[2]; Rasmus Havelund[1]; Paulina Rakowska[1]; Alan Race[1]; Alex Shard[1]; Andy West[4]; Stevan Horning[3]; Peter Marshall[4]; Morgan Alexander[5]; Colin Dollery[4]; Ian Gilmore[1]; *[1]National Physical Laboratory, Teddington, United Kingdom; [2]ION-TOF GmbH, Munster, Germany; [3]Thermo Fisher Scientific, Bremen, DE; [4]GlaxoSmithKline, Stevenage, UK; [5]University of Nottingham, Nottingham, UK*

ThOG pm 03:10 **Electron-induced Dissociation (EID) of Lipids: Diagnostic Product Ions for Confident Identification of Isomers**; Jace W. Jones[1]; Claire Louise Carter[1]; Maureen A Kane[1]; *[1]University of Maryland, School of Pharmacy Baltimore, MD*

ThOG pm 03:30 **Broad Characterization of Isomeric Lipids by High-Resolution Differential Ion Mobility Separations with Tandem Mass Spectrometry**; Rinat R Abzalimov[1]; Andrew Bowman[2]; Alexandre A Shvartsburg[2]; *[1]City University of New York - Advanced Science Research Center, New York City, NY; [2]Wichita State University, Wichita, KS*

ThOG pm 03:50 **Nano-DESI Imaging of Lipids and Metabolites in Developing Lung**; Son N. Nguyen[1]; Ryan L Sontag[1]; Jennifer E Kyle[1]; Sydney E Dautel[1]; Thomas O Metz[1]; Richard A Corley[1]; Charles K Ansong[1]; Mathew Thomas[1]; James Carson[2]; Julia Laskin[1]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]University of Texas at Austin, Austin, TX*

ThOG pm 04:10 **In depth Sphingomyelin and Triacylglycerol Structure Identification using Electron Impact Excitation of Ions from Organics (EIEIO) and Mass Spectrometry**; Takashi Baba[1]; Larry J Campbell[1]; Yves J C LeBlanc[1]; Paul RS Baker[2]; *[1]SCIEX, Concord ON, Canada; [2]SCIEX, Redwood City, CA*

2:30-4:30 pm THURSDAY
HYDROGEN-DEUTERIUM EXCHANGE MS
Sheena D'Arcy (University of Texas at Dallas)
Hemisfair Ballroom 1, level 3

ThOH pm 02:30 **HX-MS Epitope Mapping of a Ricin Toxin Chain A Double Mutant (RTA*)**; Ronald Toth[1]; Siva Krishna Angalakurthi[1]; John Hickey[1]; Sangeeta Joshi[1]; Charles Russell Middaugh[1]; Greta Van Slyke[2]; Nicholas Mantis[2, 3]; David Volkin[1]; David Weis[4]; *[1]Department of Pharmaceutical Chemistry and Macromolecule and Vaccine Stabilization Center; University of Kansas, Lawrence, KS; [2]Division of Infectious Disease, Wadsworth Center, New York State Department of Health, Albany, NY; [3]Department of Biomedical Sciences, University at Albany School of Public Health, Albany, NY; [4]Department of Chemistry and R. N. Adams Institute for Bioanalytical Chemistry; University of Kansas, Lawrence, KS*

ThOH pm 02:50 **The Role of Conformational Dynamics in Differing Activity and Substrate Specificity amongst Isozymes**; Andrew Fairman[1]; Peter Sidhu[1]; David Josephy[2]; Derek Wilson[1]; *[1]York University, Toronto, Canada; [2]University of Guelph, Guelph, Canada*

ThOH pm 03:10 **Structural basis for the formation and function of the complement effector protein iC3b**; Malvina Papanastasiou[1]; Sophia Koutsogiannaki[1]; Yiannis Sarigiannis[1]; Daniel Ricklin[1]; John D. Lambris[1]; *[1]Dept. Pathology & Lab. Medicine, Perelman School of Medicine, UPENN, Philadelphia, PA*

ThOH pm 03:30 **A New Automation Platform Provides Significant Improvements in Both the Capacity and Flexibility of the HDX-MS Experiment**; Ruben Haro[1]; Alfonso Espada[1]; Manuel Molina-Martin[1]; Jesus Castanon[1]; Bruce D Pascal[2]; Pat Griffin[2]; Jeffrey A Dodge[3]; Michael Chalmers[3]; *[1]Eli Lilly and Company, Alcobendas, SPAIN; [2]The Scripps Research Institute, Jupiter, Fl; [3]Eli Lilly and Company, Indianapolis, IN*

ThOH pm 03:50 **Intramolecular Interactions in Heme Oxygenase 2 in the Presence and Absence of Lipid Membranes**; Brent A Kochert[1]; Angela S Fleischhacker[2]; Stephen W Ragsdale[2]; John R Engen[1]; *[1]Department of Chemistry and Chemical Biology, Northeastern University, Boston, MA; [2]Department of Chemistry, University of Michigan, Ann Arbor, MI*

ThOH pm 04:10 **The Analytical Potential of HDXMS in Providing Localized Structural Dynamics Insight to Each Subunits of an Asymmetric Non-Crystallizable Protein Homodimer**; Morten Beck Trelle[1]; Alice Østergaard[2]; Jeppe Buur Madsen[1]; Shona Pedersen[2]; Søren Risom Kristensen[2]; Thomas J.D. Jørgensen[1]; *[1]University of Southern Denmark, Odense, Denmark; [2]Department of Clinical Medicine, Aalborg University Hospital, Aalborg, Denmark, Ålborg, Denmark*

4:45 - 5:00 PM
PLENARY LECTURE
Vicki Wysocki (The Ohio State University) presiding
Hall 1, level 1

More than the Sum of its Parts: Collective Phenomena in Living Systems, from Single Molecules to Flocks of Birds

William Bialek
Princeton University

6:30 – 9:00 PM, THURSDAY
CLOSING EVENT
BRISCOE WESTERN ART MUSEUM
Ticket is required.

ODD-NUMBERED POSTERS PRESENT 10:30 AM - 1:00 PM. EVEN-NUMBERED POSTERS PRESENT 12:00 - 2:30 PM.

MONDAY POSTERS

Set up all Monday posters ..... 7:30 – 8:00 am
Odd-numbered posters present ..... 10:30 am – 1:00 pm
Even-numbered posters present ..... 12:00 – 2:30 pm
Remove all Monday posters ..... 7:30 – 8:00 pm

TUESDAY POSTERS

Set up all Tuesday posters ..... 7:30 – 8:00 am
Odd-numbered posters present ..... 10:30 am – 1:00 pm
Even-numbered posters present ..... 12:00 – 2:30 pm
Remove all Tuesday posters ..... 7:30 – 8:00 pm

ODD-NUMBERED POSTERS PRESENT 10:30 AM - 1:00 PM. EVEN-NUMBERED POSTERS PRESENT 12:30 - 2:30 PM.

WEDNESDAY POSTERS

Set up all Wednesday posters ..... 7:30 – 8:00 am
Odd-numbered posters present ..... 10:30 am – 1:00 pm
Even-numbered posters present ..... 12:00 – 2:30 pm
Remove all Wednesday posters ..... 7:30 – 8:00 pm

THURSDAY POSTERS

Set up all Thursday posters ..... 7:30 – 8:00 am
Odd-numbered posters present ..... 10:30 am – 1:00 pm
Even-numbered posters present ..... 12:00 – 2:30 pm
Remove all Thursday posters ..... 2:30 – 3:00 pm

ANTIBODIES & ANTIBODY DRUG CONJUGATES (INTACT & CHARACTERIZATION)
001 - 020

MP 001 **Integrating Intact, Reduced and IdeS Approaches for Rapid Differentiation and Verification of Monoclonal Antibodies Using Liquid Chromatography Q-Exactive Mass Spectrometry**; Lianji Jin; *FDA, Cincinnati, OH*

MP 002 **Online Separation and Characterization of intact IgG Fabs Using Ultra Performance Liquid Chromatography Coupled with Top-down Mass Spectrometry**; Zhe Wang[1]; Kenneth Smith[2]; Si Wu[1]; *[1]University of Oklahoma, Dept. of Chem & Biochem Norman, OK; [2]Oklahoma Medical Research Foundation, Oklahoma City, OK*

MP 003 **Evaluation of Different Immunocapture Platforms for Antibody-Conjugate Drug Quantification**; Ling Xu[1]; Shaoxia Yu[2]; Jing-Tao Wu[3]; Mark Qian[3]; *[1]Millennium Pharma, Cambridge, MA; [2]Takeda Pharmaceutical International Inc., Cambridge, MA; [3]Takeda Pharmaceuticals International Inc., Cambridge, MA*

MP 004 **Intact Mass Analysis of Antibody-drug conjugates (ADCs) as a Tool to Measure Payloads of Linked Cytotoxic Drugs**; Joe Shambaugh[1]; Cassandra Wigmore[2]; Maurizio Bronzetti[1]; David Bush[1]; Arnd Brandenburg[2]; Peter Haberl[3]; *[1]Genedata Inc, Lexington, MA; [2]Genedata AG, Basel, Switzerland; [3]Genedata GmbH, Munich, Germany*

MP 005 **Characterization of Bispecific Antibodies Using Mass Spectrometry during Cell Line Development is Critical for an Optimized Final Drug Product**; Michael Bacica[1]; Jon R Fitchett[1]; Stephen J Demarest[1]; Xiufeng Wu[1]; Robert Peery[2]; Bryan Jones[1]; *[1]Lilly Biotech Center-San Diego, San Diego, CA; [2]Lilly BioTDR, Indianapolis, IN*

MP 006 **Developability Assessment of Multispecific Biopharmaceuticals**; Kadir Ilker Sen[1]; Eric Beil[1]; Hirsh Nanda[1]; Andrew Mahan[1]; Darryl Davis[1]; *[1]Janssen Research and Development, Spring House, PA*

MP 007 **Monitoring the Critical Quality Attributes of Antibody Drug conjugates (ADCs) as Part of Biosimilar Development: Case Studies of ado-trastuzumab emtansine**; Liuxi Chen[1]; Min Du[1]; Henry Y Shion[1]; Ying-Qing Yu[1]; Lan Wang[2]; Kai Gao[2]; Weibin Chen[1]; *[1]Waters Corporation, Milford, USA; [2]National Institutes for food and drug control, Beijing, CN*

MP 008 **Detection of an Amino Acid Sequence Variant as a Function of Cell Line Stability in a Model Antibody**; Sylwia Jozwiak[1]; James Graham[1]; *[1]Lonza, Slough, UK*

MP 009 **Assessment of Critical Parameters for the Mass Spectrometric Evaluation of the Drug-to-Antibody Ratio in Antibody-Drug Conjugates**; Neil Hershey[1]; Shiyue Zhou[2]; Yunping Huang[1]; Hangtian Song[1]; Hui Wei[1]; Jacob Bongers[1]; Richard Ludwig[1]; Li Tao[1]; Tapan Das[1]; *[1]Bristol-Myers Squibb, Hopewell, NJ; [2]Texas Tech University, Lubbock, Texas*

MP 010 **An Automated Quantitative Mass Spectrometry Assay to Determine Intra-Cellular Retention Kinetics of Antibiotic Released from Anti-Staphylococcus Aureus Antibody-Antibiotic Conjugate**; Hilda Hernandez-Barry[1]; Kimberly Kajihara[2]; Daniel Tran[2]; Martine Darwish[2]; Byoung-Chul Lee[2]; Richard Vandlen[2]; Leanna Staben[2]; Thomas Pillow[2]; Wouter Hazenbos[2]; Kelly Loyet[2]; *[1]Genentech, South San Francisco, CA; [2]Genentech Inc, South San Francisco, CA*

MP 011 **An Automated Sample Extraction and Processing Method Combining Ligand Binding and Mass Spectrometry Analysis for Biotherapeutics Quantitation**; Ian Moore; *SCIEX, Concord, ON*

MP 012 **A Comprehensive Mass Spectrometric Workflow for Characterizing Therapeutic Antibodies**; Alicia Bielik[1]; Paula Magnelli[1]; Beth McLeod[1]; Colleen McClung[1]; Beth Paschal[1]; Cristian I Ruse[1]; Xiaofeng Shi[1]; Ellen Guthrie[1]; *[1]New Englanb Biolabs, Ipswich, MA*

MP 013 **Drug-to-Antibody Ratio Determination for Antibody-Drug Conjugates in Serum Enabled by a Sample Preparation Platform that Automates Affinity Purification and Deglycosylation**; Jing Chen[1]; Maryann Shen[2]; Steve Murphy[1]; *[1]Agilent Technologies, Inc. Madison, WI; [2]Agilent Technologies, Santa Clara, CA*

MP 014 **Platform Method for Identity and Characterization of Therapeutic Monoclonal and Bispecific Antibodies by Intact and Reduced Mass Spectrometry**; Richard Seipert[1]; Lisa Patterson[2]; George Tsui[2]; Chris Yu[2]; *[1]Genentech, South San Francisco, CA; [2]Genentech Inc, South San Francisco, CA*

MP 015 **A Tag-free Collisionally-Induced Fragmentation Technique Applied to Studies of Antibody-drug Conjugate Lysosomal Processing**; Andrew Bessire[1]; Chakrapani Subramanyam[2]; My-Hahn Lam[3]; Frank Loganzo[3]; T. Eric Ballard[2]; *[1]Pfizer, Inc., Groton, CT; [2]Pfizer, Groton, CT; [3]Pfizer Oncology-Rinat R&D, Pearl River, NY*

MP 016 **Strategy to Rapidly and Comprehensively Characterize Innovator Biologics and their Biosimilars via Stress Testing Studies**; Esthelle Hoedt[1]; St John Skilton[2]; Yong J Kil[3]; Eric Carlson[4]; Chris Becker[3]; Beatrix M Ueberheide[1]; *[1]NYU School of Medicine, New York City, NY; [2]Protein Metrics, Hopkinton, MA; [3]Protein Metrics, San Carlos, CA; [4]Protein Metrics Inc., San Carlos, CA*

MP 017 **Method Development for the Detection and Quantitation of Monomethyl Auristatin F (MMAF) in Cell Culture Media**; Maria Christina Malinao[1]; Melissa M. Williams[1]; Cody Warhurst[1]; Julien Dugal-Tessier[1]; Josh T. Snyder[1]; Brian Mendelsohn[1]; Hui Zhao[1]; Sara Gulesserian[1]; Hosein Kouros-Mehr[1]; Kendall Morrison[1]; *[1]Agensys, Inc. Santa Monica, CA*

MP 018 **In-Depth Characterization of Monoclonal Antibodies with a Single Experiment and Fully Automated Data Analysis**; Paul Taylor[1]; Johnathan Krieger[1]; Qixin Liu[2]; Mingjie Xie[2]; Lian Yang[2, 3]; Bin Ma[3]; *[1]Hospital for Sick Children, Toronto, Canada; [2]Rapid Novor Inc., Waterloo ON, Canada; [3]University of Waterloo, Waterloo ON, Canada*

MP 019 **Antibody Variable Domains as Intramolecular Luciferase Inhibitors for the Generation of Proteolysis-Activated Biosensors**; Lining Zhu[1]; Teresa Hong[1]; Nicola McNiven[1]; Markus Kalkum[1]; *[1]City of Hope, Duarte, CA*

MP 020 **Novel Strategy Based on Dual Enrichment and Double Lists for Characterization of Host Cell Proteins**; Zheng-Xiang Zhang[1]; Jimmy Chan[1]; Shuai Zuo[1]; Tao Bo[1]; Rong An[1]; *[1]Agilent Technologies (China) Limited, Beijing, China*

BIOMOLECULAR STRUCTURE ANALYSIS: COVALENT LABELING AND RELATED SOFTWARE
021 - 039

MP 021 **Using High Resolution Structural Analysis to Determine if FPOP Modification Perturbs Native Protein Structure**; Emily Hart[1]; Lisa M Jones[1]; *[1]IUPUI Department of Chemistry & Chemical Biology, Indianapolis, IN*

MP 022 **Extension of the FPOP Method for Oxidative Modification in Live Tissue**; Jessica Arlett Espino[1]; Anthony J Baucum[1]; Lisa M Jones[2]; *[1]Indiana University-Purdue University Indianapolis, Indianapolis, IN; [2]Indiana University Purdue University Indianapolis, Indianapolis, In*

MP 023 **Epitope Map of Malarial Antigen PvDBP revealed by Fast Photochemical Oxidation of Proteins (FPOP)**; Manolo David Plasencia[1]; Yining Huang[1]; Henry W Rohrs[1]; Edwin Chen[2]; Nichole D. Salinas[2]; Niraj H. Tolia[2]; Michael L Gross[1]; *[1]Washington University in St. Louis, St. Louis, MO; [2]Washington University School of Medicine, St. Louis, MO*

MP 024 **The Application of "Droplet-Like" Methods to FPOP**; Don L. Rempel[1]; Supratik Dutta[2]; Ben Niu[2]; Yining Huang[2]; Manolo Plasencia[2]; Michael Gross[2]; *[1]Center for Biomedical and Bioorganic Mass Spectrometry, Washington University in St. Louis, St Louis, MO; [2]Center for Biomedical and Bioorganic Mass Spectrometry, Washington University in St. Louis, St. Louis, MO*

MP 025 **Normalization of High Resolution Hydroxyl Radical Protein Footprinting Data to Protein Structural Properties**; Boer Xie[1]; Amika Sood[1]; Robert J Woods[1]; Joshua S. Sharp[2]; *[1]University of Georgia, Athens, GA; [2]University of Mississippi, University, MS*

MP 026 **Automated Hydroxyl Radical Protein Footprinting for the Determination of Biopharmaceutical Protein Conformation**; Franklin E. Leach III[1]; Ron Orlando[2]; Joshua S Sharp[3]; *[1]Photochem Technologies, Athens, GA; [2]Complex Carbohydrate Research Center UGA, Athens, GA; [3]School of Pharmacy, University of Mississippi, Oxford, MS*

MP 027 **Develop Isotope-encoded Photoaffinity Footprinting Reagent for Structural Mass Spectrometry Studies**; Ming Cheng[1]; Michael L Gross[1]; *[1]Washington University in St. Louis, St. Louis, MO*

MP 028 **Exploring the Peroxidase Activation and Deactivation of Cytochrome C by Heme-Catalyzed Oxidative Labeling and ESI-MS**; Victor Yin[1]; Lars Konermann[1]; *[1]Western University, London, Canada*

MP 029 **Comprehensive Measurement of Protein Dynamics in Complex Environments Using Footprinting Mass Spectrometry with Inexpensive MS2 Quantification of Labeled Cysteines**; Jenna Gray Caldwell[1]; Pehr A. B. Harbury[1]; *[1]Stanford University School of Medicine, Palo Alto CA*

MP 030 **Using Covalent Labeling and Mass Spectrometry to Study b-2-Microglobulin-Inhibitor Binding Sites**; Tianying Liu[1]; Richard W Vachet[1]; *[1]University of Massachusetts Amherst, Amherst, MA*

MP 031 **Towards an Improved Understanding of Diazirine Labeling for Structural Mass Spectrometry Applications**; Daniel Ziemianowicz[1]; Chris Etienne[2]; David Schriemer[1]; *[1]University of Calgary, Calgary, Canada; [2]Thermo Fisher Scientific, Rockford, IL*

MP 032 **Characterisation Proteolytic Process by Protein N-Terminal Derivatisation in- Gel Using MS-Based Approach in Drosophila**; Nina Guillaumot[1]; Florian Veillard[2]; Jean-Marc Reichhart[2]; Alain Van dorsselaer[1]; Christine Schaeffer-Reiss[1]; *[1]Laboratoire de Spectrométrie de Masse BioOrganique, IPHC, Université de Strasbourg, CNRS, UMR7178, Strasbourg, Strasbourg, France; [2]Institut de Biologie Moléculaire et Cellulaire, IBMC, Université de Strasbourg, CNRS UPR 9022, Strasbourg, Strasbourg, France*

MP 033 **Covalent Labeling Denaturation Mass Spectrometry for Sensitive Localized Higher Order Structure Comparisons**; James A. Madsen[1]; Yan Yin[1]; Jing Qiao[1]; Vanessa Gill[1]; Kutralanathan Renganathan[1]; Wing-Yee Fu[1]; Stephen Smith[1]; James Anderson[1]; *[1]Momenta Pharmaceuticals, Cambridge, MA*

MP 034 **Xilmass: A New Approach Towards the Identification of Cross-Linked Peptides**; Şule Yılmaz[1, 2, 3]; Friedel Drepper[4, 5]; Maša Černič[6]; Kris Gevaert[1, 7]; Anastassios Economou[8, 9]; Bettina Warscheid[4, 5]; Lennart Martens[1, 7, 10]; Elien Vandermarliere[1, 7, 10]; *[1]Department of Biochemistry, Ghent University, Ghent, BELGIUM; [2]Medical Biotechnology Center, Ghent, BELGIUM; [3]Bioinformatics Institute Ghent, Ghent, BELGIUM; [4]Department of Biochemistry and Functional Proteomics, Institute of Biology II, Faculty of Biology, University of Freiburg, Freiburg, Germany; [5]BIOSS Centre for Biological Signaling Studies, University of Freiburg, Freiburg, Germany; [6]Centre of Excellence for Integrated Approaches in Chemistry and Biology of Proteins, Ljubljana, Slovenia; [7]Medical Biotechnology Center, VIB, Ghent, BELGIUM; [8]Laboratory of Molecular Bacteriology, Rega Institute for Medical Research, Department of Microbiology and Immunology, KULeuven, Leuven, BELGIUM; [9]Institute of Molecular Biology and Biotechnology-FoRTH, Department of Biology – University of Crete, Iraklio, Crete, Greece; [10]Bioinformatics Institute Ghent, Ghent University, Ghent, BELGIUM*

MP 035 **Crosslinkers with Isotope-Coding and Cleavable Spacers Improve Peptide Crosslink Identification by a Semi-Supervised Machine Learning Algorithm**; Karl A T Makepeace[1]; Evgeniy V Petrotchenko[1]; Christoph H. Borchers[2, 3]; *[1]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [2]University of Victoria - Genome BC Proteomics Centre, Victoria, BC; [3]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada*

MP 036 **A Simple Approach for Creating Protein Structural Models Based on Cross-Linking Data**; Zsuzsanna Orban-Nemeth[1]; Evelyn Rampler[1]; Thomas Stranzl[1]; David Maria Hollenstein[2]; Otto Hudecz[3]; Peter Schloegelhofer[4]; Karl Mechtler[1, 3]; *[1]Institute of Molecular Pathology, Vienna, Austria; [2]Department of Biochemistry and Cell Biology, Max F. Perutz Laboratories, University of Vienna, Vienna, Austria; [3]Institute of Molecular Biotechnology, Austrian Academy of Sciences, Vienna, Austria; [4]Department*

of Chromosome Biology, Max F. Perutz Laboratories, University of Vienna, Vienna, Austria

MP 037 **CX-Circos: A Web-Based Tool for Visualization and Analysis of Chemical Crosslinking Data**; Junjie Wang[1]; Yi Shi[1]; Brian T. Chait[1]; *[1]Rockefeller University, New York, NY*

MP 038 **In Cell Protein Footprinting Coupled with Mass Spectrometry to Probe Protein Conformational Change**; Maissa M Gaye[1]; Lisa Jones[1]; *[1]Indiana University-Purdue University Indianapolis, Indianapolis, IN*

MP 039 **High-throughput Mass Spectrometric Analysis of Covalent Protein-inhibitor Adducts, Monoclonal Antibodies and ADCs: A Complete Workflow**; Tisha San Miguel[1]; Jelly Netirojjanakul[1]; Rowe Todd[1]; Onea Daniel[1]; Victor Cee[1]; Arvedson Tara[1]; McCarter John[1]; Campuzano Iain[1]; *[1]Amgen, Inc., Thousand Oaks, CA*

CARBOHYDRATES
040 - 055

MP 040 **Quantifying Cyclodextrin-Drug Interactions by ESI-MS**; Emma-Dune Leriche[1]; Ping Zhang[2]; Aixia Wang[2]; Yuyu Yao[1]; Chang-Chun Ling[2]; Elena N Kitova[1]; John S Klassen[1]; *[1]University of Alberta, Edmonton, Canada; [2]University of Calgary, Calgary, Canada*

MP 041 **Identification and Relative Quantification C-mannosylation of Interleukin 6 (IL-6) using Liquid Chromatography-tandem Mass Spectrometry**; Anhdao Darcy; *Abbvie Bioresearch Center, Worcester, MA*

MP 042 **Development of Negative Mode Free Radical Activated Glycan Structure Elucidation Reagents**; Jinshan Gao[1]; Nikunj Desai[1]; Jungeun Lee[1]; *[1]Montclair State University, Montcalir, NJ*

MP 043 **Carbohydrate Analysis using Gas Chromatography Vacuum Ultraviolet Spectroscopy in Comparison with Gas Chromatography Mass Spectrometry**; Jamie Schenk[1]; Xiaojian Mao[1]; Jonathan Smuts[2]; Gabe Nagy[3]; Nicola L. B. Pohl[3]; Phillip Walsh[2]; Peter Kroll[1]; Kevin A Schug[1]; *[1]University of Texas at Arlington, Arlington, TX; [2]VUV Analytics, Inc., Cedar Park, TX; [3]Indiana University, Bloomington, IN*

MP 044 **Understanding the Reaction Products of Methanolysis and Butanolysis of Heparan Sulfate**; Marten F Snel[1]; Paul J Trim[2]; John J Hopwood[2]; Qi Qi He[3]; Vito Ferro[3]; *[1]South Australian Health and Medical Research Institute, Adelaide, South Australia; [2]LDRU, Nutrition and Metabolism Theme, South Australian Health and Medical Research Institute, Adelaide, Australia; [3]School of Chemistry and Molecular Biosciences, The University of Queensland, Brisbane, Australia*

MP 045 **LC-MS Analysis of the Complete Molecular Weight Distribution of Low Molecular Weight Heparins**; Yuewei Sheng[1]; Chun Shao[1]; Kshitij Khatri[1]; Joseph Zaia[2]; *[1]Boston University School of Medicine, Boston, MA; [2]Boston University, Boston, MA*

MP 046 **Size-Selective Controlled Heparin Depolymerization to Obtain Heparin Oligosaccharides**; Sandeep K Misra[1]; Joshua S Sharp[1]; *[1]Dept of Biomolecular Sciences, University of Mississippi, Oxford, MS*

MP 047 **Oxidation of Glucose at Gold Nanoparticles and Mass Spectrometric Product Analysis**; Marilyn Wooten[1]; Wendell P. Griffith[2]; Sushma Karra[2]; Waldemar Gorski[2]; *[1]Trinity University, San Antonio, TX; [2]University of Texas at San Antonio, San Antonio, TX*

MP 048 **Study of Rearrangement Products in Collision-Induced Dissociation and Surface-Induced Dissociation of Oligosaccharides and Glycoconjugates**; Forouzan Aboufazeli[1]; Eric D Dodds[1]; *[1]University of Nebraska-Lincoln, Lincoln, NE*

MP 049 **Single Stage Tandem Mass Spectrometry Assignment of the C-5 Uronic Acid Stereochemistry in Heparan Sulfate Tetrasaccharides Using Electron Detachment Dissociation**; Isaac Agyekum[1]; Chengli Zong[2, 3]; Geert-Jan Boons[2, 3]; Jon Amster[2]; *[1]University of Georgia,Chemistry Department, Athens, GA; [2]University of Georgia, Chemistry Department Athens, GA; [3]CCRC, University of Georgia Athens, GA*

MP 050 **Mass Spectrometric Quantification of Cell Wall Composition Differences in Enterococcus Using Stable Isotope Labeling by Amino Acids**; James Chang[1]; Ashley Wallace[1]; Erin Foster[1]; Alex Guinn[1]; Sung Joon Kim[1]; *[1]Baylor University, Waco, TX*

MP 051 **High Resolution CESI-MS Analysis of APTS-Labeled N-Glycans of Biopharmaceutical Interest**; Fonslow Bryan; Marton Szigeti[1]; Andras Guttman[2]; *[1]University of Debrecen, Debrecen, Hungary; [2]AB Sciex, San Diego, CA*

MP 052 **Probing Carbohydrate Isomerism through Transition Metal Ion Adduction, Gas-Phase Ion Chemistry, and Collision-Induced Dissociation**; Katherine Schumacher[1]; Yuting Huang[1]; Lauren Petrosh[1]; Eric D Dodds[1]; *[1]University of Nebraska - Lincoln, Lincoln, NE*

MP 053 **ESI-TOF-MS Study of Carbohydrate Interaction with Metal Complexes with Carboxylate-Rich Ligand**; Fangzhi Yan[1]; Christopher D. Stewart[1]; Stephan B. H. Bach[1]; Wendell P Griffith[1]; Ghezai T. Musie[1]; *[1]University of Texas at San Antonio, San Antonio, TX*

MP 054 **Fragmentation of Derivatized and Non-Derivatized Metal-Adducted Oligosaccharides**; Ranelle Schaller-Duke; *The University of Alabama, Tuscaloosa, Al*

MP 055 **A Novel Method for High-Throughput Analysis of Bioactive Oligosaccharides**; Randall Robinson[1]; Daniela Barile[1]; *[1]University of California, Davis, Davis, CA*

DATA INDEPENDENT ACQUISITION
056 - 070

MP 056 **Advances in Targeted Omics Quantitation Using a Novel Scanning Quadrupole DIA Method**; Chris Hughes[1]; Keith Richardson[1]; Jason Wildgoose[1]; Martin R Green[1]; Richard Chapman[1]; Arkadiusz Grzyb[1]; Praveen Harapanahalli[1]; Kirsten Craven[1]; *[1]Waters, Wilmslow, United Kingdom*

MP 057 **Optimisation of Data Independent Acquisition (DIA) Data Extraction for Proteome Quantification**; Gauthier Husson[1]; Alvaro Sebastian Vaca Jacome[1]; Maxime Eveque[1]; Christine Carapito[1]; *[1]Laboratoire de Spectrométrie de Masse BioOrganique (LSMBO), IPHC, Strasbourg University, CNRS, UMR7178, Strasbourg, France*

MP 058 **Improved Multiplexed Data Independent Acquisition: Sensitivity, Dynamic Range, and Full-Spectrum Demultiplexing**; Jarrett Egertson[1]; Ying Sonia Ting[1]; Philip M Remes[2]; Romain Huguet[2]; Derek Bailey[2]; Michael Senko[2]; Vlad Zabrouskov[2]; Michael J MacCoss[1]; *[1]Univ of Washington, Seattle, WA; [2]Thermo Fisher Scientific, San Jose, CA*

MP 059 **Analytical Validation of a Data-Independent Acquisition Mass Spectrometry Workflow for Quantification and Identification of Myofilament Proteoforms in Cardiac Biopsies**; Irene van den Broek[1]; Irina Tchernyshyov[1]; Vidya Venkatraman[1]; Giulio Agnetti[2, 3]; Amol Prakash[4]; Scott Peterman[5]; Jennifer E Van Eyk[1]; *[1]Advanced Clinical Biosystems Research Institute, Heart Institute, Cedars Sinai Medical Center, Los Angeles, CA; [2]Division of Cardiology. Johns Hopkins University School of Medicine, Baltimore, MD; [3]Department of Biomedical and Neuromotor Sciences, University of Bologna, Bologna, Italy; [4]Optys Tech Corporation, Brighton, MA; [5]Thermo Fisher Scientific, Cambridge, MA*

MP 060 **Computational Workflows to Improve DIA Data Analysis Without Reference Libraries for Quantitative Proteomics and PTM Analysis**; Jesse Gerard Meyer[1]; Birgit Schilling[1]; Samir Softic[2]; C. Ronald Kahn[2]; Bradford W Gibson[1]; *[1]Buck Institute for Research on Aging, Novato, CA; [2]Joslin Diabetes Center and Harvard Medical School, Boston, MA*

MP 061 **Evaluation of the Efficacy of Data-Independent Acquisition Using Hyper Reaction Monitoring in Quantitative Proteome Profiling of Diverse Species**; Jing Wang[1]; Jeong-Jin Park[1]; David R Gang[1]; *[1]Washington State University, Pullman, WA*

MP 062 **Data Independent Infrared Multiphoton Dissociation for Selective Identification of Cysteine Oxidized Peptides**; Nicholas Borotto[1]; Phillip McClory[1]; Jaimeen Majmudar[1]; Brent Martin[1]; Kristina Hakansson[1]; *[1]University of Michigan, Ann Arbor, MI*

MP 063 **Effect of Peptide Assay Library Size and Composition in Targeted Data Independent Acquisition-Mass Spectrometry Analyses**; Vidya Venkatraman[1]; Sarah Parker[1]; Jennifer E Van Eyk[1]; *[1]Advanced Clinical Biosystems Research Institute, Los Angeles, CA*

MP 064 **Spectral Library with High Confident PTM Site Localization for Phosphoproteome DIA Analysis**; Wei Zhang[1]; Yue Zhou[1]; Jing Li[1]; *[1]Thermo Fisher Scientific (China), Shanghai, China*

MP 065 **Triple Quad Two-Dimensional Scanning: A Novel Scan Approach to Highlight Relationships and Couplings between Unknowns in Complex Mixtures**; Cassandra L. Smith[1]; Vincent S. Pagnotti[2]; *[1]PPG Industries, Allsion Park, PA; [2]PPG Industries, Allison Park, PA*

MP 066 **A Case for Generating Organized and Comprehensive Digital Chromatogram Archives of Every Peptide Quantified in Large-Scale DIA Proteomics**; Michael R Heaven[1]; Archie L Cobbs[1]; Harsha P Gunawardena[2]; Adam J Funk[3]; Michael J Ford[4]; Scott A Shaffer[5]; Jeremy L Norris[6]; *[1]Vulcan Analytical, Birmingham, USA; [2]University of North Carolina, Chapel Hill, NC; [3]University of Cincinnati, Cincinnati, Ohio; [4]MS Bioworks, LLC Ann Arbor, MI; [5]University of Massachusetts Medical School, Worcester, MA; [6]Vanderbilt University, Nashville, TN*

MP 067 **Unraveling the Proteome of Differentiating Human Embryonic Stem Cells Using HDMSEDIA MS**; Elisabeth Govaert[1]; Katleen Van Steendam[1]; Maarten Dhaenens[1]; Liesbeth Vossaert[1]; Dieter Deforce[1]; *[1]Ghent University, Laboratory of Pharmaceutical Biotechnology, Ghent, Belgium*

MP 068 **Analysis of Phorphorylation Site and Occupancy Using Data Independent Acquisition with Electron Transfer Dissociation Mass Spectrometry**; Chein-Hung Chen[1]; Ya-Ping Lin[2]; Chia-Lin Wu[2]; Jung-Lee Lin[2]; Chung-Hsuan Chen[2]; *[1]Academia Sinica, Taipei, Taiwan; [2]Genomics Research Center, Academia Sinica Taipei, Taiwan*

MP 069 **Using 2-Dimensional Mass Spectrometry (2DMS) for Proteomics**; Peter B. O'Connor[1]; Maria van Agthoven[2]; Pui Yiu Lam[2]; Federico Floris[3]; Alice Lynch[3]; Marc-André Delsuc[4]; *[1]University of Warwick, Coventry, West Midlands; [2]University of Warwick, Coventry, UK; [3]University of Warwick, Covenrtry, UK; [4]University of Strasbourg, Strasbourg, France*

MP 070 **Improvements in LFQ for Reproducible Quantification of Proteomic Experiments: How DDA Outperforms DIA**; Andreas Huhmer[1]; Ignacio Ortea[2]; Michael Blank[1]; Daniel Lopez-Ferrer[1]; Romain Huguet[1]; David Horn[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]IMIBIC, Cordoba, Spain*

DIAGNOSTIC CLINICAL CHEMISTRY (APPLICATIONS) 071 - 094

MP 071 **Mass Spectrometric Identification and Clarification of the in Vesica Formation of the Diuretic Chlorazanil in Sports Drug Testing Samples**; Mario Thevis[1]; Hans Geyer[2]; Andreas Thomas[2]; Laura Tretzel[2]; Isabelle Bailloux[3]; Corrine Buisson[3]; Markus Kellmann[4]; Catharina Crone[4]; Thomas Moehring[4]; Wilhelm Schänzer[2]; *[1]German Sport University, Cologne, NRW; [2]German Sport University, Cologne, DE; [3]Agence Francaise de Lutte contre le Dopage, Chatenay-Malabry, France; [4]Thermo Fisher Scientific, Bremen, DE*

MP 072 **Development of a Sensitive and Specific LC-MS/MS Method for Rapid Diagnosis of Niemann-Pick C Disease**; Rohini Sidhu[1]; Xuntian Jiang[2]; Sarah Gale[3]; David Scherrer[3]; Jean Schaffer[3]; Daniel Ory[3]; *[1]Washington University in Saint Louis, Saint Louis , MO; [2]Washington University in St. Louis, saint louis, MO; [3]Washington University in St. Louis, St. Louis, MO*

MP 073 **A UHPLC-MS/MS Method for the Simultaneous Quantification of 10 Antihypertensive Drugs in Human Plasma**; Amedeo De Nicolò[1]; Marco Simiele[1]; Gabriele Bonifacio[1]; Valeria Avataneo[1]; Paolo Mulatero[2]; Franco Rabbia[2]; Franco Veglio[2]; Giovanni Di Perri[1]; Antonio D'Avolio[1]; *[1]Laboratory of Clinical Pharmacology and Pharmacogenetic, Unit of Infectious Diseases, University of Turin, Department of Medical Sciences, Amedeo di Savoia Hospital, Turin, Italy; [2]Unit of Internal Medicine, University of Turin, Department of Medical Sciences, "Città della Salute e della Scienza", Turin, Italy*

MP 074 **Multiplexed Enzymatic Assay for New-Born Screening of Mucopolysaccharidoses(type II, IIIB, IVA, VI, VII) and Neuronal Ceroid Lipofuscinosis II**; Yang Liu[1]; Zdenek Spacil[2]; Hsuan-Chieh Liao[1]; Martin Sadilek[1]; Michael Gelb[1]; Ronald Scott[3]; Frantisek Turecek[1]; *[1]University of Washington, Seattle, WA; [2]Masaryk University,Research Centre for Toxic Compounds in the Environment, Brno, Czech Republic; [3]University of Washington, Department of Pediatrics, Seattle, WA*

MP 075 **Early release of 1-pyrroline by *Pseudomonas aeruginosa* Cultures Discovered Using Ambient Corona Discharge Ionization Mass Spectrometry**; Juchao Liang[1]; Konstantin Chingin[1]; Longhua Hu[2]; Yaping Hang[2]; Huanwen Chen[3]; *[1]East China Institute of Technology, Nanchang, China; [2]The Second Affiliated Hospital of Nanchang University, Nanchang, China; [3]East China University of Technology, Nanchang, Mainland*

MP 076 **Skin Transplant Quality Assessment by Multiplexed 2D MRM Mass Spectrometry – A Step Forward to Improve Clinical Success Rates**; Jingzhi Yang[1]; Juncong Yang[2]; Andrew Percy[2]; Uwe vonFritschen[3]; Juliane C. Finke[3]; Christoph H. Borchers[2, 4]; Michael O. Glocker[5]; *[1]Proteome Center Rostock, Rostock, Germany; [2]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [3]HELIOS Clinic Emil von Behring, Berlin, Germany; [4]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada; [5]Proteome Center Rostock, Rostock , Germany*

MP 077 **Quantitative Clinical Chemistry Proteomics Applied to Apolipoproteins A-I / B / C-I / C-II / C-III / E in Serum**; Yuri EM van der Burgt[1]; Renee Ruhaak[1]; Nico PM Smit[1]; Fred PHTM Romijn[1]; Arnoud van der Laarse[1]; Christa M Cobbaert[1]; *[1]Leiden University Medical Center (LUMC), Leiden, The Netherlands*

MP 078 **Characterizing Traumatic Brain Injury with New Astroglial Injury Biomarkers Measured by Targeted Mass Spectrometry**; Shen Sean[1]; Julia Halford[1]; Ina-Beate Wanner[1]; Joseph A. Loo[1]; *[1]UCLA, Los Angeles, CA*

MP 079 **High-Sensitivity, High-Throughput Quantitation of Catecholamine Metabolites in Urine by LC/MS/MS for Clinical Research**; Atsuhiko Toyama[1]; Kumie Satou[2]; Yuki Nakamura[2]; Ichiro Hirano[1]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]LSI Medience Corporation, Tokyo, Japan*

MP 080 **High-Sensitivity, High-Throughput Quantitation of Catecholamines and Metanephrine in Plasma by Automated WCX-SPE Coupled to LC/MS/MS for Clinical Research**; Ichiro Hirano[1]; Atsuhiko Toyama[1]; Kumie Satou[2]; Yuki Nakamura[2]; Jun Watanabe[1]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]LSI Medience Corporation, Tokyo, Japan*

MP 081 **LC/MS/MS Determination of Plasma Catecholamine Metabolites Without Requiring Solid-Phase Extraction or Sample Dry-Up for Clinical Research**; Yusuke Inohana[1]; Atsuhiko Toyama[1]; Ichiro Hirano[1]; *[1]Shimadzu Corporation, Kyoto, Japan*

MP 082 **Discovery and Targeted Proteomics on Cutaneous Biopsies Infected by Borrelia for the Diagnosis of Lyme Disease.**; Benoit Westermann[1]; Antoine Grillon[2]; Gilles Schnell[1]; Benoit Jaulhac[2]; Nathalie Boulanger[2]; Laurence Ehret-Sabatier[1]; *[1]Laboratoire de Spectrométrie de Masse BioOrganique, Institut Pluridisciplinaire Hubert Curien (UMR 7178), CNRS-Université de Strasbourg, Strasbourg, France; [2]EA7290, Virulence bactérienne précoce, groupe Borréliose de Lyme, facultés de médecine et de pharmacie, Université de Strasbourg, Strasbourg, France*

MP 083 **Increased Levels of Serum Protein Complexes are Associated with Type 2 Diabetes**; Yujie Liu[1]; Bingchaoi Chen[2]; Yanmin Wang[2]; Mo Zhang[1]; Zhili Li[3]; *[1]Institute of Basic Medical Sciences, CAMS &PUMC, Bejing, CN; [2]Heze Municipal Hospital, Heze, CN; [3]IBMS, CAMS&PUMC, Beijing*

MP 084 **A Quantitative Assay for Serum Albumin and Creatinine in Urine Based on MALDI-TOF MS**; Stephen J. Hattan[1]; Marvin Vestal[2]; Kenneth C Parker[2]; Mark Duncan[3, 4]; Jane Yang[5]; David Herold[6]; *[1]Virgin Instruments/ SIMULTOF, Marlborough , MA; [2]Virgin Instruments/ SIMULTOF, Marlborough, MA; [3]University of Colorado, Boulder, Colorado; [4]University of Colorado School of Medicine, Aurora, CO; [5]University of California San Diego, La Jolla, CA; [6]University of California, San Diego La Jolla, CA*

MP 085 **Microorganism Identification/Classification by High Resolution Tandem Mass Spectrometry with Accurate Statistical Significance**; Gelio Alves[1]; Guanghui Wang[2]; Aleksey Ogurtsov[1]; Steven Drake[3]; Marjan Gucek[2]; Anthony Suffredini[3]; David Sacks[4]; YI-KUO YU[1]; *[1]National Center for Biotechnology Information, NLM, NIH, Bethesda, MD; [2]Proteomics Core, NHLBI, NIH, Bethesda, MD; [3]Critical Care Medicine Department, Clinical Center, NIH, Bethesda, MD; [4]Department of Laboratory Medicine, Clinical Center, NIH, Bethesda, MD*

MP 086 **Urinalysis of Opiates Using a Small Benchtop Instrument Combining Microfluidic Capillary Electrophoresis-ESI with High Pressure Mass Spectrometry**; Michael P Goodwin[1]; Scott Mellors[1]; Christopher D Brown[1]; *[1]908 Devices Inc., Boston, MA*

MP 087 **Rapid, Simultaneous Analysis of Urinary Monoamine Neurotransmitters and their Metabolites by UPLC-MS/MS**; Zhengzhi Xie[1]; Sanjay Srivastava[1]; Pawel Lorkiewicz[1]; *[1]University of Louisville, Louisville, KY*

MP 088 **Screening and Quantitation of Pain and Antidepressant Drugs in Human Urine by Liquid Chromatography-High Resolution Mass Spectrometry**; Ana Celia Grenier[1]; Lawrence Joseph Andrade[1]; *[1]Dominion Diagnostics, North Kingstown, RI*

MP 089 **LC-MS Method for Quantitation of HbA1c in the Presence of the Most Common Hemoglobin Variants (S, C, D, and E)**; Shawn Connolly[1]; Kuanysh Kabytaev[1]; Curt Rohlfing[1]; Randie Little[1]; *[1]Department of Pathology & Anatomical Sciences University of Missouri Columbia, Columbia, MO*

MP 090 **Development of a High-Throughput Hemoglobinopathies Workflow Using High Resolution Accurate Mass Analysis**; Scott Peterman; *Thermo Fisher Scientific, Grimes, IA*

MP 091 **Functionalized Surfaces for Direct Immuno-Affinity Mass Spectrometry - Detection of Haptoglobin Phenotypes**; Petr Pompach[1, 2, 3]; Jana Novakova[1]; Daniel Kavan[1, 2]; Oldrich Benada[1]; Viktor Ruzicka[4]; Michael Volny[3]; Petr Novak[1, 2, 3]; *[1]Institute of Microbiology, Prague, Czech Republic; [2]Faculty of Science, Charles University in Prague, Prague, Czech Republic; [3]AffiPro, Mratin, Czech Republic; [4]BioVendor, Brno, Czech Republic*

MP 092 **Identifying Vitamin D2 and D3, Their 25-OH Metabolites, and C3 Epimers in a Single LCMS Run**; Ken Tseng[1]; Toshi Ono[2]; Tsunehisa Hirose[3]; *[1]Nacalai USA Inc., San Diego, CA; [2]Nacalai USA Inc., San Diego, CA - California; [3]Nacalai Tesque Inc., Kyoto, Japan*

MP 093 **A Simple and Effective LC/MS/MS Method Development for the Determination of Underivatized Vitamin B1 and B6 in Human Whole Blood**; Xianrong (Jenny) Wei[1]; Sean Orlowicz[2]; *[1]Phenomenex, Torrance, ca; [2]Phenomenex, Torrance, CA*

MP 094 **Speciation of Fatty Acids in Human Serum by Gas Chromatography/Mass Spectrometry**; Bruce A. Benner[1]; Benjamin J Place[1]; Jacolin A Murray[1]; *[1]NIST, Gaithersburg, MD*

DRUG AND METABOLITE ANALYSIS: NOVEL APPROACHES FOR DRIED BIOLOGICAL SAMPLES
095 - 103

MP 095 **Insights on Microsampling Implementation in Drug Discovery: Sample Collection, Matrix Effect, Recovery, Aging and Automation's Assessment for an Emerging Technology**; Graziella Bovi[1]; Silvana Olivieri[1]; Giuseppe Santo[1]; Mariangela Corradin[1]; James Rudge[2]; Fabio Garofolo[1]; Serena Tongiani[1]; *[1]Angelini Research Center, Pomezia (Rome), Italy; [2]Neoteryx, Torrance, CA*

MP 096 **A New Microsampling Hematocrit-Compatible Dried Plasma Card for Fully Automated Online DBSA-SPE-LC-MS/MS Bioanalysis of Opioids in Blood**; Imelda Ryona[1]; Jack Henion[1]; *[1]Q2 Solutions, Ithaca, NY*

MP 097 **Bioanalysis of Emixustat (ACU-4429) in Whole Blood Collected with Volumetric Absorptive Microsampling by LC–MS/MS**; Zhixin Miao[1]; James G Farnham[1]; Glenn Hanson[1]; Terry Podoll[2]; Michael J. Reid[2]; *[1]Covance, Madison, WI; [2]Acucela, Bothell, WA*

MP 098 **Improving Transplant Patient's Welfare; Standardising and Advancing the Therapeutic Drug Monitoring of the Immunosuppressant Drug Tacrolimus**; Dima AlMekdad[1, 2]; Mark Christian Parkin[3]; Chris Mussell[2]; *[1]King's College London, London, UK; [2]LGC, Teddington, UK; [3]King's College London, London, United Kingdom*

MP 099 **Development and Validation of an UHPLC-MS/MS Method to Quantify Imatinib, Desmethylimatinib, Dasatinib, Nilotinib and Ponatinib in Dried Plasma Spots**; Alessandra Ariaudo[1]; Simiele Marco[1]; Fabio Favata[1]; Luca Paglietti[1]; Silvia De Francia[2]; Giovanni Di Perri[1]; Antonio D'Avolio[1]; *[1]Laboratory of Clinical Pharmacology and Pharmacogenetics. Department of Medical Sciences, University of Turin, Amedeo di Savoia Hospital, Turin, Italy, Torino, Italy; [2]Laboratory of Clinical Pharmacology. Department of Clinical and Biological Sciences, University of Turin, San Luigi Hospital, Orbassano (Turin), Italy, Orbassano, Italy*

MP 100 **Evaluation of Blood Fractionation Membranes for the Analysis of Dried Plasma Spots from Whole Blood Using Paper Spray Mass Spectrometry**; Brandon Bills[1]; Nicholas E Manicke[1]; *[1]IUPUI Department of Chemistry & Chemical Biology, Indianapolis, IN*

MP 101 **Method Development Considerations for Paper-Spray Mass Spectrometry - Direct Ionization Technique for Physiological Fluid Analysis**; Maria C. Prieto CONAWAY[1]; Jeff Patrick[2]; Joseph Kennedy[2]; Kristine Van Natta[3]; Marta Kozak[3]; *[1]Thermo Fisher Scientific, San Jose , CA; [2]Prosolia, Inc. Indianapolis, IN; [3]Thermo Fisher Scientific, San Jose, CA*

MP 102 **Ambient Mass Spectrometric Analysis of Herbal Medicines with Flowing Atmospheric-Pressure Afterglow**; Xinyue Liang[1]; Xiaoxia Gong[1]; Songyue Shi[1]; Mohammad Choudhury[1]; Gerardo Gamez[1]; *[1]Texas Tech University, Lubbock, TX*

MP 103 **Evaluation of Protein Stability in Dried Plasma Spots Using Targeted and Untargeted Mass Spectrometry Techniques**; Victoria David[1]; Kristine Tsantilas[1]; Matthew Rosenow[1]; Marissa Saltzman[1]; Lizzi Neylon[2]; David Carpentieri[2]; Konstantinos Petritis[2]; Patrick Pirrotte[1]; *[1]Translational Genomics Research Institute, Phoenix, AZ; [2]Phoenix Children's Hospital, Phoenix, AZ*

ENERGY: HYDROCARBON AND PETROCHEMICAL (ULTRA HI RES)
104 - 122

MP 104 **Understanding the Oxygenation Mechanism of Hydrocarbons in the Ocean Utilizing SA-TIMS-FT-ICR MS**; Paolo Benigni[1]; Rebecca Marin[1]; Kathia Sandoval[1]; Christopher J Thompson[2]; Mark E Ridgeway[2]; Melvin Park[2]; Piero Gardinali[1]; Francisco Fernandez-Lima[1]; *[1]Florida International University, Miami, FL; [2]Bruker Daltonic, Billerica, MA*

MP 105 **Unsupervised Chemical Structure Assignment Based on SA-TIMS-FTICR MS Mass and Mobility Measurements for Oxygenation Products of Hydrocarbons in the Ocean**; Rebecca Marin[1]; Paolo Benigni[1]; Francisco Fernandez-Lima[1]; Christopher Thompson[2]; Mark E Ridgeway[2]; Melvin Park[2]; *[1]Florida International University, Miami, FL; [2]Bruker Daltonic, Billerica, MA*

MP 106 **Ionization of Paraffin Samples With/Without Solvents and Analysis Using Fourier Transform Ion Cyclotron Resonance Mass Spectrometry**; Izaak Tyson-Hirst[1]; Mark P. Barrow[1]; *[1]University of Warwick, Coventry, United Kingdom*

MP 107 **Structural Elucidation of N-Containing Compounds in Crude Oil Using Positive Ion ESI FT-ICR MS/MS**; Ammar Nasif[1]; Christianne Wicking[2]; Mike Hodges[3]; John Couves[3]; Huang Zeng[4]; John G Langley[1]; *[1]Chemistry, University of Southampton, Southampton, UK; [2]BP Pangbourne Technology Centre, Pangbourne, UK; [3]BP Sunbury ICBT, Sunbury, UK; [4]BP Houston, Houston, TX*

MP 108 **Asphaltenes Generated from Low-temperature Cracking of Type II Kerogen: Molecular Characterization by Negative ESI-FT-ICR-MS and Kinetic Parameters**; Albert Kamga[1]; Patrick G Hatcher[2]; Francoise Behar[3]; Francois Baudin[4]; *[1]ODU Research Foundation, Norfolk, VA; [2]Old Dominion University, Norfolk, VA; [3]TOTAL Refining and Chemicals, Gonfreville l'Orcher, France; [4]Universite Paris Descartes, Sorbonne Paris Cite Paris, France*

MP 109 **Structural Determination of Nitrogen-Containing Compounds in Petroleum Using Collision Cross Section Calculations (CCS) and Collision-Induced Dissociation (CID)**; Hossein Maleki[1]; Sadegh Faramarzi Ganjabad[1]; Samaneh Ghassabi Kondalaji[1]; Stephen James Valentine[1]; *[1]West Virginia University, Morgantown, WV*

MP 110 **Petroleomic Analysis of Tyre Pyrolysis Oils by Using High-Resolution ESI/APPI FT-ICR Mass Spectrometry**; Janne Janis; *University of Eastern Finland, Joensuu, NA*

MP 111 **Two-Dimensional Matrix Plots for Mapping Genealogical Links in Complex Mixtures of Lignin Degradation Products**; Yulin Qi[1]; Dietrich A Volmer[2]; *[1]Saarland University, Saarbrücken, Saarland; [2]Saarland University, Saarbrücken, Germany*

MP 112 **Adaptation of SARA Fractionation with Emphasis on Resins and Asphaltenes Characterization in Crude Oils with Different API Gravity Using FT-ICRMS**; Jandyson M Santos[1, 2]; Alberto Wisniewski Jr[3]; Marcos N Eberlin[1]; Wolfgang Schrader[2]; *[1]University of Campinas, Campinas, Brazil; [2]Max-Planck Inst für Kohlenforschung., Mülheim / Ruhr, Germany; [3]Federal University of Sergipe, São Cristóvão, SE*

MP 113 **Extrography and Column Chromatography Fractionation as Tools for Increasing Compositional Space Accessibility in HRMS Analysis of Crude Oils**; Deisy Giraldo-Davila[1]; Martha L. Chacon[2]; Marianny Y Combariza[1]; Cristian Blanco-Tirado[1]; Andrea Gomez-Escudero[3]; Jorge A Orrego-Ruiz[3]; *[1]Universidad Industrial de Santander, Bucaramanga, Santander, Colombia; [2]Universidad Industrial de Santander, Bucaramanga, Santander; [3]Ecopetrol, Instituto Colombiano del Petróleo, Piedecuesta, Colombia*

MP 114 **HRMS Analysis of Naphthenic Acids Isolated from Heavy Crude Oils Using Ion Exchange and Solid Phase Extractions**; Jeferson A. Valencia-Dávila[1]; Martha L. Chacón-Patiño[1]; Jorge A. Orrego-Ruiz[2]; Cristian Blanco-Tirado[1]; Marianny Y. Combariza[1]; *[1]Universidad Industrial de Santander, Bucaramanga, Santander, Colombia; [2]Ecopetrol, Instituto Colombiano del Petróleo, Piedecuesta, Colombia*

MP 115 **New Approaches in Petroleomics:Extending the Characterization of Nitrogen in Vacuum Residue via SPE Fractionation and Analysis by ESI FT-ICR MS**; Gessica Vasconcelos[1]; Veronica Vale Carvalho[1]; Carla Santos Freitas[1]; Lilian Valadares Tose[2]; Wanderson Romão[2]; Rosana Cardoso Pereira[3]; Boniek Gontijo Vaz[1]; *[1]Federal University of Goiás, Goiânia, GO; [2]Federal University of Espirito Santo, Vitoria, Brazil; [3]Petrobras, Rio de Janeiro, RJ*

MP 116 **Nitrogen Speciation in Petroleum Distillates Fractionated by SPE Using a Complementary and Powerful Approach by GC×GC-NCD and FT-ICR/MS**; Florian Albrieux[1]; Ludovic Chahen[2]; Lyes Assam[2]; Fabien Chainet[2]; Vincent Souchon[2]; *[1]IFPEN, Solaize, 69360; [2]IFPEn, Solaize, France*

MP 117 **Asphaltene Adsorption, Aggregation and Occlusion from a High-Resolution Mass Spectrometry Point of View**; Martha Liliana Chacon-Patiño[1, 2]; Marianny Yajaira Combariza[1]; Cristian Blanco-Tirado[1]; Andrea Gómez-Escudero[2]; Jorge A Orrego-Ruiz[2]; *[1]Universidad Industrial de Santander, Bucaramanga, Santander, Colombia; [2]Ecopetrol, Instituto Colombiano del Petróleo, Piedecuesta, Colombia*

MP 118 **Petroleum Aromatic Compounds by APPI, FI, and GCEI; a Sensitivity Study**; Michael T. Cheng[1]; Matthew Hurt[1]; *[1]Chevron Research, Richmond, CA*

MP 119 **Coupling of APCI / CS2 with Collisionally Activated Dissociation of Model Compounds for Structural Determination of Asphaltenes in Crude Oil**; Mark Romanczyk[1]; Xueming Dong[1]; Hilkka Kenttämaa[2]; *[1]Purdue University, West Lafayette, IN; [2]Purdue University, West Lafayatte, IN*

MP 120 **High-field FT Orbitrap MS as a Competitive Alternative for the Analysis of Complex Mixtures**; Alessandro Vetere[1]; Wolfgang Schrader[1]; *[1]Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany*

MP 121 **High-Field FT Orbitrap Mass Spectrometric Investigation on Photooxidation Processes of Crude Oil**; Ruoji Luo[1]; Wolfgang Schrader[1]; *[1]Max-Planck Inst für Kohlenforschung., Mülheim / Ruhr, Germany*

MP 122 **Kendrick Mass Defect Visualization of Asphaltenes Pre- and Post-Reaction with Bromine**; Michael Spiegel[1]; Ian Anthony[1]; Matthew Brantley[1]; Alton Hassell[1]; Claire Moffett[1]; Subin Yoon[1]; Marie Stephensen[1]; Patrick Farmer[1]; Touradj Solouki[1]; *[1]Baylor University, Waco, TX*

ENVIRONMENTAL ANALYSIS: GENERAL (PART 1) 123 – 147

MP 123 **Determination of Nitro Polycyclic Aromatic Hydrocarbons in PM2.5 Using GC-MS/MS**; Sun Qian[1]; Fan Jun[2]; Deng XiaoLi[3]; Li Yueqi[4]; Yang Guixiang[5]; Huang Taohong[2]; Yuki Hashi[2]; *[1]Shimadzu (China) Co., Ltd., Shanghai, shanghai; [2]Shimadzu (China) Co., Ltd., Shanghai, China; [3]Shimadzu (China) Co., Ltd, Shanghai, China; [4]Shimadzu (China) Co., Ltd, Beijing, China; [5]Shimadzu (China) Co., Ltd., Beijing, China*

MP 124 **Detection of Picogram or Sub-Picogram Semi-Volatile Compounds by Full Scan GCMS Using a High Efficiency Source – A Game Changer?** ; Dale Walker[1]; Harry Prest[2]; *[1]Agilent Technologies, Little Falls, DE; [2]Agilent Technologies, Santa Clara, CA*

MP 125 **Lewisite and VX Degradation By-Product Method Development for Environmental Remediation by Liquid Chromatography/Tandem Mass Spectrometry**; Stuart Willison[1]; Carolyn Koester[2]; Deon Anex[2]; Romy Campisano[3]; Terry O'Neill[4]; Sandip Chattopadhyay[5]; Matthew Magnuson[3]; *[1]EPA/NHSRC, Cincinnati, OH; [2]Lawrence Livermore National Laboratory, Livermore, CA - California; [3]U.S. Environmental Protection Agency, Cincinnati, Ohio; [4]MRIGlobal, Kansas CIty, Missouri; [5]TetraTech, Cincinnati, OH*

MP 126 **Atmospheric Contaminant Source Identification Using Chemometric Approaches with Mobile Membrane Introduction Mass Spectrometry (MIMS)**; Larissa C. Richards[1, 2]; Nicholas G Davey[1, 2]; Erik T Krogh[1, 2, 3]; Christopher G. Gill[4]; *[1]Appl. Env. Res. Labs. (AERL), Nanaimo BC, Canada; [2]University of Victoria, Victoria BC, Canada; [3]Vancouver Island University, Nanaimo BC, Canada; [4]Appl. Env. Res. Labs. (AERL), Nanaimo , BC*

MP 127 ***In vivo* Real-time Monitoring of Aphrodisiac Pheromone Release of Small White Cabbage Butterflies (Pieris rapae)**; Yue Li[1]; Robert A Mathews[2]; *[1]The University of Maryland, College Park, MD; [2]Department of Entomology, Smithsonian Institution, National Museum of Natural History, Washington, D.C*

MP 128 **Molecular Identification of Natural Organic Matter Interactions with Mercury by Ultrahigh Resolution Mass Spectrometry**; Hongmei Chen[1]; Benjamin F Mann[1]; Rosalie K Chu[2]; Nikola Tolic[2]; Baohua Gu[1]; *[1]Oak Ridge National Laboratory, Oak Ridge, TN; [2]Environmental Molecular Sciences Laboratory, PNNL Richland, WA*

MP 129 **Quantification of 1-Hydroxypyrene in Undiluted Human Urine Samples Using Magnetic Solid-Phase Extraction Coupled with Internal Extractive Electrospray Ionization Mass Spectrometry**; Hua Zhang[1]; Haiyan Lu[1]; Xiaowei Fang[1]; Bi-Feng Yuan[2]; Yu-Qi Feng[2]; Huanwen Chen[3]; *[1]East China Institute of Technology, Nanchang, China; [2]Key Laboratory of Analytical Chemistry for Biology and Medicine (Ministry of Education), Department of Chemistry, Wuhan University, Wuhan, China; [3]East China University of Technology, Nanchang, Mainland*

MP 130 **High Throughput Detection and Identification of Chemical Excursions via GC-MS**; Parminder Kaur[1]; Corey Stedwell[1]; Daniel DeBord[1]; *[1]1st Detect Corporation, Webster, TX*

MP 131 **That's the Law : Tracking Down Trace Levels of HBCD Isomers in Recycled Polystyrene**; Claude-Paul LaFrance[1]; Maxim Maheux[2]; *[1]TransBIOTech, Levis, QC; [2]TransBIOTech, Levis, Canada*

MP 132 **Quantification of Twelve Polyfluoroalkyl Chemicals in Human Urine**; Kayoko Kato[1]; Janice Ma[1]; Antonia M. Calafat[1]; Xiaoyun Ye[1]; *[1]CDC, Atlanta, GA*

MP 133 **Quantification of Triazole Biocides in Treated Wood Using Solid-Phase Extraction Coupled with Liquid Chromatography – Electrospray High Resolution Mass Spectrometry**; Klára Ondrušová[1]; Brianna Gysbers[1]; Alena Kubátová[1]; *[1]University of North Dakota, Department of Chemistry, Grand Forks*

MP 134 **Tandem GC/MS Analysis of sub-pg/µL Quantities of PBDEs, Including BDE-209 Using the Novel High Efficiency EI Source** ; Stephan Baumann; *Agilent Technologies, Inc., Alpharetta, GA*

MP 135 **Accurate Mass Analysis of Naphthenic Acids by Ammonia NCI**; Matthew Curtis[1]; Stephan Baumann[1]; Mark Hewitt[2]; Richard Frank[2]; Dayue Shang[3]; Marcus Kim[1]; *[1]Agilent Technologies, Santa Clara, CA; [2]Environment Canada, Burlington, Canada; [3]Environment Canada, North Vancouver, BC*

MP 136 **Method optimization for Rapid Analysis of Brominated Flame Retardants in Polymers: with DART-Orbitrap HRAM**; Antonella Guzzonato[1]; Olaf Scheibner[2]; Tabiwang Arrey[3]; Thomas Moehring[3]; Stuart Harrad[4]; *[1]University of Birmingham, Bremen, Bremen, Bremen; [2]Thermo Fisher Scientific, Dreieich, Germany; [3]Thermo Fisher Scientific, Bremen, DE; [4]University of Birmingham, Birmingham, United Kingdom*

MP 137 **SIFT-MS: A Complete Real-Time Solution for Analysis of Ambient Air**; Daniel B Milligan[1]; David Hera[1]; Thomas G Hughes[1, 2]; Nic Lamont[1, 2]; Vaughan S Langford[1]; Murray J McEwan[1, 3]; Thomas I McKellar[1]; *[1]Syft Technologies Ltd, Christchurch, New Zealand; [2]University of Canterbury, Christchurch, New Zealand; [3]University of Canterbury, Christchurch, Canterbury*

MP 138 **Determination of Trace Concentrations of Carboxylic Acids and Aldehydes in Wood Smoke Particulate Matter**; Jana Rousova; *University of North Dakota, Grand Forks, North Dakota*

MP 139 **Chlorinated Dioxins, Furans and Biphenyls Analysis in Complex Matrices Using Automated Extraction and Reduced Solvent Volume Column Chromatography**; Rudolf Addink[1]; Philip Bassignani[1]; *[1]Toxic Report, Watertown, MA*

MP 140 **Automated Pressurized Liquid Extraction and Sample Clean Up of River Sediment in POPs Analysis**; Sevag Pelanjian[1]; Rudolf Addink[1]; *[1]Toxic Report, Watertown, MA*

MP 141 **Characterization of Trihalomethanes in Meat Processing Plant Effluent**; Tiffany Liden[1]; Doug D. Carlton[2]; Kevin A Schug[2]; *[1]University of Texas at Arlington, Arlington, TX - Texas; [2]University of Texas at Arlington, Arlington, TX*

MP 142 **Method Development for the Identification of Novel Brominated Flame Retardants Using a Q Exactive HRAM Mass Spectrometer**; Aristide P Ganci[1]; Tabiwang N. Arrey[2]; Thomas Moehring[2]; Stuart Harrad[1]; *[1]University of Birmingham, Birmingham, United Kingdom; [2]Thermo Fisher Scientific (GmbH), Bremen, Germany*

MP 143 **Population Assessment of Perfluoroalkyl Acids (PFAAs) in the Plasma of Wild American Alligators at Kennedy Space Center, FL**; Jacqueline T Bangma[1]; John A Bowden[2]; Jessica Reiner[2]; Russell H Lowers[3]; Matthew P Guillette[1]; Louis J Guilletter Jr.[1]; *[1]Medical University of South Carolina, Charleston, SC; [2]NIST, Charleston, SC; [3]Integrated Mission Support Service, Titusville, FL*

MP 144 **Reducing and Normalizing Matrix Effects for the Quantification of BTEX in Contaminated Soils using Ionic Liquids in HS-GC/MS**; Emmanuel Varona-Torres[1]; Michelle Reyes[1]; Doug D Carlton Jr.[1, 2]; Kevin A Schug[1, 2]; *[1]University of Texas at Arlington, Arlington, TX; [2]Collaborative Laboratories for Environmental Analysis and Remediation, The University of Texas at Arlington, Arlington, TX*

MP 145 **Ultra Low-Level Detection of Perfluoroalkyl Sustances (PFASs) using LC MS/MS**; Sarah Dowd[1]; Lauren Mullin[2]; Jennifer A Burgess[2]; *[1]Waters Corporation, Beverly, MA; [2]Waters Corporation, Milford, MA*

MP 146 **Creation of Accurate Mass Library with GC/MS Quadrupole Data and Its Application to Higher Confidence Unknown Identification**; Ming Gu[1]; Yongdong Wang[1]; *[1]Cerno Bioscience, Norwalk, CT*

MP 147 **GC-MS/MS Determination of Synthetic Musks in Human Serum**; Ivana Kosarac[1]; Cariton Kubwabo[1]; Guru Prasad Katuri[1]; *[1]Exposure and Biomonitoring Div, Health Canada, Ottawa, ON*

ENVIRONMENTAL ANALYSIS: PHARMACEUTICALS AND PESTICIDES
148 - 176

MP 148 **Mass Spectrometric Evidence of the Carbanion Reaction Intermediate in Chlordecone Environmental Decomposition**; Andrei Starostine[1]; L Lomheim[2]; S. Gaspard[3]; E. Edwards[2]; *[1]University of Toronto, Toronto, ON; [2]University of Toronto, Toronto, Canada; [3]Universite des Antilles et de la Guyane, Pointe-a-Pitre, Guadeloupe, French West Indies*

MP 149 **Analysis of Halogenated Environmental Contaminants in Food Products by Plasma-Assisted Reaction Chemical Ionization (PARCI)**; Paolo Lecchi[1]; Yao Lu[1]; Kunyu Zheng[2]; Peter Haferl[2]; Kaveh Jorabchi[2]; *[1]DSM Nutritional Products, Columbia, MD; [2]Dept of Chemistry, Georgetown University, Washington, DC*

MP 150 **UHPLC-Liquid-EI-MS/MS Interface: A New Frontier of Multiclass Environmental Risk Factors Assessment in Sudden Infant Death Syndromes**; Veronica Termopoli[1]; Giorgio Famiglini[1]; Pierangela Palma[1]; Achille Cappiello[1]; *[1]University of Urbino, Urbino, Italy*

MP 151 **Fast and Robust 210 Multi-Residue Pesticide Screening of Five Washed and Unwashed Non-Organic Berries by LC-MS/MS with Simple QuEChERS Preparation**; Joshua Ye[1]; Frank Kero[2]; Craig Young[2]; Sharanya Reddy[2]; *[1]ionics Mass Spectrometry GRO, Bolton , ON; [2]PerkinElmer, Shelton, CT*

MP 152 **A Highly Specific and Robust Multi-residue Analysis of Pesticides in Water Using Time of flight in All Ion Acquisition Mode.**; Padma Marwah[1]; Ashok Marwah[2]; Sue D'antonio[3]; Paul Zimba[1]; *[1]Texas A&M University, Corpus Christi, TX; [2]Self, Corpus Christi, TX; [3]Agilent technologies Inc, Cedar Creek, TX*

MP 153 **Multiplexed Analysis of 215 Pesticides Using Scout-MRM**; Romain Carriere[1]; Blandine Rougemont[1]; Christelle Margoum[2]; Mathieu Le Dréau[2]; David Cox[3]; Yves J C LeBlanc[3]; Jerome Lemoine[1]; *[1]Institut des Sciences Analytiques, UMR 5280 CNRS, Université de Lyon, Villeurbanne, France; [2]IRSTEA, Villeurbanne, France; [3]SCIEX, Concord, ON*

MP 154 **Automated Multi Residue Pesticides Analysis Using Pressurized Liquid Extraction and Gel Permeation Chromatography**; Philip Bassignani[1]; Ruud Addink[1]; *[1]Fluid Management Systems, Watertown, MA*

MP 155 **Target and Not-target Screening of Pesticides and Metabolites in Paddy Water**; Eleonora Mazzucco[1]; Fabio Gosetti[2]; Bianca Bolfi[2]; Marcello Manfredi[3]; Arianna Facchi[4]; Marco Romani[5]; Simone Silvestri[5]; Elisa Robotti[2]; Emilio Marengo[2]; *[1]università Del Piemonte Orientale, Alessandria, Alessandria; [2]University of Piemonte Orientale, Alessandria, IT; [3]ISALIT-DISIT, University of Piemonte Orientale, Alessandria, IT; [4]Dipartimento di Scienze Agrarie e Ambientali, Università degli Studi di Milano, Milano, IT; [5]Ente Nazionale Risi, Pavia, IT*

MP 156 **Rapid and Easy Comparison of Quechers Sample Preparation Methods for the Analysis of Pesticide Residues In Pear Using LC-ESI-QQQ**; Victor Manuel Mondragon Olguin[1]; Jose Luis Freire[1]; *[1]Agilent technologies Inc, Mexico, DF*

MP 157 **Comprehensive, Sensitive, and Quantitative Screening of Pesticides in Selected Swiss Headwater Catchments by an Online-SPE-LC-Orbitrap Method**; Heinz Singer[1]; Rahel Comte[2]; Simon Mangold[2]; Christioph Moschet[2]; Christian Stamm[2]; Tobias Doppler[2]; Irene Wittmer[2]; *[1]Eawag, Duebendorf, CH; [2]Eawag, Duebendorf, Switzerland*

MP 158 **LC-MS/MS Method Development and Validation for the Quantification of LB-100 and Endothall Metabolite in Biological Matrices**; Changyu Quang[1]; Jennifer L. Simko[1]; William C Nethero[1]; Elizabeth A Groeber[1]; John S Kovach[2]; *[1]WIL Research, Ashland, OH; [2]Lixte Biotechnology Holdings, Inc., East setauket, NY*

MP 159 **Ultra-Sensitive and Rapid Assay of Neonicotinoids, Fipronil and Some Metabolites in Honey by UHPLC-MS/MS.**; Mikael Levi[1]; Aurore Jaffuel[1]; Stephane Moreau[2]; *[1]shimadzu France, Noisiel, France; [2]Shimadzu Europe GmbH, Duisburg, Germany*

MP 160 **Parts-per-trillion (ppt) Level High-Throughput Quantitation of Glyphosate, Aminomethylphosponic Acid (AMPA) and Glufosinate in Water Samples by LC-MS/MS**; Javier Lopez[1]; Miguel Angel Perez[1]; Carsten Baessmann[2]; Louis Maljers[3]; Joe Anacleto[4]; *[1]Bruker Espanola, S.A., Madrid, Spain; [2]Bruker Daltonik GmbH, Bremen , -; [3]Bruker, Fremont, CA; [4]Bruker Ltd., Milton, Canada*

MP 161 **Direct Analysis of Formulated Pesticide Product Matrices by Paper Spray Mass Spectrometry**; Khang To[1]; Steven L Reeber[1]; Gary Glish[1]; *[1]University of North Carolina Chapel Hill, Chapel Hill, NC*

MP 162 **Human Biomonitoring for Pesticide Exposure and Effects on Metabolism using Convergence Chromatography-Mass Spectrometry**; Zdenek Spacil[1]; Garry Codling[1]; Petra Booij[1]; Jana Klanova[1]; *[1]Masaryk University, Brno, Czech Republic*

MP 163 **Multiresidue Determination of non-HPLC-ESI-MS-Amenable Organochlorine Pesticides with Liquid Chromatography Dielectric Barrier Discharge Ionization Mass Spectrometry (LC-DBDI-TOFMS)**; José Robles-Molina[1]; Felipe J Lara-Ortega[1]; Bienvenida Gilbert-López[2]; Antonio Molina-Díaz[1]; Juan F Garcia-Reyes [3]; Alexander Schutz[4]; Sebastian Brandt[4]; Joachim Franzke[4]; *[1]University of Jaen, JAEN, ES; [2]CSIC-CIAL, Madrid, ES; [3]University Of Jaen, Jaen , Andalucia; [4]Leibniz-Institut für Analytische Wissenschaften, Dortmund, Germany*

MP 164 **An Unknown Screening Approach to Analyze Micropollutants Degradation by Different Disinfection Processes**; Julia Quilitzki[1]; Patricia van Baar[1]; Uwe Dünnbier[1]; Olaf Scheibner[2]; *[1]Berliner Wasserbetriebe, Berlin, Germany; [2]Thermo Fisher Scientific, Bremen, Germany*

MP 165 **Removal and Transformation of Persistent Emerging Contaminants via Advanced Oxidation Techniques**; Kristin Cochran[1]; Jorge Casado[2]; Susan Richardson[1]; Dionysios Dionysiou[3]; Daniel Schlenk[4]; Gianluca Li Puma[5]; Danilo Russo[6]; Danilo Spasiano[6]; Marianna Vaccaro[6]; Roberto Andreozzi[6]; Nuno Reis[5]; Raffaele Marotta[6]; *[1]University of South Carolina, Columbia, SC; [2]Universal Diagnostics SL, Seville, Spain; [3]University of Cincinnati, Cincinnati, Ohio; [4]University of California, Riverside, Riverside, CA; [5]Loughborough University, Loughborough,*

United Kingdom; [6]University of Naples Federico II, Naples, Italy

MP 166 **Quantitation and Identification of Legal and Illicit Drugs in Wastewater in the Low ng/L Range using Large-Volume Injection and LC-MS/MS**; Paul Winkler[1]; Andre Schreiber[2]; Michael Scherer[3]; *[1]SCIEX, Redwood City, CA; [2]SCIEX, Concord, ON; [3]Sciex Switzerland, Rotkreuz, Switzerland*

MP 167 **Sensitive Screen of Pharmaceuticals and Personal Care Products (PPCPs) in Water Using Agilent 6545 LC/Q-TOF High Resolution Mass Spectrometer**; Dan-Hui Dorothy Yang[1]; Craig Marvin[2]; mark Murphy[3]; Yue Song[4]; Jimmy Chan[4]; *[1]Agilent Technologies, Santa Clara, CA; [2]Agilent Technologies, Wilmington, DE; [3]EPA, Golden, CO; [4]Agilent, Shanghai, China*

MP 168 **Non-Target Screening using Liquid Chromatography Coupled to High Resolution MS/MS (LC-HR-MS/MS) – Identification of Unknown Environmental Pollutants**; Andre Schreiber[1]; KC Hyland[2]; Paul Winkler[2]; *[1]SCIEX, Concord, ON; [2]Sciex, Redwood City, CA*

MP 169 **LCMS-MS Method for Evaluation of PPCPs in Environmental Water**; Katie M Pryor[1]; Jerry Byrne II[1]; Rachel Lieberman[1]; Jeremy Post[1]; Christopher Gilles[1]; *[1]Shimadzu Scientific Instruments, Columbia, MD*

MP 170 **LC–TOF-MS and GC–MS Analysis of Pharmaceuticals and Personal Care Products in Wastewaters of Eastern North Carolina**; Blake Rushing[1]; Ashley Wooten[1]; Marcus Shawky[1]; Mustafa Selim[1]; *[1]East Carolina University, Greenville, NC*

MP 171 **Analysis of Potential Genotoxic Impurities (PGI) in Active Pharmaceutical Ingredients (API) by GCMS/MS**; Prashant Hase[1]; Ankush Bhone[2]; Durvesh Sawant[2]; Dheeraj Handique[2]; Sanket Chiplunkar[2]; Ajit Datar[2]; Jitendra Kelkar[2]; Pratap Rasam[2]; *[1]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, Maharashtra; [2]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India*

MP 172 **Combining Commercial and Open-Source Accurate Mass MS/MS Library Information for Suspect and Non-Target Screening Workflows**; Sascha Lege[1]; Thomas Glauner[2]; Thierry Faye[3]; Craig Marvin[4]; Christian Zwiener[1]; *[1]Eberhard Karls University Tuebingen, Tuebingen, Germany; [2]Agilent Technologies Sales&Services GmbH, Waldbronn, Germany; [3]Agilent Technologies, Paris, France; [4]Agilent Technologies, Wilmington, DE*

MP 173 **Increased Throughput in the Determination of PPCPs in Water Using Optimized MS Cycle Times in a High Sensitivity UHPLC-QQQ System**; Behrooz Zekavat[1]; Thomas Glauner[1]; Craig Marvin[2]; André Santos[1]; Tarun Anumol[2]; Jerry Zweigenbaum[2]; *[1]Agilent Technologies, Santa Clara, CA; [2]Agilent Technologies, Little Falls, DE*

MP 174 **Fates of Known and Unknown Compounds from Full Scale Ozone and Activated Carbon Adsorption Process Using High Resolution MS**; Jaewon Choi[1]; Wonseok Choi[1]; Hyunji Jang[1]; Ilhwan Choi[1]; Yuns Kim[1]; Charles Yang[2]; Dipankar Ghosh[2]; *[1]Kwater, Daejeon, South Korea; [2]Thermo Fisher Scientific, San Jose, CA*

MP 175 **Extraction of Organochlorine Pesticides with In-line Florisil Cleanup using an Acid-Base-Neutral Solid Phase Extraction System**; Phil Germansderfer[1]; Ruud Addink[1]; *[1]Fluid Management Systems, Watertown, MA*

MP 176 **One Step Extraction, Cleanup and Concentration of Chlorinated Pesticides in Raw Coffee Beans**; Rashid Juma[1]; Ruud Addink[1]; *[1]Fluid Management Systems, Watertown, MA*

EPIGENETIC MODIFICATIONS
177 - 194

MP 177 **Improving Quantitative Analysis of Modified DNA Nucleosides by Liquid Chromatography-Triple-Quadrupole Mass Spectrometry**; Nan Dai[1]; Shengxi Guan[2]; Jeremy Foster[2]; Ivan R. Corrêa[2]; *[1]New England Biolabs, Ipswich, MA; [2]New Englanb Biolabs, Ipswich, MA*

MP 178 **Quantitative Histone Mass Spectrometry Identifies Elevated Histone H3 Lysine 27 Trimethylation in Melanoma**; Lauren Davis[1]; Deepanwita Sengupta[1]; Stephanie Byrum[1]; Nathan Avaritt[1]; Bradley Shields[1]; Fade Mahmoud[2]; Matthew Reynolds[1]; Lisa Orr[1]; Samuel Mackintosh[1]; Sara Shalin[3]; Alan Tackett[1]; *[1]Department of Biochemistry and Molecular Biology, University of Arkansas for Medical Science, Little Rock, AR; [2]Department of Hematology Oncology and Internal Medicine, University of Arkansas for Medical Sciences, Little Rock, AR; [3]Department of Pathology, University of Arkansas for Medical Sciences, Little Rock, AR*

MP 179 **Mass Spectrometric Profiling of Histone Proteins and Their Modifications in the Biofuel-Producing Microalgae Chlamydomonas Reinhardtii**; Carlo K Eikani[1]; Aliyya Khan[1]; Anthony T Iavarone[2]; James J Pesavento[1]; *[1]Department of Biology, Saint Mary's College of California, Moraga, CA; [2]QB3/Chemistry Mass Spectrometry Facility, University of California, Berkeley, Berkeley, CA*

MP 180 **Characterization of Histone H4 Post-translational Modification in the Microalgae Chlamydomonas Reinhardtii by Top Down Mass Spectrometry**; Aliyya Khan[1]; Carlo K Eikani[1]; Anthony T Iavarone[2]; James J Pesavento[1]; *[1]Department of Biology, Saint Mary's College of California, Moraga, CA - California; [2]QB3/Chemistry Mass Spectrometry Facility, University of California, Berkeley, CA*

MP 181 **Systems Level Analysis of Histone H3 Post-Translational Modifications Reveals Features of PTM Crosstalk in Chromatin Regulation**; Veit Schwämmle[1]; Simone Sidoli[2]; Chrystian Ruminowicz[1]; Xudong Wu[3, 4]; Chung-Fan Lee[3]; Kristian Helin[3]; Noerregaard Ole Jensen[1]; *[1]University of Southern Denmark, Odense, Denmark; [2]University of Pennsylvania, Philadelphia, PA; [3]University of Copenhagen, Copenhagen, Denmark; [4]Tianjin Medical University, Tianjin, China*

MP 182 **Utilizing Mass Spectrometry-Based Targeted Quantitative Proteomics to Determine the Factors that Alter the Specificity of Lysine Acetyltransferases**; Yin-Ming Kuo[1]; Ryan A Henry[1]; Andrew J Andrews[1]; *[1]Fox Chase Cancer Center, Philadelphia, PA*

MP 183 **Understanding the Origin and Evolution of the Epigenetic Code of Histones with an Orbitrap Fusion Lumos**; Arnau Sebé-Pedrós[1]; Cristina Chiva[2, 3]; Bernat Serra-Vidal[2, 3]; Iñaki Ruiz-Trillo[4]; Eduard Sabidó[2, 3]; *[1]Weizmann Institute of Science, Rehovot, Israel; [2]Proteomics Unit, Centre de Regulació Genòmica (CRG), Barcelona, SPAIN; [3]Proteomics Unit, Universitat Pompeu Fabra (UPF), Barcelona, Spain; [4]Institut de Biologia Evolutiva, Universitat Pompeu Fabra-CSIC, Barcelona, Spain*

MP 184 **Proteolytic Processing of Histone H2A by the Cathepsin L Protease**; Mariel Coradin[1]; Benjamin A Garcia[2]; *[1]University of Pennsylvania, Philadelphia, U.S.; [2]University of Pennsylvania, Philadelphia, PA*

MP 185 **Introducing Epigenomics in Systems Biology: Cross-Talk between Cell Signal Transduction and Epigenetic Mechanisms**; Simone Sidoli[1]; Pau Pascual Garcia[1]; Katarzyna Kulej[1, 2]; Brian Debo[1]; Maya Capelson[1]; Benjamin A. Garcia[1]; *[1]Department of Biochemistry and Biophysics, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA; [2]The Children's Hospital of Philadelphia, Philadelphia, PA*

MP 186 **Turnover Profiles of Histone Post-Translational Modifications in a Myogenic Model Using SILAC Labeling, Enzyme Networks and Trend Clustering Analysis**; Natarajan Bhanu[1]; Simone Sidoli[1]; Benjamin A Garcia[1]; *[1]University of Pennsylvania, Philadelphia, PA*

MP 187 **Middle-Down Characterization of Histone H4 Combinatorial Post-Translational Modification Codes for Breast Cancer Invasion**; Tingting Jiang[1]; Yu Chen[2]; Michael E Hoover[3]; Christopher L Hendrickson[1, 4]; Michael A Freitas[3]; Alan G Marshall[1, 4]; Nicolas L Young[5]; *[1]Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL; [2]The Roy J. Carver Biotechnology Center University of Illinois at Urbana-Champaign, Urbana, IL; [3]Department of Molecular Virology, Immunology and Medical Genetics, The Ohio State University, Columbus, OH; [4]Ion Cyclotron Resonance Program, National High Magnetic Field Laboratory, Tallahassee, FL; [5]Department of Biochemistry and Molecular Biology, Baylor College of Medicine, Houston, TX*

MP 188 **LC-MS/MS for the Sensitive Quantification of 5-Methylcytidine in RNA**; Gwendolyn Gonzalez[1]; Lijuan Fu[1]; Yinsheng Wang[1]; *[1]University of California - Riverside, Riverside, CA - California*

MP 189 **Less is More: Single-Neuron Epitranscriptomics using a Tandem Mass Spectrometric Approach**; Maria Basanta-Sanchez[1]; Andrea B. Kohn[2]; Lenka Halamkova[3, 4]; Igor K. Lednev[5]; Leonid L. Moroz[2, 6]; *[1]The RNA Institute, University at Albany, Albany, NY; [2]The Whitney Laboratory for Marine Bioscience, St. Augustine, FL; [3]The RNA Institute, University at Albany Albany, NY; [4]The RNA Institute, Albany, NY; [5]The RNA Institute University at Albany, Albany, NY; [6]Department of Neuroscience and McKnight Brain Institute, University of Florida, Gainesville, FL*

MP 190 **Contributions of Quantitative Histone PTM Analysis to Target Discovery, Compound Triage, and *in vivo* Experiments into Epigenetic Drug Tolerance**; Tommy K. Cheung [1]; Tobias Maile[1]; Erin McNamara[1]; Feng Zhao[2]; Patrick Trojer[2]; Lesley Murray[1]; Marie Classon[1]; David Arnott[1]; *[1]Genentech Inc, South San Francisco, CA; [2]Constellation Pharmaceuticals, Cambridge, MA*

MP 191 **Quantitation of Post-Translational Modifications in the Nucleus: Effects of Histone Modifying Enzymes on their Histone and Non-Histone Substrates**; Anastasia Lindahl[1]; Michael Smallegan[2]; Josue Baeza[3]; James Dowell[2]; Kimberly A Krautkramer[2]; John M Denu[2]; *[1]UW-Madison, Madison; [2]University of Wisconsin Madison, Madison, Wisconsin; [3]Univ of Wisconsin, Madison, WI*

MP 192 ***in vitro* Characterization of Histone Acyl-Posttranslational Modifications Using LC-MS**; Johayra Simithy[1]; Simone Sidoli[1]; Zuo-Fei Yuan[1]; Benjamin A Garcia[1]; *[1]University of Pennsylvania, Philadelphia, PA*

MP 193 **Probing the UV-Induced Effects on RNA and RNA-Modifications by LC-MS**; Congliang Sun[1]; Zalfa Abdel-Malek[1]; Kazumasa Wakamatsu[2]; Limbach A Patrick[1]; Balasubrahmanyam Addepalli[1]; *[1]University of Cincinnati, Cincinnati, Ohio; [2]Department of Chemistry, Fujita Health University School of Health Sciences, Toyoake, Japan*

MP 194 **Parallel Reaction Monitoring Mass Spectrometry for Histone H3 Modification Analysis of Differentiating MEL cells**; Michael Sweredoski[1]; Annie Moradian[1]; Matthias Raedle[2]; Sonja Hess[3]; *[1]California Institute of Technology, Pasadena, CA; [2]Hochschule Weihenstephan-Triesdorf, Weihenstephan-Triesdorf, Germany; [3]Caltech, Pasadena, CA*

HIGH MASS ACCURACY/HIGH PERFORMANCE MS APPLICATIONS
195 - 210

MP 195 **HRAM LC/MS Screen for Prostaglandins found in Consumer Products**; Bethany Hanson[1]; Toomey Valerie[1]; *[1]FDA/Forensic Chemistry Center, Cincinnati, OH*

MP 196 **Quantitation of Potential Genotoxic Impurities in Active Pharmaceutical Ingredients, Drug Products, and Process Intermediates by High Resolution LC-MS**; Robert Menger[1]; James Winter[1]; Alwyn Forbes[1]; Andy Lo[1]; Peng Wang[1]; Shannon Higgins-Gruber[1]; Ed Bishop[1]; Naijun Wu[1]; *[1]Celgene, Summit, NJ*

MP 197 **Determination of Chemical Components of KABA Meteorite by LDI and ESI Ionization Methods Using a 15T FT-ICR Instrument**; Arpad Somogyi[1]; Mihaly M. Nagy[2]; Jozsef Posta[3]; *[1]Ohio State University, Colombus, OH; [2]High School of Protestant College, Debrecen, Hungary; [3]University of Debrecen, Debrecen, Hungary*

MP 198 **Origin Discrimination of Red Pepper Powder Using UHPLC-Q-Oribitrap HRMS with Multivariate Analysis**; Dong-Jin Kang[1]; Ji-Young Moon[1]; Seong-Hun Lee[1]; *[1]Experimental Research Institute, NAQS Gimcheon-si, Korea*

MP 199 **Orbitrap Fusion Tribrid Mass Spectrometer for Pharmaceutical Impurity Analysis**; Kate Comstock[1]; Caroline Ding[2]; *[1]Thermo Fisher Scientific, San Jose , CA; [2]Thermo Fisher Scientific, San Jose, CA*

MP 200 **MALDI spiral-TOFMS and Kendrick Mass Defect Analysis of Mycolic Acids from Bacteria which Accelerate the Formation of Antibiotics**; Kanae Teramooto[1]; Shumpei Asamizu[2]; Taro Ozaki[2]; Katsuya Satoh[3]; Hiroyasu Onaka[2]; Robert Cody[4]; *[1]JEOL Ltd., Akishima, Tokyo; [2]The University of Tokyo, Bunkyo, Tokyo, Japan; [3]Japan Atomic Energy Agency, Takasaki, Japan; [4]JEOL USA Inc., Peabody, MA*

MP 201 **Top-down analysis of Calmodulin and Lysozyme Using MS/2DMS on an FT-ICR MS**; Federico Floris[1]; Maria van Agthoven[1]; Lionel Chiron[2]; Mark P Barrow[1]; Marc-André Delsuc[2, 3]; Peter B O'Connor[1]; *[1]University of Warwick, Coventry, United Kingdom; [2]C4SC4DE, Illkirch-Graffenstaden, France; [3]IGBMC, Illkirch-Graffenstaden, France*

MP 202 **Characterization of Impurities ofHIV NNRTI Doravirine by High Resolution UPLC-MS and Tandem MS Analysis**; Li-Kang Zhang; *Merck Research Laboratories, Kenilworth, NJ*

MP 203 **Prospecting for Aqueous Gold Clusters [37.6-kDa Au144(pMBA)60, 26.8-kDa Au102(pMBA)44] using a High-Resolution Extended-Mass-Range(EMR) Orbitrap MS**; Marcos Alvarez[1]; German Plascencia-Villa[1]; Wendell P. Griffith[1]; David M. Black1[1]; Miguel José Yacamán[1]; Jenny Chen[2]; Robert Loyd Whetten[1]; *[1]University of Texas at San Antonio, San Antonio, TX; [2]Thermo Fisher Scientific, San Jose, CA*

MP 204 **Increased Identification of Extractables and Leachables Compounds by the Use of Chemical Ionization and Custom Databases**; Syed Salman Lateef[1]; Siji Joseph[1]; Ravindra Gudihal[1]; *[1]Agilent Technologies India Pvt. Ltd, Bangalore, India*

MP 205 **Molecular Depth Profiling with a New Hybrid 3D SIMS Instrument for Improved Molecular Identification**; Alexander Pirkl[1]; Rudolf Moellers[1]; Henrik Arlinghaus[1]; Ewald Niehuis[1]; Alexander Makarov[2]; Stevan Horning[2]; Rasmus Havelund[3]; Melissa Passarelli[3]; Alex Shard[3]; Ian Gilmore[3]; *[1]ION-TOF GmbH, Muenster; [2]Thermo Fisher Scientific, Bremen, Germany; [3]National Physical Laboratory, Teddington, United Kingdom*

MP 206 **LC-Quadrupole/Orbitrap MS/HRMS Enables Stable Isotope Resolved Simultaneous Quantification and Metabolic Isotope Tracing of Acyl-Coezyme A Species**;

Nathaniel W Snyder[1]; Alexander J Frey[1]; Sophie Trefely[1]; Daniel R Feldman[1]; Andrew J Worth[2]; Basu S Sankha[3]; *[1]Drexel University, Philadelphia, PA; [2]Bristol-Myers Squibb Pharmaceutical Candidate Optimization, Wallingford, CT; [3]Department of Pathology, Brigham and Women's Hospital, Harvard Medical School, Boston, MA*

MP 207 **Quantitative Evaluation of Immunosuppressant Drugs by High Resolution Accurate Mass using Selected Ion Monitoring Analysis**; Keeley Murphy [1]; Jonathan L Josephs[2]; Maciej P Bromirski[3]; *[1]Thermo Fisher Scientific, San Jose , CA; [2]Thermo Fisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific, Bremen, DE*

MP 208 **Parallel Untargeted and Targeted Quantitative Metabolomics for Microbiome Research**; Alexey V. Melnik[1]; Fernando Vargas[1]; Amina Bouslimani[1]; Ivan Protsyuk[2]; Theodore Alexandrov[1, 2, 3]; Pieter C. Dorrestein[1, 4]; *[1]Collaborative Mass Spectrometry Innovation Center, Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California, San Diego, CA; [2]European Molecular Biology Laboratory (EMBL), Heidelberg, Germany; [3]SCiLS GmbH, Bremen, Germany; [4]Departments of Chemistry, Biochemistry and Pharmacology, University of California, San Diego, CA*

MP 209 **Simultaneous Determination of Phthalic Acid Esters, Organotins, Perfluorochemicals and Flame Retardants in Plastics by HPLC-LTQ/Orbitrap Mass Spectrometry**; Li Zhang[1]; Xin Luo[2]; Zengyuan Niu[2]; Xiwen Ye[2]; Zhixu Tang[2]; Shuwei Xia[1]; *[1]Ocean University of China, Qingdao, China; [2]Shandong Entry-Exit Inspection and Quarantine Bureau, Qingdao, China*

MP 210 **Acceptance Criteria for Confirmation of Identity of Chemical Residues Using Exact Mass Data**; Hiranthi Jayasuriya[1]; Philip K Kijak[1]; Sherri Turnipseed[2]; Timothy R Croley[3]; Jon Wong[3]; Bryan Gamble[4]; Hui Li[1]; *[1]Center for Veterinary Medicine, FDA, Laurel, MD; [2]Animal Drug Research Center, Denver, Colorado; [3]CFSAN, U.S. FDA College Park, MD; [4]Forensic Chemistry Center, Cincinnati, OH*

IMAGING MS: INSTRUMENTATION
211 - 231

MP 211 **Topographical and Chemical Imaging Using a Combined Atomic Force Microscopy/Infrared Spectroscopy/Mass Spectrometry Platform**; Vilmos Kertesz[1]; Tamin Tai[1]; Orsolya Karacsony[1]; Vera Bocharova[1]; Kevin Kjoller[2]; Gary J Van Berkel[1]; *[1]Oak Ridge National Laboratory, Oak Ridge, TN; [2]Anasys Instruments, Santa Barbara, CA*

MP 212 **Development of Nanopipettes as Probes for Scanning Electrospray Microscopy (SESM)**; Elizabeth M Yuill[1]; Wenqing Shi[1]; John Poehlman[1]; Lane A Baker[1]; *[1]Indiana University Dept. Chemistry, Bloomington, IN*

MP 213 **A Reflectron Microscope-Mode Imaging Mass Spectrometer Capable of Achieving High Mass Resolution**; Ang Guo[1]; Michael Burt[1]; Robert Burleigh[1]; Steve Thompson[2]; Mark Brouard[1]; *[1]University of Oxford, UK Oxford, United Kingdom; [2]Scientific Analysis Instruments, Manchester, UK*

MP 214 **Combining Scanning Ion Conductance Microscopy and Nanospray Desorption Electrospray Ionization Mass Spectrometry for Multimodal Ambient Imaging of Biological Samples**; Julia Laskin[1]; Son N Nguyen[1]; Venkateshkumar Prabhakaran[1]; Andrey Liyu[1]; Ruichuan Yin[1]; *[1]Pacific Northwest National Lab, Richland, WA*

MP 215 **Combining Imaging Mass Spectrometry with Infrared Spectromicroscopy Screening: A New Approach to Studying Biological Tissues**; Antoine Masson[1]; Matthew J DiTucci[2]; Anna Susa[2]; Jeremy T O' Brien[1]; Evan R Williams[1, 2]; Hoi-Ying holman[1]; *[1]Lawrence Berkeley National Lab, Berkeley, CA; [2]University of California, Berkeley, CA*

MP 216 **Ambient Submicron Mass Spectrometry Imaging by Combining AFM with MS**; Jonathan Brauer[1]; Jacob Berenbeim[2]; Mattanjah de Vries[2]; *[1]Anasys Instruments, Santa Barbara, CA; [2]University of California Santa Barbara, Santa Barbara, CA*

MP 217 **Microscope Ion Imaging of Complex Surfaces Using the Pixel Imaging Mass Spectrometry Camera**; Robert J Burleigh[1]; Ang Guo[1]; Edward Halford[1]; Michael Burt[1]; Steve P Thompson[2]; Mark Brouard[1]; *[1]University of Oxford, Oxford, UK; [2]Scientific Analysis Instruments, Manchester, UK*

MP 218 **Development of Laser Capture Microdissection-Liquid Vortex Capture ESI-MS (LMD-LVC/ESI-MS) for Quantitative and Sub-Micrometer Mass Spectral Surface Sampling and Imaging**; John F. Cahill[1]; Vilmos Kertesz[1]; Gary J Van Berkel[1]; *[1]Oak Ridge National Laboratory, Oak Ridge, TN*

MP 219 **Liquid Extraction Surface Analysis (LESA) Combined with Nano-Liquid Chromatography (nLC) for In-Depth Analysis of Biological Surfaces**; Daniel Eikel[1]; Terry Wilper[2]; Karen Norton[2]; Eric Solon[3]; Sara Savage[2]; Simon J Prosser[1]; *[1]Advion, Inc. Ithaca, NY; [2]Sanofi-Genzyme, Framingham, MA; [3]QPS, Newark, DE*

MP 220 **Transmission Geometry MALDI Imaging MS: Assessing Ion Generation/Collection Efficiency at Sub-micron Laser Spot Sizes**; Andre Zavalin[1]; Junhai Yang[1]; Richard M Caprioli[1]; *[1]Vanderbilt University, Nashville, TN*

MP 221 **Desorption Electrosonic Spray Ionizationfor Ambient Mass Spectrometry Imaging**; Shuai Guo[1]; Zhili Li[2]; *[1]Institute of Basic Medical Sciences, CAMS & PUMC, Beijing, CN; [2]IBMS, CAMS&PUMC, Beijing*

MP 222 **Improved Reproducibility in MALDI Imaging using a Scanning Laser Beam**; Dagmar Niemeyer[1]; Michael Becker[1]; Shannon D Cornett[2]; Paul J Kowalski[2]; Jane-Marie Kowalski[2]; Sören-Oliver Deininger[1]; *[1]Bruker Daltonik GmbH, Bremen, Germany; [2]Bruker Daltonics, Inc., Billerica, MA*

MP 223 **Laser Ablation Electrospray Ionization Mass Spectrometry Imaging (LAESI-MSI) Using an Er:YAG Laser for Improved Spot Size Resolution and Tunable Ablation**; Matthew Powell[1]; Trust T Razunguzwa[1]; Holly Henderson[1]; Heather Anderson[1]; Nicholas J. Morris[1]; Todd W. Orndorff[1]; David W. DuBois[1]; *[1]Protea Biosciences, Inc. Morgantown, WV*

MP 224 **3D nanoSIMS: A Novel High-Mass Resolution Instrument for 3D Molecular Imaging with Sub-Micron Resolution**; Melissa K. Passarelli[1]; Alexander Pirkl[2]; Rudolf Moellers[2]; Ewald Niehuis[2]; Alexander A Makarov[3]; Henrik Arlinghaus[2]; Rasmus Havelund[1]; Paulina D. Rakowska[1]; Alan M. Race[1]; Alex Shard[1]; Andy West[4]; Stevan Horning[3]; Peter S. Marshall[4]; Morgan R. Alexander[5]; Colin Dollery[4]; Ian Gilmore[6]; *[1]National Physical Laboratory, Teddington, United Kingdom; [2]ION-TOF GmbH, Muenster, Germany; [3]Thermo Fisher Scientific, Bremen, DE; [4]GlaxoSmithKline, Stevenage, UK; [5]The University of Nottingham, Nottingham, UK; [6]National Physical Laboratory, Teddington, Middlesex*

MP 225 **Development of a Time and Position Sensitive Ion Detector for a Stigmatic Imaging Mass Spectrometer**; Jun Aoki[1]; Yosuke Kawai[1]; Yowichi Fujita[2]; Hisanao Hazama[3]; Toshinobu Hondo[3]; Kunio Awazu[3]; Michisato Toyoda[1]; Yasuo Arai[2]; *[1]Osaka University, Toyonaka, Japan; [2]High Energy Accelerator Research Organization, Tsukuba, Japan; [3]Osaka University, Suita, Japan*

MP 226 **Three Micron Resolution MALDI-MS Imaging Without Transmission Geometry or Oversampling and Its Application to Maize Root Cross-section**; Adam Feenstra[1, 2]; Young-Jin Lee[1, 2]; *[1]Ames Laboratory-US DOE, Ames, Iowa; [2]Iowa State University, Ames, IA*

MP 227 **Rapid Laser Desorption Imaging MS with Submicron Spatial Resolution**; Jerome Moore[1]; J Albert Schultz[2]; Valerie Steen[2]; *[1]Robot Nose, Lemont, IL; [2]Ionwerks, Inc. Houston, TX*

MP 228 **DESI Imaging at Varying Acquisition Rates with Real Time Imaging Display for Optimized Tissue Imaging**; Emrys Jones[1]; Mark Towers[1]; Bindesh Shrestha[2]; Philiipa Hart[1]; Richard Chapman[1]; Emmanuelle Claude[1]; *[1]Waters Corporation, Wilmslow, UK; [2]Waters Corporation, Beverly, Massachusetts*

MP 229 **Automated High Throughput 3D Imaging Using Desorption Electrospray Ionisation Mass Spectrometry**; Emrys A Jones[1, 2]; Lukasz Migas[3]; Richard Chapman[2]; Emmanuelle Claude[2]; James Langridge[2]; Steven D Pringle[2]; Zoltan Takats[4]; Mike Morris[2]; *[1]Imperial College London, London, Greater London; [2]Waters Corporation, Wilmslow, UK; [3]University of Manchester, Manchester, UK; [4]Imperial College, London, United Kingdom*

MP 230 **Maximizing Performance of Spatial Proteomics through the Fusion of Ultra-High Speed MALDI-TOF and High Mass Resolution MALDI FTICR IMS**; Jeffrey Spraggins[1, 2, 3, 4]; Raf Van de Plas[2, 4, 5]; Jessica L Moore[3, 4]; Daniel Ryan[3, 4]; Richard M Caprioli[2, 3, 4, 6]; *[1]Vanderbilt University, Nashville, TN; [2]Vanderbilt Dept. of Biochemistry, Nashville, TN; [3]Vanderbilt Dept. of Chemistry, Nashville, TN; [4]Vanderbilt University MSRC, Nashville, TN; [5]Delft University of Technology, Delft, Netherlands; [6]Vanderbilt University School of Medicine, Nashville, TN*

MP 231 **Localization and Identification of Peptides from Tissue Using High-Speed MALDI TOF/TOF Mass Spectrometry**; Michael Becker[1]; Anja Resemann[1]; Janine Beckmann[1]; Julian Langer[2, 3]; Rainer Paape[1]; Detlev Suckau[1]; *[1]Bruker Daltonik GmbH, Bremen, Germany; [2]Max-Planck-Institute for Biophysics, Frankfurt Am Main, Germany; [3]Max-Planck-Institute for Brain Research, Frankfurt Am Main, Germany*

IMAGING MS: SAMPLE PREPARATION
232 - 243

MP 232 **Analyzing the Effect of Cocaine on Lipid Localization in Drosophilabrain Tissue Using Secondary Ion Mass Spectrometry Imaging**; Mai Hoang[1]; Nhu Phan[2]; Per Malmberg[1]; Andrew G Ewing[1, 2]; *[1]Chalmers University of Technology, Goteborg, Sweden; [2]Goteborg University, Goteborg, Sweden*

MP 233 **Improvement of Peptides Imaging on Tissue by Supercritical Fluid Wash of Lipids for Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry**; Shoko Matsushita[1]; Noritaka Masaki[1]; Kohei Sato[2]; Takahiro Hayasaka[3]; Eiji Sugiyama[1]; Shu-Ping Hui[3]; Hitoshi Chiba[3]; Nobuyuki Mase[2]; Mitsutoshi Setou[1]; *[1]Department of Cell Biology and Anatomy, Hamamatsu University School of Medicine, Hamamatsu, Japan; [2]Department of Applied Chemistry and Biochemical Engineering, Faculty of Engineering, Shizuoka University, Hamamatsu, Japan; [3]Health Innovation and Technology Center, Faculty of Health Sciences, Hokkaido University, Sapporo, Japan*

MP 234 **Ammonium Sulfate Improves Detection of Hydrophilic Quaternary Ammonium Compounds through Decreased Ion Suppression in Matrix-Assisted Laser Desorption/Ionization Imaging Mass Spectrometry**; Eiji Sugiyama[1]; Noritaka Masaki[1]; Shoko Matsushita[1]; Mitsutoshi Setou[1]; *[1]Hamamatsu University School of Medicine, Hamamatsu, Shizuoka*

MP 235 **Systematic Assessment of Surfactants for MALDI Imaging Mass Spectrometry**; Bijay Banstola[1]; Fabrizio Donnarumma[1]; Fan Cao[1]; Eulalie T Grodner[1]; Kermit K Murray[1]; *[1]Louisiana State Univeristy, Baton Rouge, LA*

MP 236 **High Performance Matrix Pre-coated Targets for MALDI Imaging of Lipids**; Junhai Yang[1]; Richard M Caprioli[1]; *[1]Vanderbilt University, Nashville, TN*

MP 237 **Using MALDI Depth Profiles to Understand the Effect of ESD Sample Preparation Parameters on MALDI IMS Samples**; Brian James Malys[1]; Kevin G Owens[2]; *[1]Drexel University, Ambler, PA; [2]Drexel University, Philadelphia, PA*

MP 238 **A Combined Enzymatic Digestion and Matrix Application Approach for High Throughput MSI of FFPE Tissue**; Haddon E. Goodman[1]; Erin H. Seeley[1]; *[1]Protea Biosciences, Morgantown, WV*

MP 239 **Utilization of Soft-landing Ion Mobility for the Deposition of Clusters as Matrix Substitutes for Matrix-assisted Laser Desorption/Ionization Mass Spectrometry Imaging**; Roberto Aguilar[1]; Guido F Verbeck[1]; *[1]University of North Texas, Denton, TX*

MP 240 **Optimal Sample Preparation Method for Visualizing Global Endogenous Metabolites by Mass Spectrometry Imaging in Arabidopsis**; Tomomi Ichinose[1]; Yoshinori Fujimura[1]; Shuichi Nakaya[2]; Yuzo Yamazaki[2]; Junya Nakamura[1]; Eisuke Hayakawa[1]; Hiroyuki Wariishi[1]; Daisuke Miura[1]; *[1]Kyushu University, Fukuoka, Japan; [2]Shimadzu Corporation, Kyoto, Japan*

MP 241 **Investigation into the use of Tissue Washing Procedures and the Subsequent Outcomes for DESI-MS Imaging Analyses**; Philippa Hart[1]; Mark Towers[1]; Emmanuelle Claude[1]; *[1]Waters Corporation, Wilmslow, UK*

MP 242 **Investigation of Aging of Chemically Fixed Mammalian Cells via ToF-SIMS**; Julia Kokesch-Himmelreich[1]; Daniel J Graham[1]; Lara J Gamble[1]; *[1]University of Washington, Seattle, WA*

MP 243 **Mass Spectrometry Imaging to Better Understand the Mycoparasitic Interaction of Biocontrol Agents**; Matthias Holzlechner[1]; Zoratto Samuele[1]; Reitschmidt Sonja[1]; Zeilinger Susanne[1, 2]; Martina Marchetti-Deschmann[3]; *[1]Vienna University of Technology, Vienna, Austria; [2]University of Innsbruck, Innsbruck, Austria; [3]Vienna University of Technology, Vienna, Vienna*

IMAGING MS: SOFTWARE
244 - 249

MP 244 **High-Performance Visualization and Multivariate Analysis Software for Mass Spectrometric Imaging**; Daichi Yukihira[1]; Mitsuhiro Kanazawa[1]; *[1]Reifycs Inc., Tokyo, Japan*

MP 245 **Finding Patterns in Mass Spectrometry Images**; Daniel Graham[1]; Lara J Gamble[1]; *[1]University of Washington, Seattle, WA*

MP 246 **Software for Distributed MALDI Imaging Workflows**; Stefan Frehse[1]; Fingal Orlando Galashan[1]; Tobias Boskamp[1, 2]; Jan Hendrik Kobarg[1]; Stefan Schiffler[1]; Klaus Steinhorst[1]; Janina Oetjen[2]; Carl Evertsz[1]; Theodore Alexandrov[1, 3, 4]; Peter Maass[1, 2]; Dennis Trede[1]; *[1]SCiLS GmbH, Bremen, Germany; [2]University of Bremen, Bremen, Germany; [3]EMBL Heidelberg, Heidelberg, Germany; [4]University of California, San Diego La Jolla, CA*

MP 247 **Absolute Quantification and Customizable Database Integration for Molecular Identification with MSiReader**; Kenneth Garrard[1]; Mark T Bokhart[1]; Milad Nazari[1]; David C Muddiman[1]; *[1]North Carolina State University, Raleigh, NC*

MP 248 **Translational Data Analytics for Large Mass Spectrometry Imaging Datasets in Clinical Research**; Kirill Veselkov[1]; Mirnezami Reza[2]; Emmanuelle Claude[3]; James Kinross[2]; James McKenzie[2]; Paolo Inglese[4]; Kieran Neeson[3]; James Langridge[5]; Elaine Holmes[4]; Zoltan Takats[2]; Jeremy K Nicholson[2]; *[1]Imperial College, London, London; [2]Imperial College, London, UK; [3]Waters, Wilmslow, United Kingdom; [4]Imperial College, London, United Kingdom; [5]Waters, Manchester*

MP 249 **Characterization of Data-driven Image Fusion for Imaging MS: Exploring Image Modality Combinations that Maximize Predictive Performance for Distinct Biomolecular Classes**; Raf Van de Plas[1, 2]; Jeffrey Spraggins[2]; Nico Verbeeck[1]; Junhai Yang[2]; Richard M Caprioli[2]; *[1]Delft University of Technology, Delft, Netherlands; [2]Vanderbilt University, Nashville, TN*

INFORMATICS: METABOLOMICS
250 - 264

MP 250 **IFrID: A Novel In-Source Fragmentation Detection and Deconvolution Algorithm for LC-MS Metabolomics Data**; Tytus Mak[1]; Maryam Goudarzi[2]; Stephen Stein[1]; *[1]National Institute of Standards and Technology, Gaithersburg, MD; [2]Georgetown University Medical Center, Washington, DC*

MP 251 **Exploring Spectral Relationships and Peak Redundancy in API Mass Spectra**; Nathaniel Mahieu[1]; Gary J Patti[1]; *[1]Washington University in St. Louis, St. Louis, MO*

MP 252 **Accurate Mass Retention Time Locked Metabolomics EI Library and Workflows for Accurate Mass GC/Q-TOF Metabolomics Data Processing**; Sofia Nieto[1]; Zijuan Lai[2]; Mine Palazoglu[2]; Hong Chen[1]; Aditi Koul[1]; Vadim Kalmeyer[1]; Oliver Fiehn[2]; *[1]Agilent technologies Inc, Santa Clara, CA; [2]UC Davis, Davis, CA*

MP 253 **Rapid MS1 Formulae to Isotope Pattern Matching Using a Novel MS1 Search Engine for Metabolomics**; Scott Walmsley[1, 2]; Hyungwon Choi[3]; Samantha Bokatzian[1]; Richard Reisdorph[1]; Nichole A Reisdorph[1]; *[1]Dept. of Pharmaceutical Sci., University of Colorado Denver-Anschutz, Aurora, Colorado [CO]; [2]UCD Computational Biosciences Program, Aurora, Colorado [CO]; [3]National University of Singapore, Singapore, Singapore*

MP 254 **Optimus + `ili: Software for LC-MS Based Spatial Metabolomics in 2D, 3D, and Virtual Reality**; Ivan Protsyuk[1]; Sergey Ryazanov[1]; Garg Neha[2]; Tal Luzzatto-Knaan[2]; Amina Bouslimani[2]; Clifford Kapono[2]; Alexey Melnik[2]; Dimitri Floros[2]; Luca Rappez[1]; Prasad Phapale[1]; Pieter Dorrestein[2]; Theodore Alexandrov[1, 2]; *[1]EMBL, Heidelberg, Germany; [2]Skaggs School of Pharmacy, UC San Diego La Jolla, CA*

MP 255 **Building High Confidence Metabolite Libraries for Fast Identification in Targeted Profiling Experiments**; Gina Tan[1]; Ralf Tautenhahn[1]; Andreas Huhmer[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

MP 256 **The 1-SToP Approach to Annotation of LC-MS Metabolomics Data**; Corey D Broeckling[1]; Andrea Ganna[2]; Mark Layer[3]; Brown Kevin[3]; Ben Sutton[3]; Erik Ingelsson[4, 5]; Graham Peers[3]; Jessica E Prenni[1]; *[1]Colorado State University Proteomics and Metabolomics Facility, Fort Collins, Co; [2]Broad Institute of MIT and Harvard, Cambridge, MA; [3]Colorado State University, Fort Collins, CO; [4]Uppsala University, Uppsala, Sweden; [5]Department of Medical Sciences, Molecular Epidemiology and Science for Life Laboratory, Uppsala University, Uppsala, Sweden*

MP 257 **Utilizing Advanced Multivariate Analysis Features with Automated Database Searching Algorithms to Simplify Metabolomics Study Conduct and Understanding**; Christopher Colangelo[1]; Phillip Seitzer[2]; Rick Schneider[3]; *[1]Primary Ion, Old Lyme, CT; [2]Proteome Software, Portland, OR; [3]Pfizer, Groton, CT*

MP 258 **Automatic CCS and MS/MS Library Creation and Application for Large Scale Metabolic Profiling**; Jonathan P. Williams[1]; David Eatough[1]; Lee A. Gethings[1]; Christopher. J. Hughes[1]; Mark Towers[1]; Leanne Nye[2]; Steven Lai[3]; Richard Tyldesley-Worster[1]; Johannes PC Vissers[1]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Waters Corporation, London, United Kingdom; [3]Waters Corporation, Beverly, MA*

MP 259 **Algorithm for Metabolite Identification Based on MS/MS for Untargeted Metabolomics**; Guoan Zhang; *New York University, New York, NY*

MP 260 **A Generalizable Method for False-Discovery Rate Estimation in Mass Spectrometry-Based Lipidomics**; Grant Fujimoto[1]; Jennifer E Kyle[1]; Kevin Crowell[1]; Richard D Smith[1]; Thomas O Metz[1]; Sam Payne[1]; *[1]Pacific Northwest National Lab, Richland, WA*

MP 261 **Assessing Metabolic Pathways Using Chemical Kinetics Theory**; Ismael Zamora[1]; Guillem Plasencia[2]; Laura Goracci[3]; *[1]Lead Molecular Design, S.L., Sant Cugat del Valles, Barcelona; [2]Lead Molecular Design S.L., Sant Cugat de Valles, Spain; [3]Perugia University, Perugia, Italy*

MP 262 **A Computational Platform for Analysis of Stable Isotope Assisted Metabolomics Data Acquired on GC-MS**; Xiaoli Wei[1, 2]; Imhoi Koo[1, 2]; Biyun Shi[1, 2]; Pawel Lorkiewicz[3, 4]; Hamid Suhail[5]; Ramandeep Rattan[5]; Shailendra Giri[5]; Xiang Zhang[1, 2, 3]; *[1]Department of Chemistry, University of Louisville, Louisville, KY; [2]ulatory and Center for RegEnvironmental Analytical Metabolomics, University of Louisville, Louisville, KY; [3]Pharmacology & Toxicology, University of Louisville, Louisville, KY; [4]Institute of Molecular Cardiology, University of Louisville, Louisville, KY; [5]Henry Ford Health System, Detroit, MI*

MP 263 **Analysis of Stable Isotope Assisted Metabolomics Data Acquired by High Resolution Mass Spectrometry**; Pawel Lorkiewicz[1]; Xiaoli Wei[1]; Joshua Salabei[1]; Biyun Shi[1]; Bradford Hill[1]; Seongho Kim[2]; Craig James McClain[1, 3]; Xiang Zhang[1]; *[1]University of Louisville, Louisville, KY; [2]Wayne State University, Detroit, MI; [3]Robley Rex Louisville VAMC, Louisville, KY*

MP 264 **metaX: an Automatic and Comprehensive Pipeline for Processing Metabolomics Data**; Bo Wen[1]; Zhenyu Guo[1]; David Broadhurst[2]; Yanqun Fan[1]; Chunwei Zeng[1]; Hui Jiang[1]; Xun Xu[1]; Siqi Liu[1]; *[1]BGI-Shenzhen, Shenzhen, China; [2]University of Alberta, Edmonton, Canada*

INFORMATICS: MULTIOMICS INTEGRATION
265 - 280

MP 265 **A Multi-omics Visualization Platform (MVP) Plug-in for Galaxy-based Applications**; Thomas Mcgowan[1]; James Johnson[1]; Pratik Jagtap[2]; Getiria Onsongo[1]; Candace Guerrero[2]; Timothy Griffin[2, 3]; *[1]University of Minnesota Supercomputing Institute, Minneapolis, MN; [2]University of Minnesota, Minneapolis, MN; [3]Center for Mass Spectrometry and Proteomics, UMN St.Paul, MN*

MP 266 **From Start to Finish: a Complete Proteogenomic Informatics Environment Implemented in the Galaxy Platform**; Getiria Onsongo[1]; Pratik D Jagtap[2]; James E Johnson[3]; Thomas McGowan[3]; Mohammad Heydarian[4]; Karen Reddy[5]; Timothy J Griffin[2]; *[1]University of Minnesota, Minneapolis, MN; [2]University of Minnesota at Twin Cities, Saint Paul, MN; [3]University of Minnesota Supercomputing Institute, Minneapolis, MN; [4]Johns Hopkins University, Baltimore, Maryland; [5]Johns Hopkins University, Baltimore, MD*

MP 267 **A Multi-Omic Approach to Reveal the Effect of Low-Level Gamma Radiation on Rice Seeds**; Gohei Hayashi[1]; J Shibato[2]; A Kubo[3]; T Imanaka[3]; GK Agrawal[4]; S Shioda[2]; M Fukumoto[5]; G Oros[6]; Randeep Rakwal[7]; Sa Deepak[8]; Gundimeda Seetaram[9]; Upendra Simha[10]; Padmanaban Arunkumar[10]; *[1]Institute of Development, Aging and Cancer, Tohoku University, Sendai, Japan; [2]Hoshi University, Tokyo, Japan; [3]NIES, Tsukuba, Japan; [4]RLABB, Kathmandu, Nepal; [5]Tohoku University, Sendai, Japan; [6]Plant Protection Institute, Budapest, Hungary; [7]Tsukuba University, Tsukuba, Japan; [8]Agilent Technologies, Bangalore, Bangalore; [9]Agilent technologies, Bangalore, India; [10]Agilent Technologies (India) Pvt. Ltd., Bangalore, India*

MP 268 **Global Analysis of Lipidomics, Oxylipin and Metabolomics Data Sets in Paediatric Plasmodium Falciparum Malaria**; Izabella Surowiec[1]; Sandra Gouveia-Figueira[1]; Tomas Skotare[1]; Judy Orikiiriza[2]; Elisabeth Lindquist[3]; Sven Bergström[3]; Johan Normark[3]; Johan Trygg[1]; *[1]Computational Life Science Cluster (CLiC), Umeå University, Umeå, Sweden; [2]Infectious Diseases Institute, School of Medicine and Health Sciences, Makerere University, Kampala, Uganda; [3]Department of Molecular Biology, Umeå University, Umeå, Sweden*

MP 269 **An NGS-Independent Strategy for Proteome-Wide Identification of Single Amino Acid Polymorphisms by Mass Spectrometry**; Wenqing Shui[1]; Yun Xiong[2]; Yufeng Guo[2]; Weidi Xiao[3]; *[1]Tianjin Institute of Industrial Biotechnology, Chinese Academy of Sciences, Tianjin, Tianjin; [2]Tianjin Institute of Industrial Biotechnology, Chinese Academy of Sciences, Tianjin, CN; [3]Nankai university, Tianjin, China*

MP 270 **The Fragmentarium: A Universal Query Service Enabling Partial Matching of Unidentified Spectra across the Full Gamut NIST MS Spectral Libraries**; Manor Askenazi[1]; Stephen Stein[2]; *[1]Biomedical Hosting LLC, Arlington, MA; [2]NIST, Gaithersburg, MD*

MP 271 **Precise Label-Free Quantitative Proteomes in High-Throughput Using microLC-SWATH-MS**; Jakob Vowinckel[1]; Aleksej Zelezniak[1, 2]; Markus Ralser[1, 2]; *[1]University of Cambridge, Cambridge, UK; [2]The Francis Crick Insitute, London, UK*

MP 272 **ProteoGenomics: Linking between Ensembl and PRIDE using ProteoAnnotator**; Fawaz Ghali[1]; Simon Perkins[1]; Tobias Ternent[2]; Juan Antonio Vizcaino[2]; Henning Hermjakob[2]; Andy Yates[2]; Paul Flicek[2]; Andy Jones[1]; *[1]University of Liverpool, Liverpool, United Kingdom; [2]EMBL-EBI, Hinxton, UK*

MP 273 **Crosstalker: A Biological Network Analysis Platform With an Emphasis on Openness**; Sean Maxwell[1, 2]; Mark R Chance[1, 2]; *[1]Case Western Reserve University, Cleveland, OH; [2]NeoProteomics, Inc. Cleveland, OH*

MP 274 **Looking for Black Sheep: Identifying Significant Proteogenomic Outliers**; Emily Kawaler[1]; Kelly V Ruggles[1]; David Fenyo[1]; *[1]Center for Health Informatics and Bioinformatics, New York University Medical School, New York, NY*

MP 275 **proBAMsuitea Bioinformatics Framework for Genome-Based Representation and Analysis of Proteomics Data**; Xiaojing Wang[1]; Robbert J Slebos[1]; Matthew C. Chambers[1]; David L. Tabb[1]; Daniel C. Liebler[1]; Bing Zhang[1]; *[1]Vanderbilt University, Nashville, TN*

MP 276 **Systematic Analysis of Phosphosignaling-Affecting Mutations in a Large Clinical Breast Cancer Cohort**; Karsten Krug[1]; Philipp Mertins[1]; Lauren Tang[1]; Jana Qiao[1]; Filip Mundt[1]; Karl R Clauser[1]; Michael A Gillette[1]; Li Ding[2]; Kelly V Ruggles[3]; David Fenyo[3]; Matthew Ellis[4]; D.R. Mani[1]; Steven A Carr[1]; *[1]Broad Institute of MIT and Harvard, Cambridge, MA; [2]Washington University School of Medicine, St. Louis, MO; [3]New York University, New York, NY; [4]Baylor College of Medicine, Houston, TX*

MP 277 **Detection of Colorectal Cancer Related Antibody Peptides Using Proteogenomics**; Seong Won Cha[1]; Vineet Bafna[2]; *[1]UCSD, La Jolla, California; [2]UCSD, La Jolla, CA*

MP 278 **A Comprehensive Proteogenomic Workflow Reveals Novel Insights into Leukemogenesis**; Jarrod Sandow; *The Walter & Eliza Hall Institute, Parkville, VIC*

MP 279 **Taxonomic Characterization of Metaproteomes Using Databases of Translated Metagenomic Sequencing Reads**; Damon May[1]; Emma Timmins-Schiffman[1]; Molly Mikan[2]; Rodger Harvey[2]; Elhanan Borenstein[1]; Brook Nunn[1]; William S Noble[1]; *[1]University of Washington, Seattle, WA; [2]Old Dominion University, Norfolk, VA*

MP 280 **Integrating Global Proteome and Phosphoproteome Expression into the Cancer Cell Line Encyclopedia**; David Nusinow[1]; John Szpyt[1]; Christopher M Rose[1]; Mahmoud Ghandi[2]; Levi A Garraway[2, 3]; Steven P Gygi[1]; *[1]Harvard Medical School, Boston, MA; [2]Broad Institute of MIT and Harvard, Cambridge, MA; [3]Dana Farber Cancer Institute, Boston, MA*

INSTRUMENTATION: NEW CONCEPTS
281 - 302

MP 281 **Microfabrication and Evaluation of the T-Probe: A Novel Device for Online *in situ* Live Single Cell MS Analysis**; Renmeng Liu[1]; Yanlin Zhu[1]; Ning Pan[1]; Zhibo Yang[1]; *[1]University of Oklahoma, Dept. of Chem & Biochem Norman, OK*

MP 282 **An Alternative to a Direct Insertion Probe using a Traditional GCMS Pyrolyzer Instrument**; Ben Peters[1]; Karen Sam[1]; Gary Deger[1]; *[1]CDS Analytical, Oxford, PA*

MP 283 **Development of Automated Screening and Quantitation Method on Novel On-Line SFE-SFC-MS/MS Platform – (I) For 24 Restricted Perflurocompounds**; Jie Xing[1]; Jun Xiang Lee[1]; Peiting Zeng[1]; Zhaoqi Zhan[1]; *[1]Shimadzu (Asia Pacific) Pte Ltd, 79 Science Park Drive #02-01/08, Singapore*

MP 284 **Facilitating Disulfide Bond Assignments in a Bottom-Up Proteomics Procedure Combined with Online LC–Electrochemistry–MS**; Linda Switzar[1]; Arnoud de Ru[1]; Agnieszka Kraj[2]; Jean-Pierre Chervet[2]; Annemieke Aartsma-Rus[1]; Yuri EM van der Burgt[1]; Peter A van Veelen[1]; *[1]Leiden University Medical Center (LUMC), Leiden, The Netherlands; [2]Antec, Zoeterwoude, The Netherlands*

MP 285 **Novel Ion Optics Boosting the Sensitivity of Proton-Transfer-Reaction - Time-of-Flight Mass Spectrometry (PTR-TOFMS)**; Alfons Jordan[1]; Christian Lindinger[1]; Stefan Feil[1]; Paul Mutschlechner[1]; Gernot Hanel[1]; Eugen Hartungen[1]; Jens Herbig[1]; Lukas Märk[1]; Simone Jürschik[1]; Philipp Sulzer[1]; *[1]IONICON Analytik GmbH., Innsbruck, Austria*

MP 286 **Digitally-Driven Ion Funnels to Enhance High Mass Ion Collection**; Bojana Opacic[1]; Liang Wang[1]; Brian H Clowers[1]; Peter Ta Reilly[1]; *[1]Washington State University, Pullman, WA*

MP 287 **A Segmented Linear Quadrupole Ion Trap for Enhanced Activation and Storage**; Dimitris Papanastasiou[1]; Emmanuel Raptakis[1]; Diamantis Kounadis[1]; Ioannis Orfanopoulos[1]; Alexander Lekkas[1]; Andreas Mpozatzidis[1]; *[1]Fasmatech, Athens, Greece*

MP 288 **Analysis of Species of N2 in Environmental Samples and H2 in Inorganic Samples by New Type of Quadrupole Mass-Spectrometer**; Adolf Goetz Dr.[1]; Michael Laessig[2]; Thimo Post[3]; Bernd Apelt[4]; Peter Paplewski[5]; *[1]Inprocess Instruments, Bremen,, Germany; [2]Bremen, Bremen,, Germany; [3]Bremen, Bremen, Germany; [4]Helmholtz Centre for Environmental Research - UFZ, Leipzig, Germany; [5]Bruker, Karlsruhe, Germany*

MP 289 **A Simple Ion Funnel-Based Device for the Thermalization and Transmission of Megadalton Ions**; Staci N Anthony[1]; Benjamin E Draper[1]; Martin F Jarrold[1]; *[1]Indiana University Dept. Chemistry, Bloomington, IN*

MP 290 **Ion Confinement in a Fourier Transform Electrostatic Linear Ion Trap via Mirror-Switching: Correction of a Voltage-Induced Frequency Drift**; Eric Dziekonski[1]; Joshua T.K. Johnson[1]; Santini Robert[1]; Scott A McLuckey[1]; *[1]Purdue University-Department of Chemistry, West Lafayette, IN*

MP 291 **Mass Manipulation of Ions in a Cryogenic Linear Ion Trap: Simulations and Experiment**; Larry Tesler[1]; Nicolas C Polfer[1]; *[1]University of Florida, Gainesville, Florida*

MP 292 **Ion Journey in a Mass Spectrometer: Simulation of the Ion Trajectories from an Atmospheric Pressure source to the mass analyzer**; Xiaoyu Zhou[1]; Zheng Ouyang[2]; *[1]Purdue University, west lafayette, Indiana; [2]Purdue University, West Lafayatte, IN*

MP 293 **Maximizing Linear Quadrupole Resolution and Sensitivity Using Digital Waveform Manipulation**; Zachary Philip Gotlib[1]; Gregory Forrest Brabeck[1]; Peter Ta Reilly[1]; *[1]Washington State University, Pullman, WA*

MP 294 **Mapping the Pseudopotential Well at all Points in**

the Stability Diagram; Peter Ta Reilly[1]; Gregory Forrest Brabeck[1]; *[1]Washington State University, Pullman, WA*

MP 295 **Lead-Free Ceramic Continuous Dynode Electron Multiplier**; Hiroshi Kobayashi[1]; Motohiro Suyama[2]; *[1]Hamamatsu Photonics K.K., Iwata, Shizuoka; [2]Hamamatsu Photonics K.K., Iwata, Japan*

MP 296 **Vacuum Ultra-Violet (VUV) Detection as a Complement to Mass Spectrometry (MS) Analysis of Biological Metabolites**; Shinji Kenneth Strain[1]; James Diekmann[2]; Brooke Barnette[3]; Mark Emmett[3, 4, 5, 6]; *[1]Dept of Neuroscience and Cell Biology, University of Texas Medical Branch, Galveston, TX; [2]VUV Analytics, Austin, TX; [3]Dept of Biochemistry and Molecular Biology, University of Texas Medica Branch, Galveston, TX; [4]Dept of Pharmacology & Toxicology, University of Texas Medical Branch, Galveston, TX; [5]Dept of Radiation Oncolog, University of Texas Medical Branch, Galveston, TX; [6]UTMB Cancer Center, University of Texas Galveston, USA*

MP 297 **A Modular Data Station for Radio-Frequency Ionization FT-ICR Mass Spectrometry Built on Robust and Expandable Commercial Architectures for Imaging Applications**; Matthew R Brantley[1]; Solouki Touradj[1]; *[1]Baylor University, Waco, TX*

MP 298 **Multiplexed Targeted Assays Using Ion Trap Waveform Isolation**; Philip M Remes; *Thermo Fisher Scientific, San Jose , CA*

MP 299 **Deconvolution Method for Multiple Harmonics FTMS Spectra**; Sergey Smirnov[1]; Aleksandr Rusinov[2]; Li Ding[1]; *[1]Shimadzu Research Laboratory (Europe) Ltd., Manchester, United Kingdom; [2]Shimadzu Research Laboratory (Europe) Ltd., Manchester, Manchester*

MP 300 **Novel Tandem Ionization GCxGC-TOF MS for Characterization of Allergens in Cosmetics**; Matthew Edwards[1]; Joe Blanch[1]; Laura McGregor[1]; Nick Bukowski[1]; Pete Grosshans[2]; Chris Hall[2]; Massimo Santoro[1]; David Wevill[2]; *[1]Markes International, Cardiff, UK; [2]Markes International Inc., Cincinnati, OH*

MP 301 **Design and Simulation for a Novel Wedge Ion Guide (WIG) to Achieve Ion Compression and Ion Bending**; Yupeng Cheng[1]; Xiaoqiang Zhang[2]; Wenjian Sun[2]; *[1]Shimadzu Research Laboratory (Shanghai) Co., Ltd., Shanghai, Shanghai; [2]Shimadzu Research Laboratory (Shanghai) Co., Ltd., Shanghai, China*

MP 302 **Scout-MRM; a Method to Acquire Large Numbers of MRM without Predefined Retention Time**; Cox Dave[1]; Blandine Rougemont[2]; Romain Carriere[3]; J.C. YVES LEBLANC[4]; Lemoine Jerome[2]; *[1]SCIEX, Concord ON, Canada; [2]Institut des Sciences Analytiques - UMR CNRS, Villerbanne (Lyon), France; [3]Institut des Sciences Analytiques - UMR CNRS, Villerabnne (Lyon), France; [4]SCIEX, Concord, ON*

INTACT PROTEINS
303 - 319

MP 303 **Making Heavy Peaks With a Pinch of Sugar: A Strategy for Intact Protein MS Quantitation in Any Feed**; Jeniffer Quijada[1, 2]; Jared R. Auclair[1, 2]; Joseph P. Salisbury[1, 2]; Jeffrey Agar[1, 2]; *[1]Barnett Inst., Northeastern University Boston, MA; [2]Northeastern University, Boston, MA*

MP 304 **An LC-MS based method for monitoring the activation of Mesotrypsin and a Strategy for Quantitation in Cellular Secretions**; Derek Wachtel[1]; Sushmit Maitra[2]; Keith Goodman[2]; Dan Warren[2]; Lyle Burton[2]; Marco Kessler[1]; Sanjeev Forsyth[1]; Maria Ribadeneira[1]; *[1]Ironwood Pharmaceuticals, Cambridge, MA; [2]SCIEX, Concord ON, Canada*

MP 305 **Separation of Native Proteins and Protein Complexes using Capillary Electrophoresis Coupled with Mass Spectrometry**; James Wilkins[1]; Jonathon Johnston[2]; Michael J Trnka[2]; Alma Burlingame[2]; *[1]UCSF, San Francisco, CA; [2]UCSF, San Francisco, CA*

MP 306 **Development of a high quality intact protein standard for LC and MS quality control and application development**; Helene Cardasis[1]; Rosa Viner[2]; Vikrant Gohil[3]; Kay Opperman[4]; John Rogers[4]; Kelly Flook[5]; Alexander Cherkassky[3]; Jim Stephenson[3]; Egle Capkauske[6]; Kestutis Bargaila[6]; Agne Alminaite[6]; Viktorija Vitkovske[6]; Juozas Siurkus[6]; *[1]Thermo Scientific, New York, NY; [2]Thermo Fisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific, Cambridge, MA; [4]Thermo Fisher Scientific, Rockford, IL; [5]Thermo Fisher Scientific, Sunnyvale, CA; [6]Thermo Fisher Scientific, Vilnius, Lithuania*

MP 307 **Novel Strategy for Quality Assessment of Glycosylation on a Biotherapeutic Glycoprotein by Intact Protein Analysis**; Unyong Kim[1, 2]; Myung Jin Oh[1, 2]; Hyun Joong Kim[2]; Youngsuk Seo[1, 2]; Hyun Joo An[1, 2]; *[1]Asia Glycomics Reference Site, Daejeon, Korea; [2]Graduate School of Analytical Science and Technology, Daejeon, Korea*

MP 308 **The Use of Methionine Sulfoxide Reductases to Reverse Oxidized Methionine for Mass Spectrometry Applications**; Robert Cunningham[1]; Kratika Singhal[2]; Ryan T Fellers[3]; Luca Fornelli[3]; Henrique Dos Santos Seckler[3]; Bhavin Patel[1]; Egle Capkauske[4]; Juozas Siurkus[4]; Philip Compton[3]; John C Rogers[1]; Neil L Kelleher[3]; *[1]Thermo Fisher Scientific, Rockford, IL; [2]University of Illinois at Chicago, Rockford, IL; [3]Northwestern University, Evanston, IL; [4]Thermo Fisher Scientific, Vilnius, Lithuania*

MP 309 **Top-Down sequence-specific copper and zinc retention from ECD and ETD of superoxide dismutase for ALS spinal cord**; Joe Beckman[1]; Yury V Vasil'ev[2, 3]; Nathan I Lopez[2, 3]; Valery G Voinov[3, 4]; *[1]Linus Pauling Institute, Corvallis, OR; [2]e-MSion, Inc, Corvallis, Oregon; [3]Oregon State University, Corvallis, OR; [4]Linus Pauling Institute, Oregon State University Corvallis, OR*

MP 310 **Two-Dimensional Time-Resolved LC-MS Deconvolution for Intact Mass Analysis of Biological Drugs**; Peter Haberl[1]; Joe Shambaugh[2]; David Bush[2]; Maurizio Bronzetti[2]; Cassandra Wigmore[3]; Arnd Brandenburg[3]; *[1]Genedata GmbH, Munich, Germany; [2]Genedata Inc, Lexington, MA; [3]Genedata AG, Basel, Switzerland*

MP 311 **Development of LC/MS/MS Bioanalytical Method for Quantitative Determination of Intact Insulin Glargine and Human Insulin in Plasma**; ZHAOQI ZHAN[1]; Zhe Sun[2]; Jie Xing[1]; Edwin Zhi Wei Ting[1]; *[1]Shimadzu (Asia Pacific) Pte Ltd, Singapore, Science Park 1; [2]Customer Support Centre, Shimadzu (Asia Pacific) Pte Ltd 79 Science Park Drive #02-01/08, Singapore*

MP 312 **Enabling Mass Spectrometric Analysis of Intact Proteins in Native Conditions on A Hybrid Quadrupole-Orbitrap Mass Spectrometer**; Kai Scheffler[1]; Eugen Damoc[2]; Aaron Bailey[3]; Jonathan L Josephs[3]; *[1]Thermo Fisher Scientific, Dreieich, DE; [2]Thermo Fisher Scientific, Bremen, DE; [3]Thermo Fisher Scientific, San Jose, CA*

MP 313 **Is Online Detection by Native ESI MS Beneficial to Size Exclusion Chromatography?**; Cedric Bobst[1]; Igor A Kaltashov[1]; *[1]University of Massachusetts Amherst, Amherst, MA*

MP 314 **BAC-PAGE: A Novel Proteomics Workflow Using Dissolvable Polyacrylamide Gel Electrophoresis**; Nobuaki Takemori[1]; Ayako Takemori[1]; Piriya Wongkongkathep[2]; Rachel R Ogorzalek Loo[2]; Joseph A Loo[2]; *[1]Ehime University, Toon, Japan; [2]UCLA, Los Angeles, CA*

MP 315 **Impact of Phosphorylation on the Ionization Efficiency of Intact Proteins: A Systematic Investigation**; Zhijie Wu[1]; Wenxuan Cai[2]; Bifan Chen[1]; Ziqing Lin[2]; Zachery Gregorich[2]; Ying Ge[1]; *[1]Department of Chemistry, UW-Madison Madison, WI; [2]University of Wisconsin Madison, Madison, WI*

MP 316 **Magnetic Resin Microreactor for Affinity-Capture Top-Down Mass Spectrometry**; Delafield Daniel[1]; Zhe Wang[1]; Woodard Toni[1]; Si Wu[1]; *[1]University of Oklahoma, Dept. of Chem & Biochem Norman, OK*

MP 317 **High Resolving Power Isoelectric Focusing for Routine and Comprehensive Proteoform Interrogations**; Michael Tran[1]; John Corbett[1, 2]; Daniel A Plymire[2]; Casey Wing[1]; Steven M Patrie[1, 2]; *[1]University of Texas at Dallas, Richardson, TX; [2]University of Texas Southwestern, Dallas, TX*

MP 318 **On the Reliability and Reproducibility of 2D Isoelectric Focusing and Reversed-Phase Chromatography with FTMS for Intact Label-free Proteoform Quantitation**; John Corbett[1, 2]; Michael Tran[1]; Casey Wing[1]; Daniel Plymire[2]; Steven Patrie[1, 2]; *[1]University of Texas at Dallas, Richardson, TX; [2]University of Texas Southwestern Medical Center, Dallas, TX*

MP 319 **Data Independent Characterization of Proteins from 2D CID Fingerprints Generated through Collision Energy Scanning**; Boris Kozlov[1]; Jeff Brown[1]; John Hoyes[1]; *[1]Waters, Wilmslow, United Kingdom*

ION ACTIVATION/DISSOCIATION
320 - 340

MP 320 **Potential Fragmentation of the Hydroxy Carbene**; Sabyasachy Mistry; *Purdue University, West Lafayette, IN*

MP 321 **Photodissociation of Triethylphosphonium Charge Tagged Peptides**; Nick DeGraan-Weber[1]; James P Reilly[1]; *[1]Indiana University Dept. Chemistry, Bloomington, IN*

MP 322 **Structural Determination of Peptides Containing Multiple Acceptors using Action-EET**; Lance E Talbert[1]; Ryan R Julian[1]; *[1]University of California, Riverside, Riverside, CA*

MP 323 **Implementation and Bench-Marking of Dual-Polarity 193 nm UVPD for Bottom-Up Proteomics on the Thermo Orbitrap Fusion Tribrid Mass Spectrometer**; Sylvester Greer[1]; Jennifer S Brodbelt[2]; *[1]Univ of Texas at Austin, Austin, Texas; [2]University of Texas at Austin, Austin, TX*

MP 324 **Reaction Dynamics of Small Sulfur-Containing Molecules with a Hydrated Electron in the Gas Phase**; Chi-Kit Siu[1]; Wai-Kit Tang[2]; *[1]City University of Hong kong, Hong Kong; [2]City University of Hong Kong, Hong Kong SAR, Hong Kong*

MP 325 **Kinetic Energy Release and Fragmentation Pattern of Substituted Anilines after Collision Activation**; Sarah Seulen[1]; Tassilo Muskat[1]; Jürgen Grotemeyer[1]; *[1]Institute for Physical Chemistry, Christian-Albrechts-University at Kiel, Kiel, Germany*

MP 326 **Photodissociation Action Spectroscopy of Fluorescent Dye Molecules in the Gas Phase**; Elena Mitrofanov[1]; Tassilo Muskat[1]; Claus Gernert[1]; Jurgen Grotemeyer[1]; *[1]Institute for Physical Chemistry, Christian-Albrechts-University at Kiel, Kiel, Germany*

MP 327 **Difference of Electron Capture and Transfer Dissociation Mass Spectrometry on Zn2+-Polyhistidine Complexes in the Absence of Remote Protons**; Daiki Asakawa[1]; Edwin De Pauw; *[1]AIST, Tsukuba, Ibaraki*

MP 328 **Glycan and Peptide Analysis with Iron Oxide Nanoparticle MALDI Matrices**; Joseph Mercer Wilson[1]; Qiaoli Liang[1]; Jennifer Sherwood[1]; Thomas Macher[1]; Yuping Bao[1]; Carolyn J Cassady[1]; *[1]University of Alabama, Tuscaloosa, AL*

MP 329 **Characterized Fragmentation of Neutral Carbohydrates Induced by Quartz-Tungsten-Halogen Light Prior to MALDI Mass Spectrometry**; Yu-Meng Ou[1]; Yin-Hung Lai[1]; Yi-Sheng Wang[1]; *[1]Genomics Research Center, Academia Sinica Taipei, Taiwan*

MP 330 **Optimizing Production of Selected Product Ions for SRM Analysis in a Quadrupole Collision Cell**; Bennett Kalafut[1]; Harald Oser[1]; *[1]Thermo Fisher Scientific, San Jose, California*

MP 331 **Cationized Polymer Fragmentation: Energetic and Mechanistic Effects of End-group Substitution**; Jordan M. Rabus[1]; Benjamin Bythell[1]; *[1]University of Missouri-St. Louis, St. Louis, MO*

MP 332 **The Collision of a Hypervelocity Massive Projectile with Free-Standing Graphene: Investigation of Secondary Ion Emission and Projectile Fragmentation**; Sheng Geng[1]; Stanislav S Verkhoturov[1]; Michael J Eller[1]; Emile A Schweikert[1]; *[1]Texas A&M University, College Station, TX*

MP 333 **Comparison of Ion Temperatures in a Linear Trap using the Ambient Ionization Techniques: ESI, DART and APCI**; George N. Khairallah[1]; Morphy Dumlao[2]; Richard A J O'Hair[3]; William A Donald[2]; *[1]Bio21 Inst,Uni of Melbourne and Accurate Mass Scientific P/L, Melbourne, VIC; [2]University of New South Wales, Sydney, Australia; [3]University of Melbourne, Victoria, Australia*

MP 334 **Exploring the Combination of Helium Charge Transfer Dissociation (He-CTD) and Hydrogen Deuterium Exchange Tandem Mass Spectrometry (HDX-MS/MSn)**; Gregory C. Donohoe[1]; Li Pengfei[1]; Glen P. Jackson[1]; Stephen J Valentine[1]; *[1]West Virginia University, Morgantown, WV*

MP 335 **Dissociation of Gas-Phase, Triply-Charged Lanthanide and Doubly-Charged Actinide Complexes by Multiple-Stage Tandem Mass Spectrometry**; Cassandra Hanley[1]; Michael Van Stipdonk[1]; *[1]Duquesne University, Pittsburgh, PA*

MP 336 **Chemical Derivatization to Enhance 266 nm Ultraviolet Photodissociation for Proteomics**; M. Montana Quick[1]; Rachel Mehaffey[1]; Lucas D. Akin[1]; Jennifer S Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX*

MP 337 **Dissociation of Gas-Phase, Doubly-Charged Uranyl-Acetone and Uranyl-Dimethyl Sulfoxide Complexes by Collisional Activation and Infrared Photodissociation**; Theodore Corcovilos[1]; Cassandra Hanley[1]; Evan Perez[1]; Benjamin J Bythell[2]; Michael J. Van Stipdonk[1]; *[1]Duquesne University, Pittsburgh, PA; [2]University of Missouri-St.Louis, St. Louis, MO*

MP 338 **General Rules of Fragmentations Evidencing Lasso Structures in CID and ETD**; Kevin Jeanne Dit Fouque[1]; Helene Lavanant[1]; Severine Zirah[2]; Julian D. Hegemann[3]; Marcel Zimmermann[3]; Mohamed A. Marahiel[3]; Sylvie Rebuffat[2]; Carlos Afonso[1]; *[1]Normandie Univ, CNRS UMR 6014 COBRA Mont St Aignan, France; [2]National Museum of Natural History, CNRS-MNHN UMR 7245 Paris, FRANCE; [3]Philipps University Marburg, Department of Chemistry Biochemistry LOEWE Marburg, Germany*

MP 339 **A Novel Macrobicyclic Polyether with Carbon Bridgehead Atoms: Complexation with Alkali Metals**; Anupriya Anupriya[1]; David V Dearden[1]; *[1]Brigham Young University, Provo, UT*

MP 340 **Ab InitioPrediction of Collision-Induced Dissociation Mass Spectra**; Li Li[1]; Rodger Mensing[2]; Benjamin Janesko[2]; *[1]University of Texas at Arlington, Arlington, TX; [2]Texas Christian University, Fort Worth, TX*

ION MOBILITY: APPLICATIONS (OTHER/INSTRUMENTATION)
341 - 373

MP 341 **Characterization of i-motif DNA Kinetically Trapped Folding Intermediates Using nanoESI-TIMS-MS and Molecular Dynamics**; Alyssa Garabedian[1]; David Butcher[1]; Jennifer Lippens[2]; Jaroslava Miksovska[1]; Prem Chapagain[1]; Daniele Fabris[2]; Mark E Ridgeway[3]; Melvin Park[3]; Francisco Fernandez-Lima[1]; *[1]Florida International University, Miami, FL; [2]The RNA Institute, University at Albany Albany, NY; [3]Bruker Daltonic, Billerica, MA*

MP 342 **Analysis of Synthetic Nucleotides using Accurate Mass and Ion Mobility**; Cynthia Sanderson[1]; Sushmit Maitra[1]; Keith Goodman[1]; *[1]SCIEX, Concord ON, Canada*

MP 343 **High Resolution Ion Mobility-Mass Spectrometry for Separation of isomers in Natural Products and Complex Mixtures**; Michael Groessl[1]; Sonja Klee[1]; Stephan Graf[1]; *[1]TOFWERK, Thun, Switzerland*

MP 344 **Frequency Encoding the Mobility of Isomeric Glycans: Separations Using Drift Tube Ion Mobility and Tandem Mass Spectrometry**; Kelsey A Morrison[1]; Brad K Bendiak[2]; Brian H Clowers[1]; *[1]Washington State University, Pullman, WA; [2]University of Colorado, Denver - Anschutz Medical Campus, Denver, CO*

MP 345 **Rapid and High-Throughput Detection and Quantitation of Radiation Biomarkers in Human and Nonhuman Primates by Differential Mobility Spectrometry-Mass Spectrometry**; Zhidan Chen[1]; Stephen L. Coy[1]; Evan L. Pannkuk[2]; Evagelia C. Laiakis[2]; Adam B. Hall[1]; Albert J Jr Fornace[2]; Paul Vouros[1]; *[1]Northeastern University, Boston, MA; [2]Georgetown University, Washington, DC*

MP 346 **Enhancing Carbohydrate Isomer Separation with Ion Mobility Spectrometry-Mass Spectrometry**; Xueyun Zheng[1]; Xing Zhang[2]; Nathaniel S Schocker[3]; Roger A Ashmus[3]; Igor C Almeida[3]; Keqi Tang[1]; Catherine E Costello[4]; Richard D Smith[1]; Katja Michael[3]; Erin Baker[1]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]University of Colorado, Denver, CO; [3]University of Texas, El Paso, TX; [4]Boston University School of Medicine, Boston, MA*

MP 347 **Evaluation of Collision Cross Section Calibrants for Structural Analysis of Lipids by Traveling Wave IM-MS**; Kelly M Hines[1]; Jody C May[2]; John A McLean[2]; Libin Xu[1]; *[1]University of Washington, Seattle, WA; [2]Vanderbilt University, Nashville, TN*

MP 348 **Rapid Differentiation of Bile Acid Isomers Using Sodiated Multimer Complexes with Ion Mobility - Mass Spectrometry**; Robin H.J. Kemperman[1]; Christopher D Chouinard[1]; Richard A Yost[1]; *[1]University of Florida, Gainesville, FL*

MP 349 **Machine Learning-Enabled Collisional Cross Section Predictor (CCSP) for Identification of Unknown Lipids**; Molly T Soper-Hopper[1]; Nga Lee Ng[1]; Nicholas V Hud[1]; Charles Liotta[1]; Facundo M Fernandez[1]; *[1]Georgia Institute of Technology, Atlanta*

MP 350 **Reducing Isobaric Species by Differential Mobility Spectrometry (DMS) for infusion-based lipidomics**; Goncalo Vale[1]; Jeff McDonald[1]; Paul RS Baker[2]; *[1]UT Southwestern Medical Center, Dallas, TX; [2]Sciex, Framingham, MA*

MP 351 **Characterization of Exposome Compounds in Human Biofluids Using LC-ESI-Ion Mobility QTOF Mass Spectrometry**; Yunjia Lai[1]; Mine Palazoglu[1]; Oliver Fiehn[1]; *[1]UC Davis Genome Center, Davis, CA*

MP 352 **Increasing the Resolving Power of Differential Mobility to Supplement (or Eliminate) LC Separation**; J.C. Yves Leblanc[1]; Chang Liu[2]; Larry J Campbell[2]; Brad Schneider[2]; *[1]SCIEX, Concord, ON, ON; [2]SCIEX, Concord ON, Canada*

MP 353 **Enhanced Ion Mobility Separation of Derivatized Isobaric Steroids by DESI and MALDI TOF Mass Spectrometry**; Mark Towers[1]; MicShazia Khan[2]; C.Logan C Mackay[3]; Ruth Andrew[2]; Emmanuelle Claude[1]; *[1]Waters Corporation, Wilmslow, UK; [2]Queen's Medical Research Institute, University of Edinburgh, Edinburgh, UK; [3]SIRCAMS, University of Edinburgh, Edinburgh, UK*

MP 354 **Rapid separation of Vitamin D epimers in human serum by Liquid Chromatography Ion Mobility Mass Spectrometry**; Nicholas Oranzi[1]; Christopher D Chouinard[1]; Richard A Yost[1]; *[1]University of Florida, Gainesville, FL*

MP 355 **Combining Rapid Isomer Separations and Physicochemical Property Predictions for Drug Molecules with Differential Mobility Spectrometry**; CHANG LIU[1]; Yves J C LeBlanc[1]; Jefry Shields[2]; Hui Zhang[2]; John S Janiszewski[2]; Christian Ieritano[3]; Luke Melo[3]; Evan Shepherson[3]; Mitch Verbuyst[3]; Moaraj Hasan[3]; Dalia Naser[3]; Scott W Hopkins[3]; Larry J Campbell[1]; Tim Hoffman[1]; *[1]SCIEX, Concord, ON; [2]Pfizer, Groton, CT; [3]University of Waterloo, Waterloo, Ontario (ON)*

MP 356 **Complicated Natural Product Analysis Using Liquid Chromatography (LC) – Drift Tube Ion Mobility (DTIM) Mass Spectrometry (MS)**; Xin Ma[1]; Tao Bo[2]; *[1]Agilent Technologies, Beijing, China; [2]Agilent Technologies (China) Limited, Beijing, China*

MP 357 **Structural Database of Secondary Metabolites for Natural Product Discovery: Ion Mobility-Mass Spectrometry Measurements in Nitrogen and Helium Drift Gases**; Andrzej Balinski[1]; Jody C May[1]; Brian O Bachmann[1]; Sarah M Stow[1]; John A McLean[1]; *[1]Vanderbilt University, Nashville, TN*

MP 358 **Determining Molecular Modifications by ESI Ion Mobility Mass Spectrometry (ESI IM-MS)**; Alfred L. Yergey[1]; Paul S Blank[1]; Stephanie M Cologna[2]; Peter S Backlund[1]; Allan Darling[3]; *[1]NIH, Bethesda, MD; [2]University of Illinois, Chicago, IL; [3]Vtesse Inc, Gaithersburg, MD*

MP 359 **Analysis of Propolis Extracts and Isomeric Flavonoid Mixtures Using Trapped Ion Mobility QTOF-MS**; Sven Wolfgang Meyer[1]; Alexander Harder[2]; Detlev Suckau[3]; Peter Sander[3]; *[1]Bruker Daltonic GmbH, Bremen, Bremen; [2]Bruker Daltonic, Bremen, Germany; [3]Bruker Daltonic GmbH, Bremen, Germany*

MP 360 **Investigation of the Cu(I) and Zn(II) Binding Characteristics of Methanobactin from *Methylosinus trichosporium* OB3b**; Jacob Watson McCabe[1]; Rajpal Vangala[1]; Laurence Ambrose Angel[1]; *[1]Texas A&M University - Commerce, Commerce, TX*

MP 361 **Single Oligomer Polyurethane Synthesis: Characterization by Ion Mobility-Mass Spectrometry and Computational Strategies**; Tiffany Crescentini[1, 2]; Sarah M Stow[1, 2]; Robert W. Davis[1, 2]; Gary A. Sulikowski[1, 2, 3]; David M Hercules[1, 2]; John A McLean[1, 2]; *[1]Vanderbilt Dept. of Chemistry, Nashville, TN; [2]Vanderbilt University, Nashville, TN; [3]Vanderbilt Institute of Chemical Biology, Nashville, TN*

MP 362 **Characterization of Conformational Isomers of Bisthienylethenes (BTEs) Using Ion Mobility Mass Spectrometry**; Xu Wang[1]; Ming Wang[1]; Alejandro Cisneros[1]; Xiaopeng Li[1]; *[1]Texas State University, San Marcos, TX*

MP 363 **Enhancing Analytical Characterization Workflows of Complex Synthetic Polymeric and Small Molecule Mixtures through Liquid Chromatography Ion Mobility Mass Spectrometry (LC-IM-MS)**; John Patrick O'Brien[1]; Jeffrey R Gilbert[2]; Bruce M Bell[1]; *[1]The Dow Chemical Company, Midland, MI; [2]Dow AgroSciences, Indianapolis, IN*

MP 364 **Comparison of Ion Mobility Mass Spectrometry Applications on Commercial Drift-Tube and Differential Mobility Based Instruments**; Jeffrey Gilbert[1]; Jesse L Balcer[1]; John O'Brien[2]; David McCaskill[1]; Yelena A Adelfinskaya[1]; Gerrit J Deboer[1]; Cassie Fhaner[2]; Krishnamoorthy Kuppannan[2]; Mary D Evenson[1]; Lisa Buchholz[1]; Bruce Bell[2]; *[1]Dow AgroSciences, Indianapolis, IN; [2]Dow Chemical Company, Midland, MI*

MP 365 **Separation of Positional Isomers of PAHSAs Using LC-MS/MS Coupled with Differential Ion Mobility Mass Spectrometry**; Shaokun Pang[1]; Liling Liu[2]; Xiaorong Liang[2]; Amos Baruch[2]; Leo Wang[1]; Brian Dean[2]; Yuzhong Deng[2]; *[1]SCIEX, Redwood City, CA; [2]Genentech Inc, South San Francisco, CA*

MP 366 **Structural Dependent Section of Calibrants for Accurate Measurement of CCS Values Obtained with Ion Mobility Mass Spectrometry**; Dongwan Lim[1]; Arif Ahmed[1]; Sunghwan Kim[1]; *[1]Kyungpook National University, Daegu, Republic of Korea*

MP 367 **Enantiomer Separation of Amino Acids through Binuclear Copper Bound Complex by Travelling Wave Ion Mobility Mass Spectrometry**; Xiang-Ying Yu[1]; Zhong-Ping Yao[1, 2]; *[1]State Key Laboratory of Chinese Medicine and Molecular Pharmacology (Incubation), Shenzhen Research Institute of The Hong Kong Polytechnic University, Shenzhen, China; [2]Department of Applied Biology and Chemical Technology, The Hong Kong Polytechnic University, Hong Kong, China*

MP 368 **Maintaining Speciation of Reactive Gas-Phase Complexes for the Metals Uranyl, Barium, Cesium and Lanthanum with Sulfoxides using AP-IMS-MS**; Austen Davis[1]; Brian H Clowers[1]; *[1]Washington State University, Pullman, WA*

MP 369 **Ion Mobility Mass Spectrometry of Polyoxometalate Anion Assemblies**; Helene Lavanant[1]; Sebastien Hupin[1]; Michael Groessl[2]; Madeleine Piot[3]; Guillaume Izzet[3]; Carlos Afonso[1]; *[1]Normandie Univ, CNRS UMR 6014 COBRA Mont St Aignan, France; [2]TOFWERK, Thun, Switzerland; [3]Sorbonnes Univ, CNRS UMR 8332 IPMC Paris, France*

MP 370 **Ion Mobility Quadrupole Time-of-Flight Mass Spectrometer Modified for Electron Capture Dissociation of Glycans, Glycoconjugates, Peptides, and Proteins**; Rebecca S. Glaskin[1]; Kenneth Newton[2]; Ruwan T. Kurulugama[2]; George C. Stafford[2]; Valery G. Voinov[3]; Joseph S. Beckman[3]; Douglas F. Barofsky[3]; Catherine E. Costello[1]; *[1]Boston University School of Medicine, Boston, MA; [2]Agilent Technologies, Santa Clara, CA; [3]Linus Pauling Institute, Oregon State University Corvallis, OR*

MP 371 **On-line Parallel Accumulation – Serial Fragmentation (PASEF) for Shotgun Proteomics on a Modified UHR-QTOF Platform**; Scarlet Beck[1]; Florian Meier[1]; Jürgen Cox[1]; Markus Lubeck[2]; Stephanie Kaspar-Schoenefeld[2]; Nicole Drechsler[2]; Niels Goedecke[2]; Melvin Park[3]; Oliver Raether[2]; Matthias Mann[1]; *[1]Max-Planck-Institute of Biochemistry, Martinsried (near Munich), Germany; [2]Bruker Daltonic GmbH, Bremen, Germany; [3]Bruker Daltonic, Billerica, MA*

MP 372 **Bio-Molecule Characterization Using a Novel Ion Mobility Orbitrap Mass Spectrometer**; Sung Hwan Yoon[1]; Thomas Schneider[1]; Tao Liang[1]; Yue Huang[2]; Robert K Ernst[1]; Mikhail E Belov[3]; David R Goodlett[2, 4]; *[1]University of Maryland, Baltimore, MD; [2]Deurion LLC, Seattle, WA; [3]Spectroglyph LLC, Kennewick, WA; [4]University of Maryland Baltimore, Baltimore*

MP 373 **Improvement of Selectivity and Detection Capabilities in Non-Targeted Metabolomics Using Liquid Chromatography with Drift Tube Ion Mobility Mass Spectrometry**; Tim Causon[1, 2]; Teresa Mairinger[1, 2]; Stephan Hann[1, 2]; *[1]University of Natural Resources and Life Sciences (BOKU Vienna), Vienna, AT; [2]Austrian Centre of Industrial Biotechnology (acib), Vienna, AT*

ION MOLECULE, ION/ION, ION/ELECTRON INTERACTIONS 374 - 398

MP 374 **Radical Cations of Nucleobases: A Gas-Phase Reactivity and Structural Elucidation Study**; Michael Lesslie[1]; Lawler T John[1]; Courtney Kanak[1]; Ryzhov Victor[1]; *[1]Northern Illinois University, DeKalb, IL*

MP 375 **Gas-Phase Reactions of the Deprotonated Nucleobases with H, N, and O Atoms**; Charles Nichols[1]; Zhe-Chen Wang[1]; Carl W Lineberger[1]; Veronica M Bierbaum[1]; *[1]University of Colorado, Boulder, CO*

MP 376 **Charge Transfer Dissociation (CTD) of Phosphocholines: Gas-Phase Ion/Ion Reactions between Helium Cations and Phospholipid Cations**; Pengfei Li[1]; Glen P Jackson[1]; *[1]West Virginia University, Morgantown, WV*

MP 377 **DNA/Peptide Complex Ion Dissociations: Survivor Non-Covalent Sites in "Three-Body" Product Ions Independent on Charge Polarity**; Bessem Brahim[1]; Sandra Alves[1]; Jean-claude Tabet[1, 2]; *[1]University Paris VI (UPMC) case 45 UMR 8232 CNRS, Paris Cedex O5, France; [2]CEA, iBiTec-S SPI LEMM Gif Sur Yvette, France*

MP 378 **Modulating the Interaction of Non-Covalent Dimers with Conformationally Restricted Peptides in the Gas Phase**; Huong (Ivy) Thi Huynh Nguyen[1]; Frantisek Turecek[2]; *[1]University of Washington, Department of Chemistry Seattle, WA; [2]University of Washington, Seattle, WA*

MP 379 **Ion/Ion Proton-Transfer Reaction for Improved Negative-Ion Electron Capture Dissociation Efficiency in the Structural Characterization of Nucleic Acids and Proteins**; Kevin M Ileka[1]; Jeremy J Wolff[2]; Kristina Hakansson[1]; *[1]University of Michigan, Ann Arbor, MI; [2]Bruker Daltonic, Billerica, MA*

MP 380 **Origin of the Regioselective [NH3+CO2] Concomitant Losses from Aspartate Predicted by Calculations and Evidenced by 13C and D Labeling**; Pierre Saint Hilaire[1]; Anna Warnet[1]; Ulli Martin Hohenester[1]; Yves Gimbert[2]; Marie-Françoise Olivier[1]; Francois Fenaille[1]; Benoit Colsch[1]; Christophe Junot[1]; Jean-Claude Tabet[3, 4]; *[1]CEA, iBiTec-S, SPI, LEMM,, Gif Sur Yvette Cedex, France; [2]Université Grenoble Alpes et CNRS UMR 5052, Grenoble, France; [3]University Paris VI (UPMC) case 45 UMR 7201 CNRS, Paris Cedex O5 , Ile de France; [4]CEA, iBiTec-S SPI LEMM Gif-sur-Yvette, France*

MP 381 **Cation Influence on the Competitive Ion-Dipole and Ion-Ion Interaction: Distinction of Hexose Phosphate Structural Isomers Using Basic Amino Acids**; Ekaterina Dariy[1]; Sandra Alves[2]; Alain Perret[3]; Jean-claude Tabet[2]; *[1]CEA-Genoscope/UMR8030, Evry, Île-de-France; [2]UPMC-IPCM/CSOB/UMR8232, Paris Cedex 05, France; [3]CEA-Genoscope/UMR8030, Evry, France*

MP 382 **Distinguishing Hexose Isomers by Lithiated Ion Adduction to Water**; Matthew Campbell[1]; Chen Dazhe[2]; Gary L. Glish[2]; *[1]UNC, Chapel HIll, NC; [2]UNC-Chapel Hill, Chapel Hill, NC*

MP 383 **Ion-Molecule Reactions of Fe+ and FeO+ with Ozone: Temperature Dependent Kinetics and Reaction Pathways**; Tri Le[1]; Gregory Miller[1]; Joshua Melko[1]; *[1]University of North Florida, Jacksonville, FL*

MP 384 **Bimolecular Reactions between Water and Metal Dioxide Cations, MO2+: Energetics and Mechanisms of Hydration, Hydrolysis and oxo-Exchange**; Phuong D. Dau[1]; John Gibson[1]; David Dixon[2]; Kirk A. Peterson[3]; Monica Vasiliu[2]; Richard E Wilson[4]; *[1]Lawrence Berkeley National Laboratory, Berkeley, California; [2]University of Alabama, Tuscaloosa, AL; [3]Washington State University, Pullman, WA; [4]Argonne National Laboratory, Argonne, IL*

MP 385 **Dual-Electrospray Synthesis and Reactions**; Shaan Rashid[1]; Paul Michael Mayer[2]; *[1]University of Ottawa, Ottawa, Canada; [2]University of Ottawa, Ottawa, ON*

MP 386 **Efficient and Direct Amide Bond Formation Using a Novel Alcohol/Amine Cross-Coupling Reaction Mediated by Electrospray-Based Photo-catalysis**; Savithra Jayaraj[1]; Qiongqiong Wan[1]; Abraham Badu-Tawiah[1]; *[1]The Ohio State University, Columbus, OH*

MP 387 **Phenylnitrenium Ions: Gas-phase Synthesis, Properties in Selective Alkane Activation, Gas-phase acidity, Hydride Affinity, Electron Affinity, and Electronic states**; Lei Yue[1]; Pan Yuanjiang[1]; Ding Chuanfan[2]; *[1]Zhejiang University, Hangzhou, China; [2]Fudan University, Shanghai, China*

MP 388 **Gas-phase Generation of Protonated CO2by Collision-Induced Elimination of Benzene from Protonated Benzoic Acid**; Sihang Xu[1]; Athula Attygalle[1]; *[1]Stevens Institute of Technology, Hoboken, NJ*

MP 389 **Reactions of Substituted Benzene Anions with N and O Atoms: Chemistry in Titan's Upper Atmosphere and the Interstellar Medium**; Zhechen Wang[1]; Veronica M. Bierbaum[1]; *[1]University of Colorado, Boulder, CO*

MP 390 **Selective Cleavage at Sulfur-Containing Residues via Gas-Phase Platination of Protonated Peptides upon Ion/Ion Reactions with Platinum Trichloride Anion**; David Foreman[1]; Alice L Pilo[1]; Scott A McLuckey[1]; *[1]Purdue University-Department of Chemistry, West Lafayette, IN*

MP 391 **Substituent Effects on the Reactivity of the 2,6-Didehydropyridinium Cation, an Unusual meta-Benzyne**; Xin Ma[1]; Joann P. Max[1]; Duanda Wang[1]; John J. Nash[1]; Hilkka I. Kenttämaa[1]; *[1]Department of Chemistry, Purdue University, West Lafayatte, IN*

MP 392 **Differentiation of Deprotonated Dihydroxybenzene Regioisomers via Ion-Molecule Reactions with Thionyl Chloride**; Hanyu Zhu[1]; Hilkka I Kenttämaa[1]; *[1]Purdue University, West Lafayette, IN*

MP 393 **Reactions of Fe+ with Ozone: Mapping Reaction Pathways**; Gregory Miller[1]; Tri Le[1]; Joshua Melko[1]; *[1]University of North Florida, Jacksonville, FL*

MP 394 **Attempted Generation of the2,4-Didehydro-5-oxyquinolinium Cation Leads to an Oxygen Peribridged Quinolinium Monoradical**; Raghavendhar R Kotha[1]; John J Nash[1]; Hilkka I Kenttamaa[1]; *[1]Department of Chemistry, Purdue University, West Lafayette, IN*

MP 395 **Comparison of the OH-(H2O)n + CH3I, n = 0-2, Rate Constants. Experiment and Simulation**; Jing Xie[1]; Xinyou Ma[2]; Michael J Scott[2]; Olivia Harris[2]; William L Hase[2]; Peter M Hierl[3]; Albert A Viggiano[4]; *[1]Department of Chemistry, University of Minnesota, Minneapolis, MN; [2]Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX; [3]Department of Chemistry, University of Kansas, Lawrence, KS; [4]Air Force Research Laboratory, Space Vehicles Directorate, Kirtland AFB, NM*

MP 396 **Gas-Phase Reactivity of Isomeric σ,σ-Biradicals: A Comparison of 1,4-, 1,3-, and 3,4-Didehydroisoquinolinium Cations**; Lucas Szalwinski[1]; Nelson R Vinueza[1]; John Nash[1]; Hilkka Kenttämaa[1]; *[1]Purdue University-Department of Chemistry, West Lafayette, IN*

MP 397 **Racemization and Isomerization Reactions Induced by High-Velocity Molecular Impacts in the Gas Phase**; Sandra Osburn[1]; Daniel Austin[1]; *[1]Brigham Young University, Provo, UT*

MP 398 **Calculation of Average-Dipole-Orientation Rate Constants for Proton Transfer Reactions between H3O+ and Organic Compounds Using Molecular Mass and Elemental Composition**; Kanako Sekimoto[1, 2]; Shao-Meng Li[3]; Bin Yuan[1, 4]; Abigail Koss[1, 4]; Matthew Coggon[1, 4]; Carsten Warneke[1, 4]; Joost De Gouw[1, 4]; *[1]NOAA Earth System Research Laboratory, Boulder, CO; [2]Yokohama City Univ., Yokohama, Japan; [3]Environment Canada, Tronto, Canada; [4]Cooperative Institute for Research in Environmental Sciences, University of Colorado Boulder, Boulder, CO*

ION SPECTROSCOPY
399 - 411

MP 399 **Action-Excitation Energy Transfer Illuminates the Impact of Amino Acid Epimerization and Isomerization on Peptide Structure**; Dylan Riggs; *University of California - Riverside, Riverside, CA*

MP 400 **Microsolvation by 18-Crown-6 as a Method for Preserving Native-Like Protein Structure**; James Bonner[1]; Nathan Hendricks[1]; Ryan R Julian[1]; *[1]UC Riverside, Riverside, CA - California*

MP 401 **Thermochemical Differences in Isomeric Oligopeptides: Structural Insights Using IRMPD Spectros**; Patrickhenry Batoon[1]; Jianhua Ren[2]; Jos Oomens[3]; Giel Berden[3]; *[1]University of the Pacific , Stockton, CA; [2]University of the Pacific, Stockton, CA; [3]FELIX Laboratory - IMM - Radboud University, Nijmegen, The Netherlands*

MP 402 **Deep Molecular Structure Probing in MSn by IR Ion Spectroscopy: Deamidation Reaction Networks of Gln and Asn-Containing Dipeptides**; Jos Oomens[1, 2]; Lisanne JM Kempkes[1]; Jonathan Martens[1]; Josipa Grzetic[1]; Giel Berden[1]; *[1]Radboud University, Nijmegen, Netherlands; [2]University of Amsterdam, Amsterdam, The Netherlands*

MP 403 **Infraredspectroscopy of Protonated and Radical Cationic Triphenylamine**; Giel Berden[1]; Md. Musleh Uddin Munshi[1]; Jonathan Martens[1]; Jos Oomens[1]; *[1]FELIX Laboratory - IMM - Radboud University, Nijmegen, The Netherlands*

MP 404 **The Remarkable Ionic Coordinating Ability of All-cis 1,2,3,4,5,6 Cyclohexane in the Gas Phase**; Terry Mcmahon[1]; Blake Ziegler[2]; Michael Lecours[2]; Rick Marta[2]; Eric Filliion[2]; Scott W Hopkins[3]; David O'Hagan[4]; Keddie Neil[4]; *[1]University of Waterloo, Waterloo, ON; [2]University of Waterloo, Waterloo ON, Canada; [3]University of Waterloo, Waterloo, Ontario (ON); [4]University of St. Andrews, St. Andrews, UK*

MP 405 **Laser Spectroscopic Investigation on Dichlorofluorobenzenes by Means of Resonance Enhanced Multiphoton Ionization and Mass Analyzed Threshold Ionization**; Sascha Krüger[1]; Jürgen Grotemeyer[1]; *[1]Institute for Physical Chemistry; Christian-Albrechts-University at Kiel, Kiel, Germany*

MP 406 **New Insights into the Combustion Chemistry of Butane Isomers in Premixed Low-Pressure Hydrogen Flames by Imaging Photoelectron Photoion Coincidence Spectroscopy**; Thomas Bierkandt[1]; Yasin Karakaya[1]; Dominik Krüger[2]; Patrick Hemberger[3]; Patrick Oßwald[2]; Markus Köhler[2]; Tina Kasper[1]; *[1]University of Duisburg-Essen, Duisburg, Germany; [2]Institute of Combustion Technology, German Aerospace Center, Stuttgart, Germany; [3]VUV Spectroscopy Group, Swiss Light Source, Paul Scherrer Institute, Villigen, Switzerland*

MP 407 **Förster Resonance Energy Transfer as a Distance Probe for Gas-phase Ubiquitin Ions**; Jocky Chun Kui Kung[1]; Martin F Czar[1]; Benjamin Schuler[2]; Rebecca A Jockusch[1]; *[1]University of Toronto, Toronto ON, Canada; [2]University of Zurich, Zurich, Switzerland*

MP 408 **Alkali Cation Chelation in Cold β-O-4 Tetralignol Complexes**; Andrew F DeBlase[1]; Eric T Dziekonski[1]; John R Hopkins[1]; Nicole L Burke[1]; Huaming Sheng[1]; Hilkka I Kenttamaa[1]; Scott A McLuckey[1]; Timothy S Zwier[1]; *[1]Purdue University-Department of Chemistry, West Lafayette, IN*

MP 409 **Development and Performance of a Mass Selective Linear Ion Trap for Infrared Predissociation Spectroscopy of Metabolites**; Adam Cismesia[1]; Nicolas C Polfer[1]; *[1]University of Florida, Gainesville, Florida*

MP 410 **Photodissociation Dynamics in Infrared Multiple Photon Dissociation Monitored by Time-of-Flight Mass Spectrometry**; Matthew Bell[1]; Nicolas C Polfer[1]; *[1]University of Florida, Gainesville, FL*

MP 411 **Gas Phase Fluorescence Spectroscopy for the Study of Catalytic Nitrogen-Containing Heterocycles**; Alessandra Ferzoco[1]; Vaishnavi Rajagopal[1]; *[1]Rowland Institute at Harvard, Cambridge, MA*

LC-MS: CHROMATOGRAPHY AND SOFTWARE (PART 1)
412 - 440

MP 412 **Demonstration of Automated On-The-Fly Retention Time Updating and SRM Method Visualization for Targeted Peptide Quantitation**; Susan Abbatiello[1]; Qingyu Song[2]; Mary Blackburn[2]; Jacek W Sikora[3]; Paul

Martin Thomas[3]; Neil Kelleher[3]; Yupeng Zheng[3]; Vane Dhevi Sanghvi[2]; *[1]Thermo Fisher Scientific, Cambridge, MA; [2]Thermo Fisher Scientific, San Jose, CA; [3]Kelleher Research Group, Evanston, IL*

MP 413 **An Interactive Skyline Tool for Flagging Incorrectly Chosen Peptides Peaks Across Data-Independent Acquisition Experiments: AT-Peptide Peak Picking (AT-P3)**; Andy Lin[1]; Jarrett D Egertson[1]; Brooke Nuun[1]; Michael J MacCoss[1]; *[1]University of Washington, Seattle, WA*

MP 414 **Column Performance:Comparison of Superficially Porous Particle (SPP) to Fully Porous Particles (FPP)** ; Rob Freeman[1]; Sharon Lupo[1]; Shun-Hsin Liang[1]; Frances Carroll[1]; Ty Kahler[1]; Susan Steinike[1]; *[1]Restek Corporation, Bellefonte, PA*

MP 415 **High Resolution LC/MS analysis of Therapeutic Oligonucleotides on a New Porous Polymer-Based Reversed Phase Column**; Shanhua Lin[1]; Julia Baek[1]; Jim Thayer[1]; Hongxia Wang[2]; Jonathan L Josephs[2]; Xiaodong Liu[1]; *[1]Thermo Fisher Scientific, Sunnyvale, CA; [2]Thermo Fisher Scientific, San Jose, CA*

MP 416 **Slightly Bigger is Better: Nano-LCMS with 100um ID columns**; Brett Larsen[1]; Joshua Sandor[1]; Meghan McFadden[1]; Anne-Claude Gingras[1, 2]; *[1]LTRI, Toronto, Canada; [2]Department of Molecular Genetics, University of Toronto, Toronto, Canada*

MP 417 **Improving Sensitivity in LC/MS with Multi-Dimensional Chromatography**; Thomas E. Wheat[1]; Amanda B. Dlugasch[2]; Patricia R. McConville[2]; *[1]Waters Corporation, Hopedale, MA; [2]Waters, Milford, MA*

MP 418 **Maximizing Flexibility: A Gas and Temperature Enabled Chip-Based Solution for Nanoflow and Microflow LC-MS**; Helena Svobodova[1]; Aaron Dewberry[1]; Amanda Berg[2]; Gary A Valaskovic[1]; *[1]New Objective, Woburn, MA; [2]New Objective, Inc., Woburn, MA*

MP 419 **Achieving High Proteome Coverage by Miniaturization of HPLC Columns**; Annie Moradian [1]; Roxana Eggleston-Rangel[1]; Michael Sweredoski[1]; Sonja Hess[1]; *[1]California Institute of Technology, Pasadena, CA*

MP 420 **Sphingolipid Profiling Using Robust and Sensitive LC-MS-MS Method**; Shachi Saluja[1]; DIpankar Malakar[2]; Manoj Pillai[2]; Avinash Bajaj[1]; Ujjaini Dasgupta[3]; *[1]Regional Centre for Biotechnology, Faridabad, India; [2]Sciex, Gurgaon, India; [3]Amity University, Gurgaon, India*

MP 421 **Evaluation of Critical Column Parameters for Use in Supercritical Fluid Chromatography by SFC-MS**; Alison Wicker[1]; Doug D. Carlton Jr. [1]; Ty Kahler[2]; Kevin A Schug[1]; *[1]University of Texas at Arlington, Arlington, TX; [2]Restek Corporation, Bellefonte, PA*

MP 422 **Advancing Separation Sciences under Alkali Conditions Using a Novel C18 Column for LC-MS**; Itaru Yazawa[1]; Yasuo Yamamori[2]; Hiroshi Tachikawa[2]; *[1]Imtakt Corporation, Kyoto, Japan; [2]Imtakt Corporation, Kyoto, Japan*

MP 423 **Analysis of Antioxidants in Yam (Dioscorea alata L. var. Purpurea (Roxb.) M. Pouch.) by HILIC- UV-ECD-MS**; Chih-Hsien Wang[1]; Gao-Fong Chang[1]; Wenlung Chen[1]; Tsai-Fei Yu[1]; Ya-Chi Feng[1]; Kuo-Lung Ku[2]; *[1]Department of Applied Chemistry,National Chiayi University, Chiayi City, Taiwan; [2]National Chiayi University, Chiayi City, Chiayi*

MP 424 **Displacement Chromatography Applied for Two-Dimensional Liquid Chromatography Coupled to Tandem Mass Spectrometry for Analysis of Complex Biomolecule Mixtures**; Hartmut Schlüter[1]; Marcel Kwiatkowski[2]; *[1]UKE - Mass Spec Proteomics, Hamburg, Hamburg; [2]UKE - Mass Spec Proteomics, Hamburg, Germany*

MP 425 **Combined New Approaches for Improved Quantitative and Qualitative LC-MS**; Stephan Altmaier[1]; Hans Griesinger[1]; Michael Schulz[1]; *[1]Merck, Darmstadt, Germany*

MP 426 **Rapid Separation and Determination Of 25-Hydroxy Vitamin D2 / D3 in Serum By UHPLC-MS/MS Using A Novel C18-PFP Stationary Phase** ; Geoffrey Faden[1]; Alan P McKeown[2]; *[1]MACMOD Analytical Inc., 103 Commons Court PO Box 587 Chadds Ford, PA 19317; [2]Advanced Chromatography Technologies Ltd, Aberdeen, -*

MP 427 **Separation and Low Level Determination Of Catecholamines: Epinephrine, Norepinephrine and Dopamine from Plasma By UHPLC-MS/MS Using A Novel C18-PFP Column**; Edward Faden[1]; Alan P McKeown[2]; *[1]MACMOD Analytical Inc., 103 Commons Court PO Box 587 Chadds Ford, PA 19317; [2]Advanced Chromatography Technologies Ltd, Aberdeen, -*

MP 428 **LC/MS as a Monitoring Technique for (semi) Preparative Electrochemical Metabolite Synthesis**; Lisa Frensemeier[1]; Uwe Karst[1]; *[1]University of Münster, Münster, DE*

MP 429 **Increased MS Protein Identification Rates Using 75 cm Long nano LC C18 Separation Columns: Pushing the Limits of Bottom-Up Proteomics**; Daniel Lopez-Ferrer[1]; Michael Blank[1]; Stephan Meding[2]; Aran Paulus[1]; Romain Huguet[1]; Remco Swart[2]; Andreas FR Huhmer[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Germering, Germany*

MP 430 **Influencing the Selectivity of Small Proteins and Peptides on the Raptor™ ARC-18**; Susan Steinike[1]; Shun-Hsin Liang[1]; Sharon Lupo[1]; Frances Carroll[1]; Ty Kahler[1]; *[1]Restek Corporation, Bellefonte, PA*

MP 431 **Extraction and Ionization Efficiency in On-line Supercritical Fluid Extraction and Chromatography–Mass Spectrometry for Protease Inhibitors and Steroids in Blood**; Laura Akbal[1]; Michel Raetz[1]; Kyoko Watanabe[2]; Yasuhiro Funada[2]; Gérard Hopfgartner[1]; *[1]University of Geneva, Geneva, Switzerland; [2]Shimadzu, Kyoto, Japan*

MP 432 **Maximizing Throughput of Shotgun Proteomics by Increasing the Internal Diameter of Nano-Capillary Columns**; Yuan-wei Nei[1]; Danielle B Gutierrez[1]; William J Burns[2]; Ashley T Jordan[2]; Jeremy L Norris[1]; Richard M Caprioli[1]; *[1]Vanderbilt University MSRC, Nashville, TN; [2]Vanderbilt University Medical Center, Nashville, TN*

MP 433 **Fast Chromatography For Quantitative Proteomics Workflows**; Alina Astefanei[1]; Garry Corthals[2]; Petra Jansen[1]; Michelle Camenzuli[1]; Andrea Gargano[1]; *[1]University of Amsterdam, Amsterdam, The Netherlands; [2]University of Amsterdam, Amsterdam, ZH*

MP 434 **Improved Sensitivity for Characterization of Sulfonamides and Trimethoprim in Honey Using QuEChERS Extracts with LC-MS/MS**; Hernando Escobar[1]; Jeffrey H Dahl[1]; Eddie Medina[1]; Christopher T Gilles[1]; *[1]Shimadzu Scientific Instruments, Inc., Columbia, MD*

MP 435 **Quantitative Analysis of Oligonucleotides Using Liquid Chromatography Coupled with High Resolution/ Accurate Mass (HR/AM) Mass Spectrometry**; Nidhi Jaiswal[1]; David M Good[2]; Marc Browning[1]; Benjamin Johnson[1]; Emily Measom[1]; Cassidy Hatch[1]; Min Meng[1]; Scott A Reuschel[1]; Troy Voelker[1]; *[1]Covance, Salt Lake City, UT; [2]Covance, Madison, WI*

MP 436 **Complementary ERLIC and RPLC Online Separations Significantly Expand Sequence Coverage in MS-Based Proteomic and Proteogenomic Studies**; Candace Guerrero[1]; Pratik D Jagtap[1]; James Johnson[2]; Thomas F McGowan[2]; Tim Griffin[3]; *[1]University of Minnesota, Minneapolis, MN; [2]University of Minnesota Supercomputing Institute, Minneapolis, MN; [3]University of Minnesota at Twin Cities, Saint Paul, MN*

MP 437 **A Direct Comparison between Ultrafiltration and Online Size Exclusion Affinity Selection Mass Spectrometry Methods**; Christopher Reutter[1]; Manuel Molina-Martin[2];

Elizabeth Wright[1]; Jibo Wang[1]; Ryan Bernhardt[1]; Kevin McLeaster[1]; Eduardo Harguindey[2]; Miriam del Prado[2]; Alfonso Espada[2]; Juan Espinosa[2]; Michael J Chalmers[1]; Keith Burton[1]; *[1]Eli Lilly and Company, Indianapolis, IN; [2]Eli Lilly and Company, Alcobendas, Spain*

MP 438 **An Online 2D RP-RP LC/MRM-MS Method Provides Higher Sample Throughput for the Analysis of the Human Plasma Proteome**; Richard R Vincent[1]; Andrew J Percy[2]; Dominik Domanski[1, 3]; Christoph H. Borchers[1, 2, 4]; *[1]Segal Cancer Proteomics Center, Lady Davis Institute, McGill University, Montreal, QC, Canada; [2]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, CANADA; [3]University of Victoria - Genome BC Proteomics Centre, Victoria, BC; [4]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada*

MP 439 **NanoLC-MS of Intact Histones by 0.5 µm Nonporous Silica Particles for Top-Down Proteomics**; Ximo Zhang[1]; Michael E Hoover[2]; Luca Fornelli[3]; Philip Compton[3]; Michael A Freitas[2]; Neil L Kelleher[3]; Mary Wirth[1]; *[1]Purdue University, West Lafayette, IN; [2]The Ohio State University, Columbus, Ohio; [3]Northwestern University, Evanston, IL*

MP 440 **Autopiquer – Introducing a New Approach to High Confidence Peak Detection**; David Kilgour[1]; Sam Hughes[2]; David J Clarke[3]; Quoc Bao Tran[4]; Clare Coveney[1]; David J Boocock[1]; Logan C Mackay[3]; Young Ah Goo[4]; David R Goodlett[4]; *[1]Nottingham Trent University, Nottingham; [2]University of Edinburgh, Edinburgh, UK; [3]University of Edinburgh, Edinburgh, United Kingdom; [4]University of Maryland School of Pharmacy, Baltimore, MD*

LIPIDS: GENERAL
441 - 456

MP 441 **Selective Extraction of Phospholipids from Biological Sample with Metal Oxide Chromatography for Mass Spectrometry-Based Analysis**; Shota Miyazaki[1]; Yuko Yui[1]; Shigenori Ota[1]; Kosuke Osaka[2]; Mamoru Kyogashima[3]; Atsushi Sato[1]; *[1]GL Sciences Inc., Saitama, Japan; [2]GL Sciences Inc., Tokyo, Japan; [3]Nihon Pharmaceutical University, Saitama, Japan*

MP 442 **Evaluation of Docosahexaenoic Acid Derived Lipid Mediators after Traumatic Brain Injury by a Global LC-MS/MS Method**; Tamil Selvan Anthonymuthu[1]; Lewis Jesse[1]; Andrew A Amoscato[1]; Patrick M Kochanek[1]; Kagan E Valerian[1]; Hulya Bayir[1]; *[1]University of Pittsburgh, Pittsburgh, PA*

MP 443 **Lipidomic Analyses of CEACAM1 Knockout Mouse Liver and Adipose Tissue**; Gabriel Gugiu[1]; Deirdre La Placa[1]; Zhifang Zhang[1]; John E. Shively[1]; *[1]City of Hope, Duarte, CA*

MP 444 **Multiclass Lipid Profiling Using Liquid Chromatography High Resolution Mass Spectrometry with Dielectric Barrier Discharge Ionization**; Felipe J Lara-Ortega[1]; José Robles-Molina[1]; Bienvenida Gilbert-López[2]; Juan F Garcia-Reyes [3]; Antonio Molina-Díaz[1]; Alexander Schütz[4]; Sebastian Brandt[4]; Joachim Franzke[4]; *[1]University of Jaen, Jaen, Es; [2]Csic-Cial, Madrid, Es; [3]University of Jaen, Jaen , Andalucia; [4]Leibniz-Institut für Analytische Wissenschaften, Dortmund, Germany*

MP 445 **Comparison of Different Stationary Phases for Gangliosides Separation**; Ashta Lakshmi Prasad Gobburi[1]; Renliang Zhang[2]; Denise Inman[3]; Anderson J David[4]; *[1]Cleveland State University, Department of Chemistry, Cleveland, OHIO; [2]Cleveland Clinic Lerner Research Institute, Cleveland, OH; [3]Northeast Ohio Medical University, Rootstown, Ohio; [4]Cleveland State University, Department of Chemistr Cleveland, OH*

MP 446 **High Throughput Solid Phase Microextraction: A New Alternative for Lipid Analysis and Cellular Lipidomics**; Afsoon Pajand Birjandi[1]; Vincent Bessonneau[1]; Pawliszyn Janusz[1]; *[1]University of Waterloo, Waterloo ON, Canada*

MP 447 **Characterization of Triglycerides and Lipogenesis of Serum Lipids from Dietary or Hepatic Origin: A LC-MS/MS and GC/MS Stable-Isotope Tracer Approach**; Sergiu P Palii[1]; Grace M Jones[2]; Russell Caccavello[1]; Alejandro Gugliucci[1]; Jean-Marc Schwarz[2, 3]; *[1]Department of Research, College of Osteopathic Medicine, Touro University California, Vallejo, CA 94592; [2]Department of Basic Sciences, College of Osteopathic Medicine, Touro University California, Vallejo, CA 94592; [3]Department of Medicine, University of California San Francisco, San Francisco, CA*

MP 448 **Steroid Profiling Method for Rat Serum and Plasma by Gas Chromatography/Tandem Mass Spectrometry with Large Volume Injection**; Udi Jumhawan[1]; Toshiyuki Yamashita[2]; Motonao Nakao[1]; Kuniyo Sugitate[3]; Takeshi Serino[3]; Ryoichi Sasano[4]; Yoshihiro Izumi[1]; Takeshi Bamba[5]; *[1]Kyushu University, Fukuoka, Japan; [2]Osaka University, Suita, Japan; [3]Agilent Technologies Co. Ltd, Hachioji, Japan; [4]AiSTI SCIENCE CO.,Ltd., Wakayama, Japan; [5]Kyushu University, Fukuoka, Fukuoka*

MP 449 **Unsaturated Cholesteryl Ester Analysis from Human Plasma via Online Photochemical Reaction and nanoESI-MS/MS**; Jia Ren[1]; Elissia Franklin[1]; Yu Xia[1]; *[1]Purdue University, West Lafayette, IN*

MP 450 **Discovery of Endocannabinoids by Untargeted All-Ions Fragmentation High Resolution LC-MS/MS Screen**; Mesut Bilgin[1, 2]; Petra Born[2]; Fezza Filomena[3, 4]; Michael Heimes[5]; Nicolina Mastrangelo[6]; Nicolai Wagner[2]; Carsten Schultz[5]; Mauro Maccarrone[6, 7]; Suzanne Eaton[2]; Andre Nadler[2]; Matthias Wilm[8]; Andrej Shevchenko[2]; *[1]Danish Cancer Society Research Center, Copenhagen, DK; [2]Max Planck Institute for Cell Biology and Genetics, Dresden, DE; [3]Department of Experimental Medicine and Surgery, University of Rome Tor Vergata, Rome, IT; [4]European Center for Brain Research/Fondazione Santa Lucia, Rome, IT; [5]European Molecular Biology Laboratory (EMBL), Heidelberg, DE; [6]Department of Medicine, Campus Bio-Medico University of Rome, Rome, IT; [7]European Center for Brain Research/Fondazione Santa Lucia, via del Fosso di Fiorano 65, Rome, IT; [8]Conway Institute of Biomolecular and Biomedical Research, University College Dublin, Dublin, IE*

MP 451 **Role of Ammonium Salts in the Ionization and Fragmentation of Phosphatidylcholines Found in Krill Oil**; Michael Rush[1]; Richard van Breemen[1]; *[1]University of Illinois College of Pharmacy, Chicago, IL*

MP 452 **Determination of β-Glucocerebrosidase (GBA) Activity through Global and Targeted Lipid Profiling**; Yi Zeng[1]; Sangwon Min[1]; Baris Bingol[1]; Wendy Sandoval[1]; *[1]Genentech Inc, South San Francisco, CA*

MP 453 **Separation of Metalated Lipid IsomersUsing Linear and Nonlinear Ion Mobility Spectrometry**; Andrew Bowman[1]; Julia Kaszycki[2]; Rinat Abzalimov[3]; Gordon A Anderson[4]; Alexandre A Shvartsburg[2]; *[1]Wichita State University, Wichita, KS - Kansas; [2]Wichita State University, Wichita, KS; [3]City University of New York, New York City, NY; [4]GAA Custom Engineering, LLC Benton, WA*

MP 454 **Analysis of Lipids from Biological Samples by Laser Desorption Ionization from Silicon Nanopost Arrays**; Andrew Korte[1]; Akos Vertes[1]; *[1]George Washington University, Washington, DC*

MP 455 **Polar Lipids from Insect and Tick Cuticle. Analysis and Discovery of their Roles in Semiochemical Signaling**; Robert Renthal; *University of Texas at San Antonio, San Antonio, TX*

MP 456 **Natural Variation of Blood Plasma Lipids in Healthy Asian Individuals**; Husna Begum[1, 2]; Federico Torta[3]; Pradeep Narayanaswamy[3]; Piyushkumar Mundra[2]; Yik-Ying Teo[4]; Peter Little[1]; Peter Meikle[2]; Markus Wenk[1, 3]; *[1]Life Sciences Institute, National University of Singapore,*

Singapore, Singapore; [2]Baker IDI Heart and Diabetes Institute, Melbourne VIC, Australia; [3]Department of Biochemistry, Yong Loo Lin School of Medicine, National University of Singapore, Singapore, Singapore; [4]Saw Swee Hock School of Public Health, National University of Singapore, Singapore, Singapore

METABOLOMICS: GENERAL
457 - 495

MP 457 **Validating the Roles of FraD and FraB in the Metabolism of F-Asn by Salmonella**; Jikang Wu[1]; Anindita Sengupta[1]; Anice Sabag-Daigle[1]; Pradip Biswas[1]; Brian Ahmer[1]; Venkat Gopalan[1]; Edward Behrman[1]; Vicki Wysocki[1]; *[1]Ohio State University, Columbus, OH*

MP 458 **Exploiting the Sensitivity of Structural Mass Spectrometry as a Next Generation Platform for Metabolomics**; Olga Gorlova[1]; Conrad Wolke[1]; Sean Colvin[1]; Scott Miller[1]; Mark Johnson[1]; *[1]Yale University, New Haven, CT*

MP 459 **Globally Optimized Targeted Mass Spectrometry (GOT-MS): Reliable Metabolomics Analysis with Broad Coverage**; Haiwei Gu [1]; Ping Zhang[1]; Jiangjiang Zhu[1]; Daniel Raftery[1, 2]; *[1]University of Washington, Seattle, WA; [2]Fred Hutchinson Cancer Research Center, Seattle, WA*

MP 460 **Targeted Metabolomics to Characterize Lipopolysaccharide Biosynthetic Intermediates in Gram-Negative Bacteria in Response to Chemical and Genetic Perturbations**; William Sawyer[1]; Jade Bojkovic[1]; Charles R. Dean[1]; Brian Y. Feng[1]; Daryl L. Richie[1]; David A. Six[1]; Lisha Wang[1]; Christopher M Rath[1]; *[1]Novartis Institutes for Biomedical Research, Emeryville, CA*

MP 461 **Internal Extractive Electrospray Ionization Mass Spectrometry based- Metabolomics for Lung Cancer Analysis**; Yun Li[1]; Zhihao Wang[1]; Qian Li[1]; Yiping Wei[2]; Haiwei Gu[1]; Huanwen Chen[3]; *[1]East China Institute of Technology, Nanchang, China; [2]Department of Cardiothoracic Surgery of Second Affiliated Hospital to Nanchang University, Nanchang, China; [3]East China University of Technology, Nanchang, Mainland*

MP 462 **Study of Untargeted Metabolite Degradation in Plasma using Isotopic Ratio Outlier Analysis by uHPLC-HRMS**; Elizabeth Dhummakupt[1]; Casey Chamberlain[2]; Chris Beecher[3]; Timothy Garrett[2]; *[1]University of Florida, Gainesville, FL; [2]Department of Pathology, University of Florida Gainesville, FL; [3]IROA Technologies, Ann Arbor, MI*

MP 463 **A Step Forward in GC-HRAM-MS Based Metabolomics - A Novel Atmospheric Pressure GC-APCI Source Increases Quantitative and Qualitative Performance**; Christian J. Wachsmuth[1]; Aiko Barsch[2]; Christoph Gebhardt[2]; Peter J. Oefner[1]; Katja Dettmer[1]; *[1]University of Regensburg, Institute of Functional Genomics, Regensburg, Germany; [2]Bruker Daltonics Ltd, Bremen, Germany*

MP 464 **Novel Strategies for the Analysis of Isotopologue and Isotopomer Fractions of Primary Metabolites in 13C Based Metabolic Flux Analysis Experiments**; Teresa Mairinger[1, 2]; Gunda Koellensperger[3]; Stephan Hann[1, 2]; *[1]Austrian Centre of Industrial Biotechnology (acib), Vienna, Austria; [2]Department of Chemistry, University of Natural Resources and Life Sciences - BOKU Vienna, Vienna, Austria; [3]Institute of Analytical Chemistry, Faculty of Chemistry, University of Vienna, Vienna, Austria*

MP 465 **13C-Metabolic Flux Analysis of Microbes by Using Novel Fragmentations of tert-Butyldimethylsilyl (tBDMS)-Amino Acid Derivatives with GC-MS/MS.**; Nobuyuki Okahashi[1]; Shuichi Kawana[2]; Junko Iida[2]; Hiroshi Shimizu[1]; Fumio Matsuda[1]; *[1]Osaka University, Suita, Japan; [2]Shimadzu Corporation, Kyoto, Japan*

MP 466 **Analysis of Plasma Metabolites Using Gas-Chromatography Tandem Mass Spectrometry System with Automated TMS Derivatization** ; Shuichi Kawana[1]; Yumi Unno[2]; Yukihiko Kudo[3]; Takero Sakai[3]; Takashi Kobayashi[4]; Shin Nishiumi[4]; Masaru Yoshida[4]; Noriyuki Ojima[5]; *[1]Shimadzu Corporation, Osaka, Japan; [2]Shimadzu Corporation, Kanagawa, Japan; [3]Shimadzu Corporation, Kyoto, Japan; [4]Kobe University Graduate School of Medicine, Kobe, Japan; [5]Shimadzu Corporation, Tokyo, Japan*

MP 467 **LC-HRMS Metabolic Flux Analysis Reveals Mechanistic-Based Changes after Muscle AMPK Activation**; John Kenji Meissen[1]; Russell Alan Miller[2]; Matt Blatnik[1]; *[1]Pfizer, Groton, CT; [2]Pfizer, Cambridge, MA*

MP 468 **Metabolic Analysis of Single Human Cells in Different Mitotic Phases by Capillary Microsampling Electrospray Ionization Mass Spectrometry**; Linwen Zhang[1]; Akos Vertes[1]; *[1]The George Washington University, Washington, DC*

MP 469 **Evaluating the Impact of Environmental Ultrafine Particles to Gut Bacterial Metabolism by targeted LC-MS/MS Metabolic Profiling**; Julia Roubidoux[1]; Katie Schelli[1]; Joshua Rutowski[1]; Britt Holmén[2]; Jiangjiang (Chris) Zhu[1]; *[1]Department of Chemistry and Biochemistry, Miami University, Oxford, OH; [2]Civil & Environmental Engineering, School of Engineering, University of Vermont, Burlington, VT*

MP 470 **Ion-pairing LC-MS with Automated Sample Prep for Metabolomics**; Jason L. Richardson[1]; Bhavana Shah[1]; Zhongqi Zhang[1]; *[1]Amgen, Inc., Thousand Oaks, CA*

MP 471 **Application of Data-Dependent MS/MS in Structural Analysis of Isomeric Acylsugar Metabolites from Solanaceous Plants**; Xiaoxiao Liu[1]; A. Daniel Jones[1, 2]; *[1]Department of Chemistry, Michigan State University, East Lansing, MI; [2]Department of Biochemistry and Molecular Biology, Michigan State University, East Lansing, MI*

MP 472 **Probiotic Lactobacillus Reuteri Strains Produce L-Ethionine via a Two-Carbon-Transferring Alternative Branch of the Folate Cycle**; Daniel Röth[1]; Abby J Chiang[1]; Gabriel Gugiu[1]; James Versalovic[2]; Markus Kalkum[1]; *[1]City of Hope, Duarte, CA; [2]Texas Children's Hospital, Baylor College Houston, TX*

MP 473 **Using Isotopic Ratio Analysis (IROA) and Non-negative Matrix Factorization (NMF) to Sort Mixtures in Metabolomic Analyses**; Chris Beecher[1]; Timothy J Garrett[2]; Elizabeth Dhummakupt[2]; Vanessa Y. Rubio[2]; *[1]IROA Technologies, Gainesville, Florida; [2]University of Florida, Gainesville, FL*

MP 474 **MS Profiling of Molecular Composition Inside live 3D Artificial Tumors Using the Single-Probe Device**; Wei Rao[1]; Ning Pan[1]; Haiqing Yu[1]; Xuewei Qu[1]; Chuanbin Mao[1]; Zhibo yang[1]; *[1]University of Oklahoma, Dept. of Chem & Biochem Norman, OK*

MP 475 **5a-Reductase Type 3 (SRD5A3) Δ4-3-keto Steroid Metabolism Using Triple Quadrapole Mass Spectroscopy**; sumankalai ramachandran; *Department of Genitourinary Medical Oncology, David H. Koch Center for Applied Research of Genitourinary Cancers, The University of Texas MD Anderson Cancer Center, Houston, Texas., Houston, TX*

MP 476 **LC-SWATH/MS Metabolomics Platform with Hyphenation of Extraction and Analysis of Polar and Non-Polar Metabolites in Plasma and Urine**; Michel Raetz[1]; Renzo Picenoni[2]; Guenter Boehm[2]; Gerard Hopfgartner[1]; *[1]University of Geneva, Geneva, Switzerland; [2]CTC Analytics AG, Zwingen, Switzerland*

MP 477 **What Are We Eating? Differential Metabolomic Profiles Reveal an Insight into our Dietary Habits**; Paul Clemens[1]; Baljit Ubhi[1]; *[1]SCIEX, Redwood City, CA*

MP 478 **Molecular Network Analysis of Environmental Samples for Drug Discovery**; Stefano Bonissone[1]; Natalie E Castellana[1]; *[1]Digital Proteomics, LLC. San Diego, CA*

MP 479 **Labeling of Specialized Metabolites in the Medicinal Plant Camptotheca acuminata using 13CO2 to Track Intermediates in the Biosynthetic Pathway**; Sujana Pradhan[1]; Daniel A Jones[2]; Zhenzhen Wang[2]; *[1]Michigan State University, Haslett, MI; [2]Michigan State University, East Lansing, MI*

MP 480 **Development of an LC-MS Method for the Kinetic Flux Profiling of a Diverse Set of Metabolic Pathways**; Jay Kirkwood[1, 2]; Corey Broeckling[1, 2]; Jordan Steel[1, 3]; Becky Gullberg[1, 3]; Rushika Perera[1]; Jessica Prenni[1, 2]; *[1]Colorado State University, Fort Collins, CO; [2]Proteomics and Metabolomics Facility, Fort Collins, Colorado [CO]; [3]Arthropod-borne & Infectious Diseases Laboratory, Fort Collins, CO*

MP 481 **Δ9-THC Metabolites and Other Cannabinoid Detection**; Toshi Ono[1]; Ken Tseng[2]; Tsunehisa Hirose[3]; *[1]Nacalai USA, San Diego, CA; [2]Nacalai USA Inc., San Diego, CA - California; [3]Nacalai Tesque Inc., Kyoto, Japan*

MP 482 **Determining Pentose Phosphate Pathway Metabolism in VHL (-) Clear Cell Renal Carcinoma (ccRCC)**; Collin Wetzel[1]; Megan Bischoff[1]; Johnson Chu[1]; Patrick A Limbach[1]; David R Plas[1]; Maria F Czyzyk-krzeska[1]; *[1]University of Cincinnati, Cincinnati, OH*

MP 483 **An Optimized Acquisition Database and LC-MS/MS Method Targeting Central Carbon Pathway Metabolites**; Mark Sartain[1]; Amy Caudy[2, 3]; Adam Rosebrock[2, 3]; *[1]Agilent Technologies, Santa Clara, CA; [2]Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto ON, Canada; [3]Department of Molecular Genetics, University of Toronto, Toronto ON, Canada*

MP 484 **Lanthanide-Chelator Barcode for Combinatorial Screening Applications**; Todd Duncombe[1]; Kai Deng[1]; Paul D Adams[2]; Anup K Singh[1]; Trent R Northen[2]; *[1]Sandia National Laboratories, Albuquerque, NM; [2]Lawrence Berkeley National Lab, Berkeley, CA*

MP 485 **Chromatographic performance for high resolution metabolomics**; Vilinh Tran[1, 2]; Ken Liu[1, 2]; Dean Jones[1, 2]; *[1]Clinical Biomarker, Emory School of Medicine Atlanta, GA; [2]Emory University School of Medicine, Atlanta, GA*

MP 486 **Development of Chemical Isotope Labeling Liquid Chromatography Mass Spectrometry for Metabolomic Analysis of Small Numbers of Mammalian Cells**; Xian Luo[1]; Liang Li[2]; *[1]University of Alberta, Edmonton, Alberta; [2]University of Alberta, Edmonton, Canada*

MP 487 **Cow Milk Metabolome Profiling and Determination of its Dietary Effects on the Human Urine Metabolome Using Chemical Isotope Labeling LC-MS**; Dorothea Mung[1]; Liang Li[1]; *[1]University of Alberta, Edmonton, Canada*

MP 488 **Metabolic Profiling of Human Sweat from Various Epidermal Locations Using Non-occlusive Sample Collection and Chemical Isotope Labeling LC-MS**; Kevin Hooton[1]; Liang Li[1]; *[1]University of Alberta, Edmonton, Canada*

MP 489 **Metabolic Phenotyping of Platelet-Rich Plasma Using the AbsoluteIDQ™p180 kit**; Lisa St John Williams[1]; Guido Dallmann[2]; Will J Thompson[1]; Therese Koal[2]; *[1]Duke University Medical Center, Durham, NC; [2]Biocrates Life Science AG, Innsbruck, Austria*

MP 490 **Metabolomic Analysis of 13C/15N Labeled Metabolites Utilizing High Resolution OrbitrapTM Mass Spectrometry and Compound Discoverer Software**; Anastasia Kalli[1]; Bryson Bennett[2]; Junhua Wang[1]; Caroline Ding[1]; Ralf Tautenhahn[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Calico Labs, South San Francisco, CA*

MP 491 **Development of Ion Pair-Reverse Phase Chromatography Mass Spectrometry Method to Maximize Isomer Separation and Coverage of Endogenous Metabolite Classes**; Yuqin Dai; *Agilent Technologies, Santa Clara, CA*

MP 492 **Formate Tetrahydrofolate Ligase of *Lactobacillus reuteri*: A Multifaceted Player of the Folate Cycle?**; Abby Chiang[1]; Daniel Röth[1]; James Versalovic[2]; Markus Kalkum[1]; *[1]City of Hope, Duarte, CA; [2]Texas Children's Hospital, Baylor College Houston, TX*

MP 493 **Development of MRM-Based Detection of the Plant Metabolome Using Liquid Chromatography/Tandem Mass Spectrometry**; Satoshi Yamaki [1]; Junichi Masuda[2]; Yoshihiro Hayakawa[3]; Muneo Sato[4]; Yuji Sawada[4]; Masami Yokota Hirai[4]; *[1]Shimadzu Corporation, Kanagawa , E; [2]Shimadzu Corporation, Kanagawa, Japan; [3]Shimadzu Corporation, Kyoto, Japan; [4]RIKEN, Yokohama, Japan*

MP 494 **Fractionation and Untargeted Metabolomics of Human Plasma by Off-Line Coupling of Reversed-Phase and Hydrophilic Interaction Liquid Chromatography LC/MS**; Stefanie Wernisch[1]; Subramaniam Pennathur[1, 2]; *[1]University of Michigan, Ann Arbor, MI; [2]University of Michigan Medical School, Ann Arbor, MI*

MP 495 **Wine Flavonoids Identified and Analyzed by Composite Neutral Loss Scan and Novel Data-Dependent Scans for Metabolomics Discovery by LC/MS/MS**; Bennett Kalafut[1]; Rae Ana Snyder[1]; Mark Dreyer[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

MICROORGANISMS: IDENTIFICATION AND CHARACTERIZATION
496 - 517

MP 496 **Utility of Random Forest Combined with Infusion Electrospray MS and MALDI-TOF MS for Rapid Classification of Neisseria Meningitidis Strains**; Adrian R Woolfitt[1]; Hercules Moura[1]; Bryan A Parks[1]; Ramnath Gowrishankar[1]; Conrad P Quinn[1]; Brian H Harcourt[1]; Xin Wang[1]; John R Barr[1]; *[1]CDC, Atlanta, GA*

MP 497 **Identification of Microorganisms in Biofluids and Saliva of Individuals with Periodontitis and Chronic Kidney Disease Using MALDI Biotyper**; Levy Anderson Cesar Alves[1]; Rafael Celestino Souza[1]; Taciana Mara Couto Silva[1]; Marcelo Fava[2]; Meriellen Dias[3]; Maria Anita Mendes[3]; Ana Lidia Ciamponi[1]; *[1]Orthodontics and Paediatric Department – Dental School – University of São Paulo, Sao Paulo, SP - BR; [2]Paediatric Nephrology Department – Medical School – University of São Paulo (USP), Sao Paulo, SP/BRAZIL; [3]LSCP - Chemical Engineering Department - Polytechnics School – University of São Paulo (USP), Sao Paulo, SP/ Brazil*

MP 498 **A Peptide-Based LC-MS/MS Method for Detection and Identification of *Salmonella serovars***; Shu-Hua Chen[1]; Christine H. Parker[1]; Melinda A. McFarland[1]; Timothy R Croley[1]; *[1]FDA/CFSAN, College Park, MD*

MP 499 **Detection of Penicillin Binding Protein 2a for the Identification of Methicillin Resistant S.aureus Using Top-down Proteomics**; Jason Neil[1]; James Jr L Stephenson[2]; Alexander Cherkassky[3]; *[1]Thermo Fisher Scientific, Cambridge, MA; [2]Thermo Fisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific, San Jose CA, CA*

MP 500 **Reliable Biomarkers for Identification of Mycobacterium Tuberculosis Complex in Broth Culture Media with Nanodiamond**; Hsi-An Chen[1]; Ya-Chin Chin[1]; Po-Chi Soo[2]; Wen-Ping Peng[1]; *[1]National Dong Hwa University, Shoufeng Hualien, Taiwan; [2]Tzu Chi University, Hualien, Taiwan*

MP 501 **Deciphering Multifactorial Resistance in *Acinetobacter baumannii* Combining Whole-Genome Sequencing and Targeted Label-Free Proteomics**; Tiphaine Cecchini[1]; Eun-Jeong Yoon[2]; Corinne Beaulieu[1]; Yannick Charretier[1]; Chloe Bardet[1]; Xavier Lacoux[1]; Zack Blair[3]; Patrice Courvalin[2];

Jerome Lemoine[4]; Catherine Grillot-Courvalin[2]; Jean-Philippe Charrier[1]; *[1]Biomerieux, Marcy L'Etoile, France; [2]Institut Pasteur, Paris, France; [3]bioMerieux, Saint Louis, Missouri; [4]ISA, Unit 5280 CNRS/UCBL-1 Villeurbanne, France*

MP 502 **Novel Genetic Determinants for Complex Head Composition in a Giant Salmonella Phage**; Susan T Weintraub[1]; Adriana Coll[2]; Martine Bosch[2]; Kevin Hakala[3]; Sammy Pardo[1]; Dana Molleur[1]; Stephen C Hardies[1]; Lindsay W Black[4]; Julie A Thomas[2]; *[1]Univ. of Texas HSC, San Antonio, TX; [2]Rochester Institute of Technology, Rochester, NY; [3]Thermo Fisher Scientific, San Jose, CA; [4]University of Maryland School of Medicine, Baltimore, MD*

MP 503 **Thermal Desorption Electrospray/Ionization Mass Spectrometry Combined with Principal Component Analysis for Rapid Characterization of Bacterial Species**; Shiang Jiun Lin[1]; Sung Pin Tseng[2]; Hung Su[1]; Yang Kuang Pan[1]; Jentaie Shiea [1]; *[1]National Sun Yat-Sen University, Kaohsiung, Taiwan; [2]Kaohsiung Medical University, Kaohsiung, Taiwan*

MP 504 **Application of Matrix-Assisted Laser Desorption/Ionization Time-Of-Flight Mass Spectrometry for Differentiation of Cacao Phytopathogen Strains Growing in Different Tissues and Hosts**; Fábio Santos[1]; Alessandra Tata[1]; Kátia Belaz[1]; Dilze Magalhães[2]; Edna Luz[2]; Marcos Nogueira Eberlin[1]; *[1]University of Campinas, Campinas SP, Brazil; [2]CEPLAC, Ilhéus Bahia, Brazil*

MP 505 **MALDI Profiling of Cyanobacteria by Monitoring Large Molecules**; Hirohiko Asukabe[1]; Takuma Nakayama[1]; Ken-ichi Harada[1]; Susumu Y. Imanishi[2]; *[1]Meijo University, Nagoya, Japan; [2]Meijo University, Nagoya, Aichi*

MP 506 **Identification of Fungi using Rapid Evaporative Ionisation Mass Spectrometry**; Frances Bolt[1]; Simon Cameron[1]; Ali Abdolrasouli[1]; Johanna Rhodes[1]; Tony Rickards[2]; Kate Hardiman[1]; Adam Burke[1]; Julia Balog[3]; Tamas Karancsi[3]; Daniel Simon[3]; Richard Schaffer[3]; Zsolt Bodai[1]; Monica Rebec[2]; Zoltan Takats[1]; *[1]Imperial College, London, United Kingdom; [2]Imperial College Healthcare Trust, London, UK; [3]Waters Research Center, Budapest, Hungary*

MP 507 **Identification and Species Delineation of Bacteria Using MALDI-TOF MS Based on Ribosomal Protein Sequences in DNA Databases**; Kenneth Parker; *SimulTOF/ VIC Instruments, Marlborough, MA*

MP 508 **Differentiation of Bacteria at the Strain Level by MALDI-MS of Proteins >15kDa**; Franco Basile[1]; Anthony Maus[1]; Bledar Bisha[1]; *[1]University of Wyoming, Laramie, WY*

MP 509 **Liquid Extraction Surface Analysis Mass Spectrometry for Protein Analysis Directly from *Escherichia coli* and *Staphylococcus epidermidis***; Klaudia I Kocurek[1, 2]; Josephine Bunch[2]; Robin C May[1]; Helen J. Cooper[1]; *[1]University of Birmingham, Birmingham, United Kingdom; [2]National Physical Laboratory, Teddington, United Kingdom*

MP 510 **High-velocity Impact Survival and Bouncing Kinetics of Electrosprayed Bacterial Spores Studied using Novel Asymmetric Image Charge Detectors**; Brandon Barney[1]; Daniel Austin[1]; *[1]Brigham Young University, Provo, UT*

MP 511 **Probing Protein Interaction Dynamics between Asian Citrus Psyllid and *Candidatus Liberibatcter asiaticus* by Chemical Crosslinking Mass Spectrometry**; Xuefei Zhong[1]; John Ramsey[2, 3]; Juan Chavez[1]; Arti Navare[1]; Jared Mohr[4]; Michelle Cilia[2, 3, 4]; James Bruce[1]; *[1]University of Washington, Seattle, WA; [2]USDA Agricultural Research Service, Ithaca, NY; [3]Boyce Thompson Institute for plant research, Ithaca, NY; [4]Cornell University, Ithaca, NY*

MP 512 **High Yielding Spin Column Isolation of Total Proteins from Microbial Cultures for Proteomic Applications**; Victoria Nieciecki[1]; Heather Callahan[1]; Eddie Adams[2]; *[1]MO BIO Laboratories, Carlsbad, CA - California; [2]MO BIO Laboratories, Carlsbad, CA*

MP 513 **Simultaneous DNA, RNA, and Protein Extraction from Microbial Cells: Sequential Isolation of Complex Biomolecules from a Single Source**; Heather Callahan[1]; Victoria Nieciecki[1]; Eddie Adams[1]; *[1]MO BIO Laboratories, Carlsbad, CA*

MP 514 **Characterizing the Formation of Electrophilic Fatty Acid Derivatives During Influenza Infection and Determining their Role in Pathogenesis**; Greg Buchan; *University of Pittsburgh, Pittsburgh, PA*

MP 515 **Integrated Omics Reveals Dynamic Nature of the Arabidopsis Rhizosphere Microbiome**; Ljiljana Pasa-Tolic[1]; Abigail Ferrieri[2]; Charles K. Ansong[2]; Heather M. Brewer[2]; Angela D. Norbeck[2]; Yaya Cui[3]; Christopher Staley[4]; Malak Tfaily[2]; Rosalie Chu[2]; Jared Shaw[2]; Meng L. Markillie[2]; Richard A. Ferrieri[3]; Susannah G. Tringe[5]; Michael J. Sadowsky[4, 6]; Gary Stacey[3]; *[1]Battelle - PNNL, Richland, WA; [2]Pacific Northwest National Laboratory, Richland, WA; [3]University of Missouri, Columbia, MO; [4]University of Minnesota, St. Paul, MN; [5]DOE Joint Genome Institute, Walnut Creek, CA; [6]University of Minnesota at Twin Cities, Saint Paul, MN*

MP 516 **Development of Metaproteomics Methods for Characterization of Soil Microbial Communities**; ZHOU LI[1]; Cristina N. Butterfield[2]; Susan Spaulding[2]; Brian C. Thomas[2]; Andrea Singh[2]; K. Blake Suttle[3]; Robert Hettich[1]; Jillian Banfield[2]; Chongle Pan[1]; *[1]Oak Ridge National Laboratory, Oak Ridge, TN; [2]University of California, Berkeley, CA; [3]University of California, Santa Cruz,, Santa Cruz, CA*

MP 517 **Non-Targeted Mass Spectrometry-based Analysis for the Differentiation of Pathogenic *Escherichia coli* Strains**; Rabih Jabbour[1]; Raja Sekhar Nirujogi[2]; Kim Min-Sik[3]; Mary M Wade[4]; Babylakshmi Muthusamy[5]; Gajanan J. Sathe[5]; T.S. Keshava Prasad[6, 7]; Akhilesh Pandey[3, 8]; *[1]ECBC, APG, MD; [2]Institute of Bioinformatics, International Technology Park, Bangalore, India; [3]McKusick-Nathans Institute of Genetic Medicine, Johns Hopkins University School of Medicine, Baltimore, MD; [4]ECBC, Apg, MD; [5]Institute of Bioinformatics, Bangalore, India; [6]Institute of Bioinformatics, Banglore, India; [7]2Centre for Bioinformatics, Pondicherry University, Puducherry, India; [8]Department of Biological Chemistry, Pathology, Oncology, Johns Hopkins University School of Medicine, Baltimore, MD*

PHOSPHOPEPTIDES: ENRICHMENT METHODS
518 - 529

MP 518 **Enrichment and Identification of MHC-Associated Phosphopeptide Neoantigens in Hepatocellular Carcinoma for the Development of Novel Cancer Immunotherapeutics**; Paisley Myers[1]; Nico Buttner[2]; Jennifer G Abelin[1]; Sarah A. Penny[2]; Lora G Steadman[2]; Dina L. Bai[1]; Mark Cobbold[3]; Jeffrey Shabanowitz[1]; Donald F Hunt[1]; *[1]University of Virginia, Charlottesville, VA; [2]University of Birmingham, Birmingham, UK; [3]Harvard University, Boston, MA*

MP 519 **Phosphoproteome Changes in Altered Cholesterol Metabolism Revealed by SCX Tip Based Fractionation of Batch-Enriched Phosphopeptides**; Alireza Dehghani[1]; Markus Gödderz[1]; Volkmar Gieselmann[1]; Dominic Winter[1]; *[1]University of Bonn, Bonn, Germany*

MP 520 **Development of Enrichment Strategies for the Analysis of Phosphohistidine-Containing Peptides**; Gemma E Hardman[1]; Claire E Eyers[1]; *[1]University of Liverpool, Liverpool, United Kingdom*

MP 521 **Enrichment of Phosphorylated Peptides Using Metal-Loaded Polymeric Reverse Micelles for MALDI-MS Analysis**; Meizhe Wang[1]; Bo Zhao[1]; Sankaran Thayumanavan[1]; Richard Vachet[1]; *[1]University of Massachusetts Amherst, Amherst, MA*

MP 522 **Fabrication of MnFe2O4 Magnetic Nanoparticles for the Enrichment of Phosphopeptides in Combination with Mass Spectrometric Analysis**; Yung-Yun Huang[1]; He-Hsuan Hsiao[2]; *[1]Department of Chemistry, National Chung-Hsing University, Taichung, Taiwan; [2]Department, of Chemistry, National Chung-Hsing University, Taichung, Taiwan*

MP 523 **Dual Wield nanoLC-ESI-MS for Simultaneous Detection of Singly and Multiply Phosphorylated Peptides**; Chia-Feng Tsai[1]; Kosuke Ogata[1]; Masaki Wakabayashi[1]; Naoyuki Sugiyama[1]; Yasushi Ishihama[1]; *[1]Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, Japan*

MP 524 **Metal Ion-Immobilized Magnetic Nanoparticles for Global Enrichment and Identification of Phosphopeptides by Mass Spectrometry**; Yangjun Zhang[1, 2]; Rui Zhai[2]; XiaoHong Qian[2]; *[1]Beijing Proteome Research Ctr, Beijing, Beijing; [2]Beijing Institute of Radiation Medicine, Beijing, C.N.*

MP 525 **Excellent Sensitivity through Excellent Recovery – ERLIC Outperforms TiO2—Affinity Purification in Quantitative Phosphoproteomics with Low Sample Amounts**; Stefan Loroch[1]; Albert Sickmann[1, 2, 3]; René P Zahedi[1]; *[1]Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Dortmund, Germany; [2]Ruhr-Universität-Bochum, Medizinische Fakultät, Bochum, Germany; [3]University of Aberdeen, School of Natural & Computing Sciences, Aberdeen, Scotland*

MP 526 **ESI Tandem Mass Spectrometric Analysis of Phosphopeptide Modified by Cyclic Quaternary Ammonium Tags**; Hye Kyong Kweon[1]; Kristina Hakansson[1]; Philip Andrews[1]; *[1]University of Michigan, Ann Arbor, MI*

MP 527 **Method Development and Evaluation of the Protein Phosphatase 2 Phosphoproteome Using the Chip iFunnel QTOF Platform**; Brooke Thompson[1]; Vadiraja Bhat[2]; Chelsea E. Cunningham[3]; Paulos Chumala[1]; Frederick S. Vizeacoumar[3]; Franco J. Vizeacoumar[3]; George S. Katselis[1]; *[1]CCHSA/Medicine, College of Medicine, University of Saskatchewan, Saskatoon, SK, Canada; [2]Agilent Technologies, Wilmington, DE; [3]Department of Pathology, Cancer Cluster, College of Medicine, University of Saskatchewan, Saskatoon, SK, Canada*

MP 528 **Acid-Based SCX Fractionation for In-Depth Proteome and Phosphoproteome Analysis**; Jun Adachi[1]; Hashiguchi Kazunari[2]; Nagano Maiko[2]; Sato Misako[2]; Sato Ayako[2]; Fukamizu Kazuna[2]; Ishihama Yasushi[3]; Tomonaga Takeshi[2]; *[1]National Institutes of Biomedical Innovation, Health and Nutrition, Ibaraki, Osaka; [2]National Institute of Biomedical Innovation, Health and Nutrition, Osaka, Japan; [3]Kyoto University, Kyoto, Japan*

MP 529 **Two-Step Elution of Phosphopeptides from TiO2 Microparticles – an Improved Detection of Multiphosphorylated Peptides**; Rudolf Kupcik[1]; Pavel Rehulka[2]; Ivo Fabrik[2]; Jana Klimentova[2]; Helena Rehulkova[2]; Jiri Stulik[2]; Pavla Krulisova[1]; Zuzana Bilkova[1]; *[1]Department of Biological and Biochemical Sciences, Faculty of Chemical Technology, University of Pardubice, Pardubice, Czech Republic; [2]Department of Molecular Pathology and Biology, Faculty of Military Health Sciences, University of Defence, Hradec Kralove, Czech Republic*

POLYMERS
530 - 548

MP 530 **Characterization of Bromine Functionalized Alternating and Random Copolyesters by Tandem Mass Spectrometry**; Selim Gerislioglu[1]; Xianglin Yin[2]; Coleen Pugh[2]; Chrys Wesdemiotis[2]; *[1]The University of Akron, Akron, Ohio; [2]The University of Akron, Akron, OH*

MP 531 **The Characterization of Polymeric Methylene Diphenyl Diisocyanates (PDMIs) Using UHPSFC and FT-ICR APPI-MS**; Julie M Herniman[1]; Robert Carr[2]; John G Langley[1]; *[1]University of Southampton, Southampton, United Kingdom; [2]Huntsman (Europe), bvba, Everborg, Belgium*

MP 532 **An APCI LC-MS-MS Method for the Determination of Octamethylcyclotetrasiloxane (D4), Decamethylcyclopentasiloxane (D5), and Dodecamethylcyclohexasiloxane (D6) in Silicone Emulsions.**; Ron Tecklenburg[1]; Tanya M Habitz[1]; *[1]Dow Corning Corporation, Auburn, MI*

MP 533 **Simplification of Polysorbate 80 Spectrum: Selective Removal of Metal Cation Adducts from Polymers via Gas-Phase Ion/Ion Reactions Using Carborane Anions**; Stella Betancourt[1]; Alice L Pilo[1]; Jiexun Bu[1]; Scott A McLuckey[1]; *[1]Purdue University-Department of Chemistry, West Lafayette, IN*

MP 534 **Self-Assembly and Characterization of 2D to 3D Supramolecular Star of David Using Mass Spectrometry**; Bo Song[1]; Xiaopeng Li[1]; Ming Wang[1]; *[1]Texas State University, San Marcos, TX*

MP 535 **Analysis for Extractable and Leachable Compounds from Polymeric Materials**; Gordon Fujimoto[1]; Sarah Dowd[1]; Baiba Cabovska[2]; Marian Twohig[2]; *[1]Waters Corporation, Beverly, MA; [2]Waters Corporation, Milford, MA*

MP 536 **Identification of Poly Ethylene Glycol (PEG) and PEGylated Detergents Using Protein Search Engines**; Shiva Ahmadi[1]; Dominic Winter[1]; *[1]University of Bonn, Bonn, Germany*

MP 537 **Assembling and Characterization of Discrete Supramolecular Fractal Architectures Using ESI-MS and Ion Mobility-Mass Spectrometry** ; Yuanfang Ying[1]; Ming Wang[1]; Kendall Williams[1]; Xiaopeng Li[1]; *[1]Texas State University, San Marcos, TX*

MP 538 **Mass Spectrometry Characterization of Isomeric Biodegradable Polyesters**; sahar sallam[1]; Chrys Wesdemiotis[1]; Yuanyuan Luo[1]; Mathew L. Becker[1]; *[1]The University of Akron, Akron, OH*

MP 539 **Surface Composition of Films Made from Partially Functionalized Polymer Blends**; Kevin Endres[1]; Jacob A. Hill[1]; John Meyerhofer[2]; Qiming He[1]; Chrys Wesdemiotis[1]; Mark D Foster[1]; *[1]The University of Akron, Akron, OH; [2]Saint Vincent College, Latrobe, PA*

MP 540 **MALDI-MS Signal Enhancement of Peptides from Donor-Acceptor Interactions between Amphiphilic Polymers and MALDI Matrix**; Mahalia Serrano[1]; Huan He[1]; Sankaran Thayumanavan[1]; Richard W Vachet[1]; *[1]University of Massachusetts Amherst, Amherst, Massachusetts*

MP 541 **Investigating the Effect of Sample Preparation Parameters on the Cationization of Synthetic Polymers Using Matrix-Assisted Laser Desorption Ionization**; Michelle Piotrowski[1]; Kevin Owens[1]; *[1]Drexel University, Philadelphia, PA*

MP 542 **Revealing Topological Isomers Inside Insoluble Cyclo-Para-Phenylenes by Ion Mobility Mass Spectrometry**; Hans Joachim Raeder[1]; Wen Zhang[2]; Ali Abdulkarim[2]; Klaus Müllen[2]; *[1]MPI for Polymer Research, Mainz, Rhineland-Palatinate; [2]MPI for Polymer Research, Mainz, Germany*

MP 543 **Matrix Assisted Laser Desorption Ionization Mass Spectrometry and NMR Characterization of Plasma Polymerized Styrene**; Lee Elliott[1]; Kris Micheal Kirmess[1]; Gary Ray Kinsel[1]; *[1]Southern Illinois University Carbondale, Carbondale, IL*

MP 544 **Highly Sensitive Analysis of Residual Monomers in Adhesives Using HSGC/MS**; Sanket Chiplunkar[1]; Durvesh Sawant[2]; Dheeraj Handique[1]; Prashant Hase[1]; Ankush Bhone[1]; Ajit Datar[1]; Jitendra Kelkar[1]; Pratap Rasam[1]; *[1]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, Maharashtra; [2]Shimadzu Analytical (India) Pvt. Ltd.,*

Mumbai, India

MP 545 **Polymer and Adhesive Tape Analysis by Thermal Desorption and Pyrolysis Combined with Direct Analysis in Real Time (DART) Mass Spectrometry**; Cody Robert B.[1]; Chikako Takei[2]; Haruo Shimada[3]; Yasuo Shida[4]; Akihiko Kusai[5]; *[1]JEOL USA, Inc. Peabody, MA; [2]BioChromato, Inc. Fujisawa, Japan; [3]Shiseido Research Center, Yokohama, Japan; [4]University of Yamanashi, Kofu, Japan; [5]JEOL Ltd., Akishima, Japan*

MP 546 **Polymer Structure Investigation by Trapped Ion Mobility Mass Spectrometry**; Jan Jordens[1]; Ynze Mengerink[1]; Esra Altuntas[1]; Mark E Ridgeway[2]; Melvin Park[2]; Maarten Honing[1, 3]; *[1]DSM Resolve, Geleen, Netherlands; [2]Bruker Daltonic, Billerica, MA; [3]VU University, Amsterdam, Netherlands*

MP 547 **Improved Characterization of Complex Mixtures via Liquid Chromatography/Charge Reduction/Mass Spectrometry (LC/CR/MS)**; John Stutzman[1]; Matthew C Crowe[2]; James IV N Alexander[2]; Bruce Bell[1]; Melissa N Dunkle[3]; *[1]The Dow Chemical Company, Midland, MI; [2]The Dow Chemical Company, Collegeville, PA; [3]The Dow Chemical Company, Terneuzen, NL*

MP 548 **Characterization of Unknown Surfactant Packages in Industrial Samples by Liquid Chromatography Mass Spectrometry (LC/MS) with Electrospray Ionization (ESI)**; Dale Willcox[1]; Noelle Elliott[1]; *[1]Intertek, Allentown, PA*

PROTEINS: GENERAL AND MEMBRANE
549 - 571

MP 549 **Biophysical Characterization of the Interactions between Membrane Proteins and Lipids**; Xiao Cong[1]; Yang Liu[1]; Wen Liu[1]; David H Russell[2]; Arthur Laganowsky[1, 2, 3]; *[1]Center for Infectious and Inflammatory Diseases, Institute of Biosciences and Technology, Texas A&M Health Science Center, Houston, TX; [2]Department of Chemistry, Texas A&M University, College Station, TX; [3]Department of Microbial Pathogenesis & Immunology, College of Medicine, Texas A&M Health Science Center, Bryan, TX*

MP 550 **Protein Mass Spectra Database for Rapid Identification of Field-Caught Phlebotomine Sand Flies**; Kristyna Hlavackova[1]; Daniel Kavan[2]; Vit Dvorak[1]; Petr Volf[1]; Petr Halada[2]; *[1]Department of Parasitology, Charles University in Prague, Prague, Czech Republic; [2]Institute of Microbiology CAS, Prague, Czech Republic*

MP 551 **Developments in Analysis of GPCRs: Monitoring Protein Movement by Means of Mass Spectrometry**; Krzysztof Okrasa[1]; James Errey[1]; Rob Cooke[1]; *[1]Heptares Therapeutics Ltd., Welwyn Garden City, UK*

MP 552 **Improving the Efficiency and Rapidity of Tryptic Proteolysis: from Blood to "Unknown Stains"**; Ekta Patel[1]; Paola Cicatiello[2]; Lisa Deininger[1]; Malcolm R Clench[1]; Peter Marshall[3]; Andy West[3]; Simona Francese[1]; *[1]Centre for Mass Spectrometry Imaging, Biomolecular Research Centre, Sheffield, South Yorkshire; [2]Universita' di Napoli Federico II, Dipartimento di Scienze Chimiche, Naples, Naples; [3]GlaxoSmithKline, Stevenage, UK*

MP 553 **How Sequence Variant Analysis can be Hampered by Trypsin Side Reactions**; Georg Drabner[1]; Marco Boettger[1]; *[1]Roche Innovation Center Penzberg, Penzberg, Germany*

MP 554 **Mass spectrometry of Collagen and Casein in the Remains of the 5th to 7th Century Bamiyan Buddhas**; Takashi Nakazawa[1]; Kazuki Kawahara[2]; Shunsuke Fukakusa[3]; Mao Karino[3]; Miho Takashima[4]; Yoko Taniguchi[5]; *[1]Nara Women's University, Nara, Nara; [2]Osaka University, Suita, Japan; [3]Nara Women's University, Nara, Japan; [4]The National Museum of Western Art, Tokyo, Japan; [5]University of Tsukuba, Tsukuba, Japan*

MP 555 **Proteomic Characterization of Cell Architecture and its Preparatory Biochemical Extractions**; Li-Hua Li[1]; Cheng-Chih Richard Hsu[2]; Cheng-Hsien Yang[3]; Chen Meng[4]; Yeou-Guang Tsay[3, 5, 6]; *[1]Taipei Veterans General Hospital, Taipei, Taiwan; [2]Department of Chemistry National Taiwan University, Taipei, Taiwan; [3]Institute of Biochemistry and Molecular Biology, Taipei, Taiwan; [4]Chair of Proteomics and Bioanalytics Technische Universitaet Muenchen, Munich, Germany; [5]Proteomics Research Center, Taipei, Taiwan; [6]Department of Biotechnology and Laboratory Science in Medicine, National Yang-Ming University, Taipei, Taiwan*

MP 556 **The Interactions between N-Heterocyclic Carbene Silver Complex and Cytochrome C Studied by Electrospray Ionization Mass Spectrometry**; Yan Pan; *, Morgantown, WV*

MP 557 **A Chemical Proteomic Method for the Discovery of Novel LPA-binding Proteins**; Xuejiao Dong[1]; Yinsheng Wang[1]; *[1]University of California - Riverside, Riverside, CA*

MP 558 **Exploring the Differences in Endocytic Vesicles with the Aid of Mass Spectrometry Based Protein and Lipid Profiling**; Bini Ramachandran[1]; Krishnamurthy H[2]; Satyajit Mayor[3, 4]; *[1]National Centre for Biological Sciences, Bangalore, India, Bangalore, Karnataka; [2]Centre for Imaging and Flow Cytometry Facility, National Centre for Biological Sciences, Tata Institute of Fundamental Research, GKVK, Bangalore, India; [3]National Centre for Biological Sciences, Tata Institute of Fundamental Research, GKVK, Bangalore, India; [4]Institute for Stem Cell Biology and Regenerative Medicine, Bellary Road,, Bangalore, India*

MP 559 **Quality by Design (QbD) Based Development of a Peptide Mapping UPLC Method for Recombinant Human Serum Albumin (rHSA)**; Ashraf Madian[1]; Irish Gibson[2]; Janet G. De Los Reyes[3]; Cassandra Norton[4]; Shen Chen[5]; Lisa Cherry[2]; *[1]Global Technology Services, Hospira, a Pfizer Company, Lake Forest, IL; [2]One2One® Global Pharmaceutical R and D, Hospira, a Pfizer Company, McPherson, KS; [3]Global Established Products R and D, Hospira, a Pfizer Company, McPherson, KS; [4]Global Technical Supply, Hospira, a Pfizer Company, McPherson, KS; [5]One2One® Global Pharmaceutical R and D, Hospira, a Pfizer Company, Lake Forest, IL*

MP 560 **Using LC-MS Based Methods for Testing the Digestibility of a Non-Purified Membrane Protein in Simulated Gastric Fluid**; Wayne Skinner[1, 2]; Brett S Phinney[3]; Anthony Herren[3]; John Goodstal[1]; Isabel Dicely[1]; Daniel Facciotti[1]; *[1]Arcadia Biosciences, Davis, CA; [2]Arcadia Biosciences, Davis, Davis, CA; [3]Proteomics Core Facility, University of California, Davis, CA 95616, USA, Davis, CA*

MP 561 **Using UHPLC-ESI-HRMS to Detect Small Mass Differences in High Molecular Weight Glutenin Subunits of Wheat**; Ray Bacala[1]; Dave Hatcher[2]; *[1]Canadian Grain Commission, Winnipeg, MB; [2]Canadian Grain Commission, Winnipeg, Canada*

MP 562 **Towards a Prediction of Protein Reactivity Against Electrophile Ligands: 1. Ranking Amino Acid Side Chain Nucleophilicities**; Guillaume Gabant[1]; Yoann Richer[1]; Solène Motteau[1]; Emmanuelle Mebold[2]; Martine Cadene[1]; *[1]CBM CNRS UPR4301, Orleans, France; [2]IMMM CNRS UMR 6283, Le Mans, France*

MP 563 **Evaluation of N-terminal Labeling Protocols for Determination of Protein Cleavage Sites by Mass Spectrometry**; Michelle Gadush[1]; Maria D. Person[1]; *[1]University of Texas at Austin, Austin, TX*

MP 564 **Identification of Unique Rod Outer Segment Plasma Membrane Proteins Using a Label-Free Protein Correlation Profiling**; Nikolai P Skiba[1]; Vadim Y Arshavsky[1]; *[1]Albert Eye Research Institute, Duke University Medical Center, Durham, NC*

MP 565 **Identification of Polyglutamylation of C-Terminal Tails of Tubulins from In-Gel Double Digests with Trypsin and Subtilisin**; Hang-Gyeong Chin[1]; Colleen McClung[1]; Sriharsa Pradhan[1]; Christopher J. Noren[1]; Cristian I. Ruse[1]; *[1]New England Biolabs, Ipswich, MA*

MP 566 **Disulfide Bond Reduction on TiBlue Electrodes – a Breakthrough in Protein Analysis**; Jean-Pierre Chervet [1]; Agnieszka Kraj[2]; Hendrik-Jan Brouwer[2]; Nico Reinhoud[2]; Martin Eysberg[3]; *[1]Antec, Zoeterwoude , -; [2]Antec, Zoeterwoude, The Netherlands; [3]Antec LLC, Boston, MA*

MP 567 **Rapid Analysis of Proteins on High-Resolution Mass Spectrometers Using Matrix-Assisted Ionization**; Shameemah Thawoos[1]; Casey Daniel Foley[1]; James Wager-Miller[2]; Ken Mackie[2]; Paul Stemmer[1]; Sarah Trimpin[1]; *[1]Wayne State University, Detroit, MI; [2]Indiana University Dept. Chemistry, Bloomington, IN*

MP 568 **A New Thiol Derivatization Reactions with 2,1,3-Benzotelluradiazole Studied by Mass Spectrometry**; Chang Xu[1]; Qiuling Zheng[1]; Kehua Xu[2]; Bo Tang[2]; Hao Chen[1]; *[1]Ohio University, Athens, OH; [2]Shandong Normal University, Jinan, SD*

MP 569 **Native Mass Spectrometry Analysis of Membrane-Bound Reaction Center from *Blastochloris viridis***; Yue Lu[1]; Zhang Hao, [1]; Michael L Gross[1]; Robert E Blankenship[1]; *[1]Washington University in St. Louis, St. Louis, MO*

MP 570 **Improved Proteolytic Digestion under High Pressure Cycling: Rapid Digestion with Improved Sensitivity and Sequence Coverage**; Vera S. Gross[1]; John Wilson[2]; Alexander Lazarev[1]; *[1]Pressure BioSciences, South Easton, MA; [2]Protifi, LLC, Huntington, NY*

MP 571 **Fully Automated Digestion, Separation and Analysis of the Human Prolactin Receptor Transmembrane Protein by LC-MS/MS**; Joshua Emory[1]; Nishi Rochelle[1]; Boutaghou Nazim[1]; Feild J Brian[1]; *[1]Shimadzu Scientific Instruments, Inc. Columbia*

PROTEINS: PTMS (PART 1)
572 - 596

MP 572 **Proteomic Analysis of Protein S-Sulfhydration in *Staphylococcus aureus***; Yixiang Zhang[1, 2]; Hui Peng[1, 3]; David Peter Giedroc[1, 3]; Jonathan Cyboski Trinidad[1, 2]; *[1]Department of Chemistry, Indiana University, Bloomington, IN; [2]Laboratory for Biological Mass Spectrometry, Indiana University, Bloomington, IN; [3]Department of Molecular and Cellular Biochemistry,Indiana University, Bloomington, IN*

MP 573 **Deep Coverage of the Mouse Cysteine Sulfenome in *vivo***; Shin-Cheng Tzeng[1]; Sjoerd Van der Post[1]; Nelmi O Devarie-Baez[2]; Cristina M Furdui[2]; Jason Held[1]; *[1]Washington University in St. Louis, St. Louis, MO; [2]Wake Forest School of Medicine, Winston-Salem, NC*

MP 574 **Quantifying Oxidation in Peptides Containing Multiple Methionine Residues**; Joshua T Shipman[1]; Eden P Go[1]; Heather Desaire[1]; *[1]University of Kansas, Lawrence, KS*

MP 575 **Quantifying Reversible Oxidation of Protein Thiols in *Arabidopsis thaliana***; Evan Mc Connell[1]; Leslie M Hicks[1]; *[1]University of North Carolina, Chapel Hill, NC*

MP 576 **Energetics of S-Palmitoylation: Role of Proline and Neighboring Cysteines**; Neelam Khanal[1]; Vikas Pejaver[1]; Zhiyu Li[1, 2]; Predrag Radivojac[3]; David E Clemmer[1]; Suchetana Mukhopadhyay[3]; *[1]Indiana University Dept. Chemistry, Bloomington, IN; [2]Novilytic, West Lafayette, IN; [3]Indiana University, Bloomington, IN*

MP 577 **Elevated Level of S-Glutathionylation of Hemoglobin in Mole-Rats Determined by LC-MS**; Kuanysh Kabytaev[1]; Christiane Vole[2]; Dmitriy Shin[1]; Philip Dammann[2]; Alexandre Stoyanov[1]; *[1]Department of Pathology & Anatomical Sciences, University of Missouri, Columbia, MO; [2]Department of General Zoology, University of Duisburg-Essen, Essen, Germany*

MP 578 **Difference Gel Electrophoresis for Phosphoproteomics (DiGEP)**; Mayank Srivastava[1]; Linna Wang[1]; Weiguo Andy Tao[1]; *[1]Purdue University, West Lafayette, IN*

MP 579 **Intact Phosphorylated Protein Analysis by Microfluidic CE-ESI-MS**; Esme Candish[1]; Michael E Pacold[2]; Scott Mellors[3]; Michael J Ramsey[1]; *[1]University of North Carolina at Chapel Hill, Chapel Hill, NC; [2]Whitehead Institute for Biomedical Research, Cambridge, MA; [3]908 Devices Inc., Boston, MA*

MP 580 **Elucidating Kinase Substrate Networks in *Chlamydomonas reinhardtii***; Alex Chao[1]; Chris A Broberg[1]; Megan C Connor[1]; Leslie M Hicks[1]; *[1]UNC Chapel Hill, Department of Chemistry Chapel Hill, NC*

MP 581 **Studies of the Molecular Mechanisms in the Regulation of PRL-3 Phosphatase Activity in the Endothelial Cells**; Xinggui Shen[1]; Christopher G. Kevil[1]; *[1]LSU Health-Shreveport, Shreveport, LA*

MP 582 **Phosphoproteomic Evaluation of Chimeric Proteins**; Katelyn Ludwig[1]; Nirmalya Sen[2]; Natasha J Caplen[2]; Amanda B Hummon[1]; *[1]University of Notre Dame, Notre Dame, IN; [2]NIH, Bethesda, MD*

MP 583 **The Functions of Serine 687 Phosphorylation of Human DNA Polymerase h in UV Damage Tolerance**; Xiaoxia Dai[1]; Changjun You[1]; Yinsheng Wang[1]; *[1]UC Riverside, Riverside, CA*

MP 584 **Phosphorylation Dynamics and Interacting Proteins of MAP Kinase 4 Revealed by Proteomics**; Tong Zhang[1]; Jacqueline D Schneider[2]; Craig P. Dufresne[3]; Alice C Harmon[2]; sixue chen[2]; *[1]University of Florida, Gainesville, FL; [2]University of Florida, Gainesville, Florida; [3]Thermo Fisher Scientific, West Palm Beach, FL*

MP 585 **Perturbation of the Phosphoproteome of Colony Stimulating Factor 3 Receptor (CSF3R) in Normal Myeloid Development, Myeloid Leukemia and Neutrophilic Leukemia**; Pankaj Dwivedi[1]; David Muench[2]; Mohammad Azam[2]; Harry Leighton Grimes[2]; Kenneth D Greis[1]; *[1]University of Cincinnati, Cincinnati, OH; [2]Cincinnati Children's Hospital Medical Center, Cincinnati, OH*

MP 586 **A Panoramic Survey of Cellular Signaling in Human Gastric Cancer Cells by Monitoring both Phosphotyrosine and Acetyl-Lysine Post-Translational Modifications**; Jeffrey C Silva[1]; Cammarata John[2]; Hamza Ghaith[1]; Manor Askenazi[1]; Jun Zhu[3]; Zhongyi Cheng[3]; *[1]Lighthouse Proteomics, Beverly, MA; [2]Adeptrix Corporation, Beverly, MA; [3]PTM BioLab (Hangzhou) Co. Ltd, Hangzhou, China*

MP 587 **Updating and Expanding the PTM Catalog of Acid-Soluble Tau: A Case for Multiplexed Proteomic Analysis**; Gogce Crynen[1]; Robert Pelot[1]; Craig P Dufresne[2]; Jon M Reed[1]; Prashanthi Vallabhaneni[1]; Benoit Mouzon[1]; Laila Abdullah[1]; James E Evans[1]; Fiona Crawford[1]; *[1]Roskamp Institute, Sarasota, FL; [2]Thermo Fisher Scientific, West Palm Beach, FL*

MP 588 **Identification of Cross-Linked Peptides in Proteins Subjected to Photo-Oxidation**; Michele Mariotti[1]; Fabian Leinisch[2]; Diana Julie Oersnes-Leeming[3]; Michael J Davies[2]; Birte Svensson[4]; Per Hägglund[4]; *[1]Technical University of Denmark, Kongens Lyngby, Denmark; [2]University of Copenhagen, Copenhagen, Denmark; [3]Nordic Bioscience, Herlev, Denmark; [4]Technical University of Denmark, Lyngby, Denmark*

MP 589 **msViz, a Zero Learning Curve Graphical Software Tool for Detailed Manual Validation and Quantitation of Post-Translational Modifications**; Manfredo Quadroni[1]; Roman Mylonas[2]; Trinidad Martin Campos[2, 3]; Alexandre Masselot[2]; Patrice Waridel[1]; Ioannis xenarios[2]; *[1]CIG - University of Lausanne, Lausanne, Switzerland; [2]Vital-IT Group - Swiss Institute of Bioinformatics, Lausanne, Switzerland; [3]University of Geneva, Geneva, Switzerland*

MP 590 **Sequential Immunoaffinity Purification of Post-Translationally Modified Peptides for Improved Enrichment Specificity**; Matthew P. Stokes[1]; Charles L Farnsworth[1]; Jian Min Ren[1]; Kimberly A Lee[1]; Xiaoying Jia[1]; Hongbo Gu[1]; Vicky Yang[1]; *[1]Cell Signaling Technology, Inc. Danvers, MA*

MP 591 **Metabolomics-Assisted Proteomics Reveals the Function of Lysine Succinylation and SIRT5 in Regulation of β-Oxidation of Long-Chain Fatty Acids**; Sushabhan Sadhukhan[1]; Xiaojing Liu[1]; Ornella D Nelson[1]; John A Stupinski[2]; Sheng Zhang[1]; Robert S Weiss[1]; Jason W Locasale[1]; Hening Lin[1]; *[1]Cornell University, Ithaca, NY; [2]Cornell University, New York, NY*

MP 592 **Mass Spectrometry Based Identification and Characterization Studies of Post Translational Modification Citrullination**; Mandvi Sharma[1]; Damagard Dres[2]; Anne Christian-Bay Jensen[3]; Claus Nielsen[4]; Birte Svensson[5]; Per Hagglund[6]; *[1]PhD, Department of Systems Biology, Denmark Technical University, Copenhagen, Denmark; [2]Institute for Inflammation Research, Department of Infectious Diseases and Rheumatology, Copenhagen University Hospital, Rigshospitalet, Copenhagen, Denmark; [3]Principal Scientist, Head of Rheumatology, Nordic Biosciences, Copenhagen, Denmark; [4]Professor, Consultant Physician, Head of Department of Rheumatology, Rigshospitalet, Copenhagen, Denmark; [5]Professor Enzyme and Protein Chemistry Department of Systems Biology The Technical University of Denmark, Copenhagen, Denmark; [6]Associate Professor, Deaprtment of Systems Biology, Technical University of Denmark., Copenhagen, Denmark*

MP 593 **Characterization of Non-Heme Iron Enzymes Using Mass Spectrometry**; Yi Pu[1]; Cheng-Hsuan Wu[1]; Deborah R. Leon[1]; Pinghua Liu[1]; Catherine E. Costello[1]; *[1]Boston University, Boston, MA*

MP 594 **Evolutionary Conservation of Sirtuin Lipoamidase Activity from Bacteria to Human Mitochondria**; Elizabeth A Rowland[1]; Todd M Greco[1]; Caroline K Snowden[1]; Ileana M. Cristea[1]; *[1]Princeton University, Princeton, NJ*

MP 595 **Detecting Changes in the Epimerization of Water-Soluble and Water-Insoluble Crystallin Proteins Using Tandem LC-MS**; Yana Lyon; *, Riverside, CA*

MP 596 **Measurement of the Dynamics of Histone Methylation by One-Carbon Metabolic Isotope Labeling and HCD Methylation-Signature-Ions Detection**; Hui Tang[1]; KANGLING ZHANG[1]; *[1]University of Texas Medical Branch at Galveston, Galveston, TX*

PROTEOMICS: CLINICAL APPLICATIONS (APPLIED PROTEOMICS)
597 - 621

MP 597 **Effects of MK-801 and Clozapine on the Proteome of Cultured Human Oligodendrocytes**; Juliana Silva Cassoli[1]; Keiko Iwata[2]; Johann Steiner[3]; Paul C. Guest[1]; Juliana Minardi Nascimento[1]; Daniel Martins-de-Souza[1]; *[1]Laboratoy of Neuroproteomics, Department of Biochemistry and Tissue Biology, Institute of Biology, University of Campinas, Campinas, SP, Brazil; [2]University of Fukui, Fukui, Japan; [3]Department of Psychiatry, University of Magdeburg,, Magdeburg, Germany*

MP 598 **Proteomics of Benign and Metastatic Triple Negative Breast Cancer Cells and Cybrids**; Vadiraja B Bhat[1]; Durairaj Renu[2]; Akanksha Mishra[2]; Pramila Tata[2]; Jun Hyoung Park[3]; Santhosh Kumar[3]; Sajna A Vithayathil[3]; Nagireddy Putluri[3]; Efrosini Tsouko[3]; Taraka R Donti[3]; Daniel E Frigo[3]; Chad J Creighton[3]; Michael T. Lewis[3]; Arun Sreekumar[3]; Lee-Jun Wong[3]; Benny A Kaipparettu[3]; *[1]Agilent Technologies, Wilmington , DE; [2]Strand Life Sciences, Bangalore, India; [3]Baylor College of Medicine, Houston, TX*

MP 599 **Targeted Proteomic Analysis of FFPE Bone Metastases from Lung Cancer and Other Malignancies**; Chao Gong[1]; Fabiola Cecchi[1]; Adele Blackler[1]; Wei-Li Liao[1]; Marlene Darfler[1]; Todd Hembrough[1]; *[1]NantOmics, Rockville, MD*

MP 600 **Comprehensive Proteome Characterization of Pancreatic Cyst Fluid from Intraductal Papillary Mucinous Neoplasm (IPMN) by LC-MS/MS**; Joonho Park[1]; Dohyun Han[2]; Misol Do[3]; Mee Joo Kang[4]; Jin-Young Jang[4]; Youngsoo Kim[1]; *[1]Department of Biomedical Engineering, Seoul National University College of Medicine, Seoul, Korea; [2]Biomedical Research Institute, Seoul National University Hospital, Seoul, Korea; [3]Department of Biomedical Science, Seoul National University College of Medicine, Seoul, Korea; [4]Department of Surgery, Seoul National University College of Medicine, Seoul, Korea*

MP 601 **Epitope Identification of Human α-Galactosidase A to a Monoclonal Antibody by Affinity Mass Spectrometry**; Zdenek Kukacka[1, 2]; Marius Iurascu[1, 2]; Yannick Baschung[1, 3]; Mary Murphy[4]; Jeff Bornheim[4]; Michael Przybylski[1, 2]; *[1]Steinbeis Centre Biopolymer Analysis and Biomedica, Ruesselsheim, Germany; [2]University of Konstanz, Konstanz, Germany; [3]University of Rostock, Rostock, Germany; [4]Ametek-Reichert Technologies, Buffalo, NY*

MP 602 **Proteomics Identifies Three New Types of Amyloidosis Associated with Distinctive Clinical Phenotypes**; Surendra Dasari[1]; Jason D Theis[1]; Julie A Vrana[1]; Samih H Nasr[1]; Sanjeev Sethi[1]; Paul J Kurtin[1]; *[1]Mayo Clinic, Rochester, MN*

MP 603 **Minimal Residual Disease in Multiple Myeloma by LC-MS/MS by Analysis of Immunoglobulin Heavy and Light Chain CDR Tryptic Peptides**; Linda M Benson[1]; Angela Dispenzieri[1]; David L. Murray[1]; H. Robert Bergen, III[2]; *[1]Mayo Clinic, Rochester, MN; [2]Mayo Clinic, Rochester , MN*

MP 604 **Pharmacoproteomics Identifies the Drug Efficacy Mechanism in Acamprosate Treatment of Alcoholism**; Caroline M Germany[1]; Ashlie N Reker[1]; Hyung W Nam[1]; *[1]LSU Health Science Center, Shreveport, LA*

MP 605 **A Network Based Approach to Understand the Brain Proteome in Alzheimer's Disease**; Nicholas Seyfried[1]; Eric B Dammer[1]; Vivek Swarup[2]; Duc Duong[1]; Luming Yin[1]; Juan C Troncoso[3]; Madhav Thambisetty[4]; Daniel Geschwind[2]; James Lah[1]; Allan Levey[1]; *[1]Emory University School of Medicine, Atlanta, GA; [2]UCLA, Los Angeles, CA; [3]Johns Hopkins University School of Medicine, Baltimore, MD; [4]National Institutes of Health, Bethesda, MD*

MP 606 **To Pool or Not to Pool: Discovery of Biomarkers for Sjögren's Syndrome Using Mass Spectrometry-Based Proteomics**; Wanlu Qu[1]; Driss Zoukhri[2]; Athena Papas[2]; Markus Hardt[1]; *[1]The Forsyth Institute, Cambridge, MA; [2]Tufts University, Medford, MA*

MP 607 **Analysis of Monoclonal Immunoglobulins from Multiple Myeloma Patients by Use of 21 Tesla FT-ICR MS/MS**; Lidong He[1]; Lissa Anderson[2]; David R Barnidge[3]; David L Murray[3]; Christopher L Hendrickson[2]; Alan G Marshall[1, 2]; *[1]Florida State University, Tallahassee, Florida; [2]National High Magnetic Field Laboratory, Tallahassee, FL; [3]Mayo Clinic / DLMP, Rochester, MN*

MP 608 **Understanding the Molecular Mechanisms Underlying Cisplatin Resistance in Ovarian Cancer Cells**; Yi Huo[1]; Yuling Chen[2]; Chongdong Liu[3]; Zhenyu Zhang[3]; HAITENG DENG[4]; *[1]MOE Key Laboratory of Bioinformatics, Tsinghua University, Beijing, China, 100084, Beijing, China; [2]Tsinghua University, Beijing, China; [3]Chaoyang Hospital Affiliated to Capital Medical University, Beijing, China; [4]Tsinghua University, Beijing*

MP 609 **Apolipoprotein Kinetics Measured in Human HDL by HR/AM-PRM Unveils a Novel Picture of HDL Metabolism**; Lang Ho Lee[1]; Allison B Andraski[2]; Brett Pieper[1]; Frank M Sacks[2]; Masanori Aikawa[1]; Sasha A Singh[1]; *[1]Center for Interdisciplinary Cardiovascular Science,*

Brigham and Women's Hospital and Harvard Medical School, Boston, MA; [2]Department of Nutrition, T.H. Chan Public Health School of Harvard University, Boston, MA

MP 610 **Relevance of Albumin Bound Iron in Ovarian Cancer as Determined by ICP-MS**; Lindsay Schambeau[1]; Lauren Amable[2]; Jana Rocker[1]; Michael Finan[1]; Rodney Rocconi[1]; Lewis Pannell[1]; *[1]Mitchell Cancer Institute, Mobile, AL; [2]National Institutes of Health, Bethesda, MD*

MP 611 **Proteomic Analysis of an ALDH Sub-Population in Colorectal Cancer Identified by Liquid Chromatography-Mass Spectrometry**; Rui Yang[1]; Xinhua Liu[2]; Smathorn Thakolwiboon[3]; Jianhui Zhu[1]; Xiucong Pei[1]; Zhijing Tan[1]; Mingrui An[1]; Jun Cao[1]; Jing Wu[1]; David M Lubman[1]; *[1]University of Michigan Medical Center, Ann Arbor, MI; [2]Shanghai University, Shanghai, CHINA; [3]Mahidol University, Bangkok, Thailand*

MP 612 **Ion Current-based Proteomic Profiling in Understanding the Mechanism of Tumor Necrosis Factor Alpha on Myogenic Differentiation**; Chengjian Tu[1]; Jun Li[2]; Jun Qu[1]; *[1]University at Buffalo, Buffalo, NY; [2]University at Buffalo SUNY, Williamsville, NY*

MP 613 **Characterization of O- and N-Glycosylations of Immunoglobulin A in IgA Nephropathy**; Jean-Marie Schmitter[1]; Katell Bathany[2]; Christelle Oblet[3]; Jean-Claude Aldigier[3]; Anne Druilhe[3]; *[1]University of Bordeaux, Bordeaux, France; [2]University of Bordeaux, Bordeaux, France; [3]University of Limoges, Limoges, France*

MP 614 **Effect of Radiotherapy on Protein Levels in Blood Plasma Collected from Breast Cancer Patients**; Catherine C Going[1]; Marta Vilalta[1]; Marjan Rafat[1]; Melissa Jenkins[1]; Kathleen C Horst[1]; Edward E Graves[1]; Sharon J Pitteri[1]; *[1]Stanford University School of Medicine, Palo Alto, CA*

MP 615 **Prions in Hormonal Replacement Therapy?**; Tanja Panic-Jankovic[1]; Maria Zellner[2]; Goran Mitulovic[2]; *[1]Medizinische Universitaet Wien, Vienna, Austria; [2]Medical University of Vienna, Vienna, Austria*

MP 616 **Mass Spectrometry Based Proteomic Investigation of Annulus Fibrosus and Nucleus Pulposus of the Mature Bovine Intervertebral Disc**; Willem Duckworth[1]; Ashley Brisbin[1]; Kelly L Wormwood[1]; Emmalyn J Dupree[1]; Jessica Roberge[1]; Devika Channaveerappa[1]; Petra Kraus[1]; Thomas Lufkin[1]; Costel C Darie[1]; *[1]Clarkson University, Potsdam, NY*

MP 617 **Single Amino Acid Variation Profiles of the MCF7 Breast Cancer Cell Line Using LC-MS/MS**; Zhijing Tan[1]; Song Nie[1, 2]; Mingrui An[1]; Rui Yang[1]; Jun Cao[1]; Xiucong Pei[1]; David M. Lubman[1]; *[1]The University of Michigan, Ann Arbor, MI; [2]Pacific Northwest National Laboratory, Richland, WA*

MP 618 **Evaluation of Undifferentiated State of Human iPS Cells by Non-Invasive LC-MS/MS Analysis Approach Using Cell Culture Supernatant as Samples**; Takashi Suzuki[1]; Gamo Kentaro[2]; Hatabayashi Kunitada[2]; Takahashi Masatoshi[1]; Kagawa Kenichi[2]; Ogura Tairo[3]; Hiramaru Daisuke[1]; Toyoda Kenichi[1]; Ozaki Shigenori[2]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]Tokyo Electron Limited, Kobe, Japan; [3]Shimadzu Scientific Instruments, Inc. Columbia*

MP 619 **Quantitative Proteomics Analysis Reveals Molecular Signatures Associate with LPS, Betamethasone, and Magnesium Sulfate Treatment in E15 Murine Gastrointestinal Tract**; Elizabeth Yohannes[1]; Jesica L. Slack[1]; Vivek Ramachandran[1]; Andrew S. Thagard[2]; Mark Wingerd[1]; Avedis Kazanjian[1]; *[1]Department of Clinical Investigation, Madigan Army Medical Center, Tacoma, Washington; [2]Maternal Fetal Medicine, Madigan Army Medical Center, Tacoma, Washington*

MP 620 **Proteomics of Globo H High/Low BxPC-3 Pancreatic Cancer Cell Line**; Sheng-Ta Tsai[1]; Hsin-Ying Han[1]; Shok-Li Ng[1]; Chia-Ning Shen[1]; Chung-Hsuan Chen[1]; *[1]Genomics Research Center, Academia Sinica Taipei, Taiwan*

MP 621 **Proteomic Analysis by SILAC to Distinguish between Salmonella Lipopolysaccharide (LPS) and Monosodium Urate (MSU) Crystals Induced Inflammation in Macrophages**; Sarbjeet Makkar[1]; Rohana Liyanage[1]; Jr Jackson O Lay[1]; *[1]University of Arkansas, Fayetteville, AR*

PROTEOMICS: QUANTITATIVE
622 - 650

MP 622 **Quantitation of Immunoglobulin Alpha from Whole Gut Lavage Fluid Using the Thermo Q-Exactive Plus**; Joseph Otto[1]; Crystal Daniels[1]; Lindsay Schambeau[1]; Jana Rocker[1]; *[1]Mitchell Cancer Institute, Mobile, AL*

MP 623 **Targeted Quantitation of Crbpl in Cancer Cells through a Bottom-Up Approach**; Wenjing Li[1]; Jianshi Yu[1]; Claire Louise Carter[1]; Jace W Jones[1]; Maureen A Kane[1]; *[1]University of Maryland School of Pharmacy, Baltimore, MD*

MP 624 **Kinase Activity Profiling of Lung Adenocarcinoma to Understand Cancer Signaling and Select Targeted Therapeutics**; Melissa A. Hoffman[1, 2]; Bin Fang[1]; Stephen Brantley[1]; Fumi Kinose[1]; Eric Welsh[1]; Steven A. Eschrich[1]; Eric B. Haura[1]; John M. Koomen[1]; *[1]Moffitt Cancer Center, Tampa, FL; [2]University of South Florida, Tampa, FL*

MP 625 **Label-Free Quantitative Proteomics Profiling of Human Osteoclast Activation, Differentiation and anti-TNF Biologics Treatment**; Chenqi Hu[1]; Bohdan Harvey[1]; Zehra Kaymakcalan[1]; Edit Tarcsa[1]; Dongdong Wang[1]; Yu Tian[1]; *[1]Abbvie Bioresearch Center, Worcester, MA*

MP 626 **Protein Biomarker Quantitation from Human Blood and Plasma Using Novel Collection Technology by LCMS/MS**; Alan Barnes[1]; Neil Loftus[2]; Jérôme Vialaret[3]; Christophe Hirtz[3]; Sylvain Lehmann[3]; *[1]Shimadzu MS/BU, Manchester, Greater Manchester; [2]Shimadzu, Manchester, UK; [3]CHU de Montpellier, Montpellier, France*

MP 627 **In Depth Quantification of Extracellular Matrix Proteins from Human Pancreas for Tissue Engineering**; Fengfei Ma[1]; Christopher Lietz[2]; Sara Sackett[3]; Dan Tremmel[3]; Jon Odorico[3]; Lingjun Li[1, 2]; *[1]School of Pharmacy, University of Wisconsin-Madison, Madison, WI; [2]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [3]Department of Surgery, School of Medicine and Public Health, University of Wisconsin-Madison,, Madison, WI*

MP 628 **Identification of Interaction Networks of Mutant and Wild-Type IDH1 in Glioma Cell Lines**; Nina Overbeck[1]; Anja Stefanski[1]; Vanessa Scherbaum[2]; Christiane Knobbe-Thomsen[2]; Kai Stühler[1]; *[1]Molecular Proteomics Laboratory, Heinrich-Heine-University, Düsseldorf, Germany; [2]Department of Neuropathology, Heinrich-Heine-University, Düsseldorf, Germany*

MP 629 **Quantitative MRM Assays of Salivary Proteins for Biomarker Assessment Studies**; Andrew J Percy[1]; Darryl B Hardie[1]; Juncong Yang[1]; Armando Jardim[2]; Yassene Mohammed[1, 3]; Monica H. Elliott[1]; Christoph H. Borchers[4, 5]; *[1]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [2]Institute of Parasitology, McGill University, Montreal, QC, Canada; [3]Center for Proteomics and Metabolomics, Leiden University Medical Center, Leiden, The Netherlands; [4]University of Victoria - Genome BC Proteomics Centre, Victoria, BC; [5]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada*

MP 630 **Toward the Development of a Scheduled GeLC-MRM Method for High-Throughput Quantitative Profiling of Small GTPases in Cancer Cells**; Ming Huang[1]; Yinsheng Wang[2]; *[1]University of California, Riverside, Riverside, California; [2]University of California, Riverside, Riverside, CA*

MP 631 **Targeted Proteomic Analysis Using Parallel Reaction**

Monitoring Revealed Longitudinal Change in Level of Proteins in Activation of BV2 Mouse Microglia; Woo Jongmin[1]; Han Dohyun[2, 3]; Kim Youngsoo[2]; *[1]Department of Biomedical Sciences, Seoul National University, College of Medicine, Seoul, Korea; [2]Department of Biomedical Engineering, Seoul National University, College of Medicine, Seoul, Korea; [3]Biomedical Research Institute, SNUH, Seoul, Korea*

MP 632 **Changes in Lipid Raft Proteome upon TNF-α Stimulation of Cystic Fibrosis Cells Using SILAC**; Cerina Chhuon[1]; Iwona Pranke[2]; Florence Borot[2]; Danielle Tondelier[2]; Joanna Lipecka[3]; Janine Fritsch[2]; Marc Chanson[4]; Aleksander Edelman[2]; Mario Ollero[5]; Chiara Ida Guerrera[1]; *[1]Proteomic Platform Necker, PPN-3P5, Structure Fédérative de Recherche SFR Necker US24, 75015, Paris, France; [2]Institut Necker Enfants Malades, INSERM, U1151, Paris, France; [3]The CPN Proteomics Facility – 3P5, Center of Psychiatry and Neuroscience, UMR INSERM 894, 75014, Paris, France; [4]Geneva University Hospitals and University of Geneva, 1211, Geneva, Switzerland; [5]Institut Mondor de Recherche Biomédicale, INSERM, U955, and Université Paris Est Créteil, 94010, Créteil, France*

MP 633 **MRM Quantitation of an In-depth Panel of Candidate Disease-linked Proteins in Various Mouse Tissues**; Sarah Michaud[1]; Andrew Percy[2]; Nicholas Sinclair[2]; André LeBlanc[2]; Suping Zhang[3]; Christoph H. Borchers[2, 4]; *[1]MRM Proteomics Inc, Victoria, BC, Canada; [2]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [3]MRM Proteomics, Inc., Victoria, BC, Canada; [4]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada*

MP 634 **The Proteomic Landscape of Breast Patient-Derived Xenografts Reveals Tumor-Specific Education of the Cancer Microenvironment**; Xuya Wang[1]; Petra Erdmann-Gilmore[2]; Rosa Viner[3]; Matthew R Meyer[2]; Timothy J Stuhlmiller[4]; Sherri R Davies[2]; Shunqiang Li[2]; Qiang Zhang[2]; Arshag D Mooradian[2]; Kuan-lin Huang[5]; Ryan Bomgarden[6]; Li Ding[5]; Matthew J Ellis[7]; John C Rogers[6]; Gary L Johnson[4]; Reid R Townsend[2]; David Fenyö[1]; Jason M Held[2, 8]; *[1]NYU School of Medicine, New York City, NY; [2]Washington University School of Medicine, Saint Louis, MO; [3]Thermo Fisher Scientific, San Jose, CA; [4]Department of Pharmacology University of North Carolina, Chapel Hill, NC; [5]The Genome Institute Washington University, Saint Louis, MO; [6]Thermo Fisher Scientific, Rockford, IL; [7]Baylor College of Medicine, Houston, TX; [8]Department of Anesthesiology Washington University, Saint Louis, MO*

MP 635 **The Pathway Activity of Fatty Acid β-Oxidation is Up-Regulated in the Skeletal Muscle Mitochondria of T2DM Mouse Model**; Zhou Yang[1, 2]; Hou Guixue[1, 3]; Wu Lin[1]; Lou Xiaomin[1]; Ren Yan[2]; Su Siyuan[1, 2]; Deng Yamei[1, 2]; Li Qidan[1, 2]; Zhang Yue[1, 2]; Zi Jin[2]; Liu Siqi[1, 2]; *[1]CAS Key Laboratory of Genome Sciences and Information, Beijing Institute of Genomics, Chinese Academic of Sciences, Beijing, China; [2]BIG-Shenzhen, Shenzhen, China; [3]BGI shenzhen, Shenzhen, China*

MP 636 **In-Depth Quantitative Proteomic Analysis of Human Breast Cancer Cells in Response to Nicotinamide**; Dohyun Han[1, 2]; Ji Young Kim[3]; Joonho Park[2]; Han Suk Ryu[3]; *[1]Biomedical Research Institute, Seoul National University Hospital, Seoul, Korea; [2]Department of Biomedical Engineering, Seoul National University Hospital, Seoul, Korea; [3]Department of Pathology, Seoul National University Hospital, Seoul, Korea*

MP 637 **iTRAQ Based Quantitative Proteomics of a Brain-Enriched Cytosolic Protein Fraction in Schizophrenia**; Erika Velásquez[1]; Daniel Martins-de-Souza[2]; Ingrid Velásquez[3]; Andrea Schmitt[4]; Fabio Cs Nogueira[5]; Gilberto B Domont[1]; *[1]Federal University of Rio de Janeiro, Rio de Janeiro, Brazil; [2]Unicamp, Campinas, SP; [3]University of Carabobo, Valencia, Venezuela; [4]Ludwig Maximilian University of Munich, Munich, Germany; [5]UFRJ, Rio de Janeiro, Rio de Janeiro*

MP 638 **Challenges of Using Isobaric Labeling for In-Depth Analysis of Large Numbers of Plasma Samples in a Cardiotoxicity Biomarker Discovery Study**; Pengyuan Liu[1]; Lynn A. Beer[1]; Bonnie Ky[2]; David W Speicher[1]; *[1]The Wistar Institute, Philaldephia, PA; [2]University of Pennsylvania, Philadelphia, PA*

MP 639 **Quantitative Multiplexed Isobaric Tag-Based Proteomic and Phosphoproteomic Profiling Reveals Nicotine and Cigarette Smoke Extract-Induced Alterations in Human Pancreatic Stellate Cells**; Joao A Paulo[1]; Steven P Gygi[2]; *[1]Harvard, Boston, MA; [2]Harvard Medical School, Boston, MA*

MP 640 **SILAC-based Phosphoproteomic Analysis of PTH1R Signaling in Proliferating Osteoblasts**; Lauren E Ball[1]; Grace Williams[1]; Jennifer Bethard[1]; Louis Luttrell[1]; *[1]Medical Univ of S Carolina, Charleston, SC*

MP 641 **Quantitative Temporal Proteomics of Flow Cytometry Isolated Virus-Driven MDSCs**; Derek Clements[1]; Patrick Murphy[2]; Youra Kim[1]; Andra Sterea[3]; Shekoufeh Almasi[3]; Namit Holay[1]; Prathyusha Konda[2]; Joao Paulo[4]; Steven P Gygi[4]; Shashi Gujar[2]; Patrick Lee[1, 2]; *[1]Department of Pathology, Dalhousie University, Halifax, NS, Canada; [2]Department of Microbiology & Immunology, Dalhousie University, Halifax, NS, Canada; [3]Department of Biology, Dalhousie University, Halifax, NS, Canada; [4]Harvard University, Boston*

MP 642 **Down Regulation of Glycolysis Pathway in PICALM Depleted Cells**; Barsam Mirfattah[1]; Hui Tang[1]; Cheryl F Lichti[1]; Fernanda Laezza[1]; Kangling Zhang[1]; *[1]University of Texas Medical Branch at Galveston, Galveston, TX*

MP 643 **Phosphoproteomic and Glycoproteomic Studies of Tonic and Activated B Cell Receptor Signaling in Burkitt's Lymphoma**; Jasmin Corso[1]; Kuan-Ting Pan[1]; Roland Walter[2]; Carmen Döbele[2]; Sebastian Mohr[2]; Christof Lenz[1, 3]; Hubert Serve[2, 4]; Henning Urlaub[1, 3]; Thomas Oellerich[2, 4, 5]; *[1]Bioanal. MS Group, Max Plank Inst for Biophys Chem, Goettingen, Germany; [2]Department of Hematology/Oncology, Johann Wolfgang Goethe University, Frankfurt, Germany; [3]Bioanalytics, University Medical Center Göttingen, Institute for Clinical Chemistry, Goettingen, Germany; [4]German Cancer Consortium/ German Cancer Research Center, Heidelberg, Germany; [5]Department of Haematology, University of Cambridge, Cambridge, United Kingdom*

MP 644 **Quantitative Profiling of Peroxisome Proliferation in the Heart by Selected Reaction and Selected Ion Monitoring. Effects of High Fat Diets**; Caroline Kinter[1]; Maria Thomas[1]; David Gutierrez[1]; Szweda Luke[1]; Michael Kinter[1]; *[1]Oklahoma Medical Research Foundation, Oklahoma City, OK*

MP 645 **MS1-Based Quantitative Proteomics Investigation of Mechanisms Underlying Gemcitabine and Trabectedin Synergism with High Multiplexing Capacity and Extremely Low Missing Value**; Shichen Shen[1]; Xin Miao[1]; Jun Li[1]; Xiaomeng Shen[1]; Xue Wang[1]; William Jusko[1]; Jun Qu[1]; *[1]University at Buffalo, Buffalo, NY*

MP 646 **Understanding Proteomic Alterations in GBM Tumors Associated with the Subventricular Zone: a Quest for Better Prognosis**; Ghantasala Saicharan[1]; Gollapalli Kishore[2]; Shailendra Rane[3]; Deepti Bhandarkar[3]; Sanjeeva Srivastava[2]; Aliasgar Moiyadi[4]; *[1]Indian Insitute of Technology, Bombay, Mumbai, India; [2]Indian Institute of Technology, Bombay, Mumbai, India; [3]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, INDIA; [4]Tata Memorial Centre's-Advanced Centre for Research, Training and Education in Cancer, Kharghar, Navi Mumbai, India*

MP 647 **Exploration of Novel Mechanisms for Synergy of Paclitaxel and Birinapant through Large-scale Quantitative Label-free LC/MS Proteomics**; Xue Wang[1]; Jin niu[1]; Jun Li[2]; Shichen Shen[2]; Xiaomeng Shen[2]; Jun Qu[2]; *[1]University at Buffalo, Buffalo, NY; [2]Center of Excellence in Bioinformatics&Life Sci., Buffalo, NY*

MP 648 **ProteOMZ: Development of Biogeochemically Relevant Peptide Biomarkers for High-Throughput Marine Microbial Ecosystem Characterization in Oceanic Oxygen Minimum Zones**; Mak Saito[1]; Matt McIlvin[1]; Dawn Moran[1]; Alyson Santoro[2]; Chris Dupont[3]; Michael Rappe[4]; *[1]Woods Hole Oceanographic Institution, Woods Hole, MA; [2]University of Maryland Horn Point Laboratory, Cambridge, MD; [3]J.C. Venter Institute, La Jolla, CA; [4]Hawaii Institute of Marine Biology, University of Hawaii, Manoa, HI*

MP 649 **Sensitive, Fast and Robust Quantification of Antibodies in Complex Matrices by Capillary Flow UHPLC and High Resolution Accurate Mass MS**; Alexander Boychenko[1]; Stephan Meding[2]; Martin Samonig[2]; Remco Swart[2]; *[1]Thermo Fisher Scientific, Bremen, DE; [2]Thermo Fisher Scientific, Germering, DE*

MP 650 **Src-Family Kinase Signaling Mediating Gemcitabine Resistance in Gall Bladder Cancer Revealed by Quantitative Phosphoproteomics**; Patricia García[1]; Jun Zhong[2]; Carolina Bizama[1]; Jaime Espinoza[1]; Juan Carlos Roa[1]; Pamela Leal[3]; *[1]Department of Pathology, School of Medicine; Center for Investigation in Translational Oncology (CITO), FONDAP-ACCDIS, Pontificia Universidad Católica de Chile, Santiago, Chile; [2]Delta Omics Biotechnology, Catonsville, MD; [3]Center of Genetic and Immunological Studies (CEGIN) and Scientific and Technological Bioresource Nucleus (BIOREN). Universidad de La Frontera, Temuco, Chile*

SMALL MOLECULES: QUALITATIVE ANALYSIS
651 - 680

MP 651 **Identification of Chemical Ingredients from *Ginkgo biloba* Extract Using UHPLC-QTOF/MS Coupled with PCDL Library**; Guoqiang Liu[1]; Shan-An Chan[2]; *[1]Agilent Technology, Inc. Shanghai, China; [2]Agilent Technology, Inc. Taipei Taiwan, Taiwan*

MP 652 **Collision-Induced Dissociation MS/MS of Cimitrypazepines, A New Class of Alkaloids from Black Cohosh (*Actaea racemosa*)**; Dejan Nikolic[1]; David C Lankin[1]; Richard van Breemen[1]; *[1]University of Illinois College of Pharmacy, Chicago, IL*

MP 653 **Dereplication of Fungal Secondary Metabolites by UPLC-PDA-HRMS-MS/MS and Mass Defect Filtering**; Noemi Paguigan[1]; Tamam M. El-Elimat[1, 2]; Diana Kao[1, 2]; Huzefa A. Raja[1]; Cedric J. Pearce[3]; Nicholas H Oberlies[1]; *[1]Department of Chemistry and Biochemistry, University of North Carolina at Greensboro, Greensboro, NC; [2]Chemistry and Biochemistry Department, Greensboro, NC; [3]Mycosynthetix, Inc., Hillsborough, NC*

MP 654 **Development and Evaluation of a Dual Separation, High-Resolution, nano-ESI-LC-MS/MS Approach for Dissolved Soil Organic Matter Characterization**; Mallory P Ladd[1, 2]; Robert Hettich[1]; *[1]Oak Ridge National Laboratory, Oak Ridge, TN; [2]University of Tennessee-Knoxville, Knoxville, TN*

MP 655 **Formation of m/z 92 Ion During Fragmentation of Deprotonated N-butyl Benzenesulfonamide**; Chongming Liu[1]; Athula B. Attygalle[1]; *[1]Stevens Institute of Technology, Hoboken, NJ*

MP 656 **Gas-phase Methylation of Benzene by an Internal Electrophilic Aromatic Addition Mechanism Mediated by *in-situ* Generated Methylcarbenium Ion**; Hanxue Xia[1]; Athula Attygalle[2]; Yong Zhang[2]; *[1]SIT, jersey city, New Jersey; [2]Stevens Institute of Technology, Hoboken, NJ*

MP 657 **Non-Targeted Screening of Tattoo Ink Contaminants Using Liquid Chromatography/ High-Resolution Mass Spectrometry and Chemometrics**; Caitlin N. Kneapler[1]; Ann M. Knolhoff[1]; Clark Ridge[1]; Fred Fry[1]; Timothy R Croley[1]; *[1]FDA/CFSAN, College Park, MD*

MP 658 **Applications of Infrared Ion Spectroscopy in Bioanalytical Chemistry**; Jonathan Martens[1]; Giel Berden[1]; Jos Oomens[1]; *[1]FELIX Laboratory - IMM - Radboud University, Nijmegen, The Netherlands*

MP 659 **A Bayesian Prior Probability Model to Improve the Confidence of Chemical Identification**; Tyler A Zimmerman[1]; W.Gary Mallard[2]; Tytus D Mak[2]; Nirina Rabe Andriamaharavo[2]; Dmitrii V Tchekhovskoi[2]; Stephen E Stein[2]; *[1]National Institute of Standards and Technology, Gaithersburg, MD; [2]National Institute of Standards & Technology, Rockville, MD*

MP 660 **Investigation of the Metabolites of the HIF-Stabilizer FG-4592, Formed by Four *in vitro* Models, Using High Resolution Mass Spectrometry**; Annelie Hansson[1]; Mario Thevis[2]; Geoff Miller[3]; Daniel Eichner[3]; Ulf Bondesson[1, 4]; Mikael Hedeland[1, 4]; *[1]Uppsala University, Uppsala, SE; [2]German Sport University, Cologne, DE; [3]Sports Medicine Research and Testing Laboratory, Salt Lake City, UT; [4]National Veterinary Institute, Uppsala, SE*

MP 661 **The ETD-Like Fragmentation for Small Molecules**; Romain Huguet[1]; Chad R Weisbrod[1]; Mark Berhow[2]; Vlad Zabrouskov[1]; Jae Schwartz[1]; Tim J Stratton[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]USDA, ARS NCAUR Peoria, IL*

MP 662 **Application of TOF MS instrument in Bioanalysis – A Case Study**; Shaokun Pang[1]; Weixing Sun[2]; Adrien Musuku[2]; Xavier Misonne[3]; *[1]SCIEX, Redwood City, CA; [2]Pharmascience, Montreal, Canada; [3]SCIEX, Lorraine, QC*

MP 663 **On-Line Chiral Analysis of Reaction Mixtures Using the Kinetic Method**; Ryan M Bain[1]; Xin Yan[1]; Shannon A Raab[1]; Stephen T Ayrton[1]; Tawnya G Flick[2]; Graham R Cooks[1]; *[1]Purdue University, West Lafayette, IN; [2]Amgen, Inc., Thousand Oaks, CA*

MP 664 **Automated Correlation between Structural Isomers and Fragment Ion Spectra Using a Novel Fragmentation Prediction Engine** ; Kirsten Hobby [1]; Richard T Gallagher[2]; *[1]Shimadzu MS/BU, Manchester, Lancashire; [2]AstraZeneca, Maccelsfield, UK*

MP 665 **Effects of Low Percentage Non-Ionic Additives on Charge State and Ion Intensity in Electrospray Ionization for Small Molecule Analysis**; Jeffrey Alberts[1]; Kenneth J Ruterbories[1]; David W Bedwell[1]; Kishore K Katyayan[1]; Kenneth C Cassidy[1]; *[1]Eli Lilly and Company, Indianapolis, IN*

MP 666 **Understanding Paper Degradation: Identification of Products of Cellulosic Paper Decomposition at the Wet-Dry "Tideline" Interface Using GC-MS and LTQ Orbitrap**; Sergey Sladkevich[1]; Anne-Laurence Dupont[2]; Michel Sablier[2]; Richard B. Cole[1]; *[1]Sorbonne Universités, UPMC Univ Paris 06, Paris, France; [2]Muséum National d'Histoire Naturelle, Paris, France*

MP 667 **Development of a GC-MS Method for Structure Elucidation of Disubstituted Naphthalenes**; Kirill Tretyakov[1]; Stephen Stein[1]; Anzor Mikaia[1]; *[1]National Institute of Standards and Technology, Gaithersburg, MD*

MP 668 **Substituting Atmospheric Solid Analysis Probe Ionization for Direct Probe Electron Impact Ionization for Analysis of Alcohols and Hydrocarbons**; Martha M. Vestling[1]; Trevor C. Christenson; Stephanie N. Knezz; *[1]University of Wisconsin, Madison, WI*

MP 669 **Dosing Syringe Extractables Analysis Using Bench-top Orbitrap Mass Spectrometer**; Kenneth Wong[1]; Dujuan Lu[1]; Kate Comstock[2]; *[1]SGS, Fairfield, NJ; [2]Thermo Fisher Scientific, San Jose , CA*

MP 670 **Identification and Quantitation of IV Bag Extractables Using LC-HRMS and GCMS** ; Dujuan Lu[1]; Kenneth Wong[1]; Kate Comstock[2]; *[1]SGS, Fairfield, NJ; [2]Thermo Fisher Scientific, San Jose , CA*

MP 671 **Impurity Profiling of Pharmaceuticals Using a UPLC-ToF Data Independent Acquisition Strategy and Scientific Data and Library Information Systems**; Jayne Kirk[1]; Russell Mortishire-Smith[1]; Sean McCarthy[2]; Mark Wrona[2]; *[1]Waters Corporation, Wilmslow, UK; [2]Waters Corporation, Milford, MA*

MP 672 **The Application of Electrochemistry/MS to Pharmaceutical Stability Testing and Degradant Synthesis**; Martin Eysberg[1]; Jean-Pierre Chervet[2]; Nico Reinhoud[2]; Mark Taylor[3]; Susana da Silva Torres[3]; *[1]Antec LLC, Boston, MA; [2]Antec, Zoeterwoude, The Netherland; [3]Pfizer Worldwide Research and Development, Kent, United Kingdom*

MP 673 **Differentiating between Leachates and Process Related Compounds in Drug Substance Using Accurate Mass LC-MS and LC-MS/MS**; George L Perkins[1]; Lorraine Hill[1]; Gary Campbell[1]; Matthew Balmer[1]; *[1]Sanofi Pasteur Inc, Swiftwater, PA*

MP 674 **Analysis of Celastrol in Rat Brain Tissue and Plasma Samples Using TSQ Quantum Access MAX**; Usha Mishra; *Minnmass(Minnesota Mass Spec), Minneapolis, MN*

MP 675 **Determination of Limaprost, an Analogue of PGE1 in Human Plasma by QTRAP® 6500+ and SelexION®+ Technology**; Gangyi Liu[1]; Chao Zhang[2]; Wenhai Jin[3]; *[1]Xuhui Center Hospital, Shanghai, China; [2]SCIEX Asia Pacific Application Support Center, Beijing, China; [3]SCIEX Asia Pacific Application Support Center, Shanghai, China*

MP 676 **Effects of Temperature and Anticoagulant on the Stability of Tetracyclines in Whole Blood: Drug-Matrix Equilibrium**; Vinicio Vasquez[1]; Richard Lavallée[1]; Nikolay I Youhnovski[1]; Milton Furtado[1]; Anahita Keyhani[1]; *[1]Algorithme Pharma Inc., Laval, Canada*

MP 677 **Extremely Low LC-MS/MS Lithium Adduct Detection of Rapamycin in Animal Blood and Tissues**; Alexandre Pimenov[1]; Timothy Samuels[1]; *[1]Charles River Bioanalisys, Senneville, Canada*

MP 678 **Analyzing Zn-BDPA Probes to Detect Apoptotic Cells in Three-Dimensional Cell Culture System via Mass Spectrometry**; Jessica K Lukowski[1]; Eric M Weaver[1]; Kasey Clear[1]; Bradley D Smith[1]; Amanda B Hummon[1]; *[1]University of Notre Dame, Notre Dame, Indiana*

MP 679 **LC-MS Based Approach to Characterize Non-Specific Binding Inhibitors to Mycobacterium tuberculosis Shikimate Kinase (MtSK)**; Mansour Alturki[1]; Madison Jarrard[1]; Rene Ngouli[1]; Douglas Goodwin[1]; Angela Calderon[1]; *[1]Auburn University, Auburn, AL*

MP 680 **Synthesis and Characterization of Tetraphenylporphyrinate Manganese(III) Siloxides by Silyl Group Transfer from Silanethiols**; Zachary J Tonzetich[1]; Daniel J Meininger[1]; Zieph Kasrawi[1]; Hadi D Arman[1]; Wendell P. Griffith[1]; *[1]University of Texas at San Antonio, San Antonio, TX*

SYSTEMS BIOLOGY (MULTIOMICS AND OTHER)
681 - 707

MP 681 **Trans-omics Analysis of Yeast Central Carbon Metabolism by Integration of Metabolome, Proteome and Fluxome Data**; Fumio Matsuda[1]; Syunsuke Nishino[2]; Tairo Ogura[3]; Atsumi Tomita[2]; Ichiro Hirano[3]; Hiroshi Shimizu[2]; *[1]Osaka Univeristy, Osaka, Japan; [2]Osaka University, Osaka, Japan; [3]Shimadzu Corporation, Kyoto, Japan*

MP 682 **Proteomics and Metabolomics Demonstrate Inheritance of Key Energy Pathways in Red Blood Cells**; Erin M. Weisenhorn[1]; Thomas J. van't Erve[2]; Michael S Westphall[3]; Thomas J. Raife[4]; Joshua J Coon[5]; *[1]Integrated Program in Biochemistry, University of Wisconsin-Madison, Madison, Wi; [2]Immunity, Inflammation and Disease Laboratory, National Institute of Environmental Health Sciences, Research Triangle Park, NC; [3]University of Wisconsin-Madison Genome Center of Wisconsin, University of Wisconsin, Madison, Madison, WI; [4]Department of Pathology and Laboratory Medicine, University of Wisconsin-Madison, Madison, WI; [5]Departments of Chemistry and Biomolecular Chemistry, University of Wisconsin–Madison, Madison, WI*

MP 683 **Proteomic and Metabolomic Comparative Analyses of Plasma and Vasculature Tissue from TiO2nanoparticle Exposed Rats**; Megan M. Maurer[1]; Jinghai Yi[1]; Carroll McBride[1]; Timothy R. Nurkiewicz[1]; Stephen J Valentine[1]; *[1]West Virginia University, Morgantown, WV*

MP 684 **Combined Metabolomics-Proteomic Profiling Reveals Intermittent Hypoxia to Result in Lower Productivity on Scale-Up to a 5000-Liter Industrial CHO Bioprocess**; Yuanwei Gao[1]; Somak Ray[1]; Shujia Dai[1]; Alexander R. Ivanov[1]; Nicholas R. Abu-Absi[2]; Amanda M. Lewis[2]; Zhuangrong Huang[2]; Xing Zizhou[2]; Michael C. Borys[2]; Zheng Jian Li[2]; Barry L Karger[1]; *[1]Northeastern University, Boston, Massachusetts; [2]Bristol-Myers Squibb, Devens, MA*

MP 685 **Triomics Analysis from Cancer Cells and Tumors: Modeling the Biology of Disease through The Integration of Metabolomics, Lipidomics and Phosphoproteomics**; Susanne Breitkopf[1]; Min Yuan[1]; Ying Xu[1]; John M Asara[1,2]; *[1]Beth Israel Deaconess Medical Center, Boston, MA; [2]Harvard Medical School, Boston, MA*

MP 686 **Integrated Multi-Omic Analysis of Chinese Hamster Ovary Cells**; Joseph Longworth[1]; Javier Gonzalez[1]; Paul Dobson[2]; Josselin Noirel[3]; Neil Lawrence[1]; Mark Dickman[1]; David James[1]; *[1]The University of Sheffield, Sheffield, United Kingdom; [2]The University of Manchester, Manchester, United Kingdom; [3]Conservatoire National des Arts et Métiers, Paris, France*

MP 687 **Systematic Integration of Multiple 'Omics Data for Yeast Strains Isolated from Different Environments**; Rohith Srivas[1]; Barbara Dunn[1]; Andreas Huhmer[2]; Daniel Lopez Ferrer[3]; Michael Snyder[1]; *[1]Dept. of Genetics, Stanford University, Palo Alto, CA - California; [2]Thermo Fisher Scientific, San Jose, CA; [3]ThermoFisher, Palo Alto, CA*

MP 688 **Integrative Analysis of Proteome, Transcriptome, and MHC Class I Ligandome of Human Cancer Cell Lines**; Pedro Navarro[1]; Sebastian Boegel[2]; Jennifer Hahlbrock[1]; John C Castle[3]; Meike Wagner[2]; Hansjörg Schild[1]; Ugur Sahin[2]; Stefan Tenzer[1]; *[1]Institute for Immunology, JG University Medical Center, Mainz, Germany; [2]TRON – Translational Oncology at the University Medical Center of Johannes Gutenberg University, Mainz, Germany; [3]Agenus, 4-Antibody AG, Basel, Switzerland*

MP 689 **Differential Dynamics of the Mammalian mRNA and Protein Expression Response to Misfolding Stress**; Zhe Cheng[1]; Guoshou Teo[2]; Sabrina Krueger[3]; Tara Rock[1]; Hiromi Koh[2]; Hyungwon Choi[2]; Christine Vogel[1]; *[1]New York University, New York, NY; [2]National University of Singapore, Singapore, Singapore; [3]Max-Delbruck-Center, Berlin, Germany*

MP 690 **High Resolution Mass Spectrometry-Based Subcellular Proteomics of a Human Cell Line**; Aikaterini Geladaki[1]; Claire Mulvey[1]; Jake Beech[1]; Kathryn S Lilley[1]; *[1]Cambridge Centre for Proteomics, Department of Biochemistry, University of Cambridge, Cambridge, United Kingdom*

MP 691 **A Multi-Molecular Omics Approach to Study Metabolic Shifts in Caveolin-3 Transgenic Mice**; Cristina Coman[1]; Denisa Gabriela Hathazi[1]; Andreas Roos[1]; Robert Ahrends[1]; *[1]Leibniz-Institut für Analyt. Wissensch. - ISAS -, Dortmund, Germany*

MP 692 **Integration of Metabolomic and Proteomic Profiles with Physiological Measures to Understand the Complex Mechanisms of Sodium Fluoroacetate Toxicity**; Nadja Grobe[1, 2]; Meghan K Makley[2, 3]; Mitchell L Meade[2]; Andrea Hoffmann[2, 3]; Jeffery M Gearhart[2, 3]; *[1]The Henry M. Jackson Foundation for the Advancement of Military Medicine (HJF), Wright-Patterson AFB, OH; [2]Molecular Bioeffects Branch, Bioeffects Division, Human Effectiveness Directorate, 711th Human Performance Wing, Air Force Research Laboratory, Wright-Patterson AFB, OH; [3]The Henry M. Jackson Foundation for the Advancement of Military Medicine (HJF), Wright-Patterson AFB, OH*

MP 693 **In-Depth Secretome Analysis of Ovarian Clear Cell Carcinoma with ARID1A Knockdown and EZH2 Inhibition.**; Aaron R Goldman[1]; Benjamin G Bitler[1]; Rugang Zhang[1]; David W Speicher[1]; *[1]The Wistar Institute, Philaldephia, PA*

MP 694 **Data-independent Mass Spectrometry: An Effective Tool in Mechanistic Neurotoxicological Research**; Pallavi P Pilaka[1]; Pretal P Muldoon[1]; Pavel N Lizhnyak[1]; Andrew K Ottens[1]; *[1]Department of Anatomy and Neurobiology, Virginia Commonwealth University, Richmond, VA*

MP 695 **Data-Driven Construction of Global Drug Mechanisms Enabled by an Integrated High-Throughput Multi-Omics Platform**; Jeremy L Norris[1]; Melissa A Farrow[1]; Danielle Gutierrez[1]; Nicole Muszynski[1]; Lauren D Palmer[1]; Stacy D Sherrod[1]; James C Pino[1]; Jamie L Allen[1]; Jeffrey M Spraggins[1]; Alex Lubbock[1]; Ashley T Jordan[1]; William J Burns[1]; James C Poland[1]; Carrie E Romer[1]; Nathaniel Braman[1]; Yuan-wei Nei[1]; Kristie L Rose[1]; Salisha Hill[1]; Lisa M Manier[1]; Tina Tsui[1]; M. Ray Keller[1]; Stacey A Rutherford[1]; Nichole A Lobdell[1]; Carlos Lopez[1]; D. Borden Lacy[1]; John A McLean[1]; John P Wikswo[1]; Eric P Skaar[1]; Richard M Caprioli[1]; *[1]Vanderbilt University, Nashville, TN*

MP 696 **Applying Sequence Clustering to Facilitate Sample Comparisons in Metaproteomes Searched Against Different Metagenomes in Human Microbiome Research**; Jose Alfredo Blakeley-Ruiz[1]; Weili Xiong[2]; Yang Song[3]; Claire Fraser-Liggett[3]; Robert Hettich[2]; *[1]University of Tennessee, Knoxville, TN; [2]Oak Ridge National Laboratory, Oak Ridge, TN; [3]University of Maryland Baltimore, Baltimore, USA*

MP 697 **Rapid Changes in the Proteome of Gut Microbiota in Response to Short-Term Dietary Challenges in Baboons**; Prahlad K Rao[1]; Kimberly D Spradling-Reeves[1]; Vicki Mattern[1]; Laura Cox[1]; Anthony G Comuzzie[1]; Michael Olivier[1]; *[1]Texas Biomedical Research Institute, San Antonio, TX*

MP 698 **Mass Spectrometry Based Systems Biology Approaches to Understand Platelet Metabolism**; Ottar Rolfsson[1, 2]; Steinn Guðmundsson[1, 2]; Manuela Magnusdottir[1, 2]; Freyr Johansson[1, 2]; Ólafur Eysteinn Sigurjónsson[3, 4]; Bernard O Palsson[1, 2]; *[1]Center For Systems Biology, Reykjavik, Iceland; [2]University of Iceland, Reykjavik, Iceland; [3]Reykjavik University, Reykjavik, Iceland; [4]The Icelandic Blood Bank, Reykjavik, Iceland*

MP 699 **Exercise-Induced Protein Secretion from Muscle**; You Zhou[1]; Ji Li[1]; Sammy Pardo[1]; Dana Molleur[1]; Caleb Emmons[2]; Susan T Weintraub[1]; Nicolas Musi[1]; *[1]Univ. of Texas HSC, San Antonio, TX; [2]Proteome Software, Portland, OR*

MP 700 **Data-independent Quantitative Mass Spectrometry in Brain Injury Therapeutic Development**; Pavel Lizhnyak[1]; Andrew K. Ottens[1]; *[1]Dept Anatomy and Neurobiology, Virginia Commonwealth University, Richmond, VA*

MP 701 **Asymmetric Flow Field-Flow Fractionation Coupled with On-Line Trypsin Digestion and LC-MS/MS for Quantitative Analysis of Lipoprotein Sub-Class Composition**; John R. Barr[1]; Zsuzsanna Kuklenyik[2]; Michael Gardner[2]; Bryan A Parks[2]; Christopher Toth[3]; Jeffrey Jones[2]; Michael Andrews[3]; David M Schieltz[2]; Jon Rees[2]; Lisa G McWilliams[2]; James L. Pirkle[2]; *[1]CDC, Atlanta, GA; [2]Center for Disease Control and Prevention, Atlanta, GA; [3]Battelle Memorial Institute, Atlanta, GA*

MP 702 **Analysis of Liver and Heart Spheroids in Drug-Induced Hepatotoxicity and Cardiotoxicity**; Nathalie Selevsek[1]; Bernd Roschitzki[1]; Jens Kelm[2]; Olivia Rose Clayton[3]; Claudia Fortes[1]; Witold Wolski[1]; Jonas Grossmann[1]; Laura Kunz[1]; Paolo Nanni[1]; Adrian B. Roth[3]; Ralph Schlapbach[1]; *[1]Functional Genomics Center Zurich, University of Zurich & ETH Zurich, Zurich, Switzerland; [2]InSphero AG, Schlieren, Switzerland; [3]Roche Innovation Center Basel, Grenzacherstasse Basel, Switzerland*

MP 703 **Label Free Proteomics Profiling Unveils Down Regulation of Thrombin Mediated Signaling and Aggregation of Human Platelets upon Treatment with Thrombin Inhibitors**; Cristina Clement[1]; Ebenezer L.V. Ewul[2]; Anna Babinska[3]; Janet Gonzalez[4]; Monika Dzieciatkowska[5, 6]; Moro Salifu[7]; Manfred Philipp[2]; *[1]Albert Einstein CollegeMed, Bronx, NY; [2]Chemistry Department Lehman College CUNY, Bronx, NY; [3]Department of Medicine, State University of New York, Downstate Medical Center, Brooklyn, NY; [4]Department of Natural Sciences, LaGuardia Community College, Queens, NY; [5]Biological Mass Spectrometry Core Facility, University of Colorado at Denver, Aurora, Colorado; [6]Biological Mass Spectrometry Core Facility, University of Colorado at Denver, Aurora, Denver, CO; [7]Division of Nephrology, Department of Medicine, State University of New York, Downstate Medical Center, Brooklyn, NY*

MP 704 **Validation of a Unified Sample Preparation Platform for Multi-Omics Technologies**; Danielle Gutierrez[1]; Stacy D Sherrod[1]; Jeremy L Norris[1]; Carrie E Romer[1]; Melissa A Farrow[1]; Simona Codreanu[1]; Randi Lee Gant-Branum[1]; Yuan-wei Nei[1]; John A McLean[1]; Richard M Caprioli[1]; *[1]Vanderbilt University, Nashville, TN*

MP 705 **ChIP-MS/TMT: A Quantative Proteomic Analysis of Steroid Hormone Receptor Activation**; Andrew Holding; , *Cambridge, Cambridgeshire*

MP 706 **Proteomewide Profiling of Geranylgeranyl Pyrophosphate-Protein Interaction Network in Liver *via* Click Chemistry-Based Affinity Purification and Mass Spectrometry**; Lei Fang[1]; Jingzi Zhang[1]; Di Shen[1]; Bin Xue[1]; Lan Huang[2]; Chaojun Li[1]; *[1]Nanjing University, Nanjing, China; [2]University of California-Irvine, Irvine, CA*

MP 707 **Novel Method to Process Proteomics for Identification of Pathways Associated with Anti-Colon Cancer Properties of Anthocyanin-Rich Purple-Fleshed Potato in Mice**; Venkata Charepalli[1]; Vadiraja Bhat[2]; Lavanya Reddivari[3]; Jairam Vanamala[3, 4]; *[1]Pennsylvania State University, University Park, Pennsylvania; [2]Agilent Technologies, Wilmington, DE; [3]The Pennsylvania State University, State College, PA; [4]The Penn State Hershey Cancer Institute, Hershey, PA*

TOP DOWN PROTEIN ANALYSIS (APPLICATIONS) 708 – 727

MP 708 **TopDownLab – Proteoform-Specific Monitoring of Multi-Site Protein Phosphorylation**; Andrea Mizzi Brunner[1]; Philip Lössl[1]; Albert J R Heck[1]; Maarten A F Altelaar[1]; Richard A Scheltema[1]; *[1]Utrecht University, Utrecht, Netherlands*

MP 709 **Top-Down Proteomic Study of Sarcomere Protein Post-Translational Modifications in Aging Skeletal Muscle**; Liming Wei[1]; Ziqing Lin[1]; Yutong Jin[2]; Wenxuan Cai[1]; Zachery R. Gregorich[1]; Ying Ge[1]; *[1]Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison; [2]Department of Chemistry, University of Wisconsin-Madison, Madison*

MP 710 **Ultra-Fast Analysis of Hemoglobin Isoforms Using Capillary Electrophoresis Coupled to Mass Spectrometry and Ultraviolet Photodissociation**; Andreas Krupke[1]; Chien-Hsun Chen[1]; Xiaolei Xie[1]; Chad R Weisbrod[1]; Romain Huguet[1]; Shiaw-Min Chen[2]; Achim Karger[2]; Steve Williams[2]; Michael Wenz[2]; Andreas Huhmer[1]; Aran Paulus[1]; Daniel Lopez-Ferrer[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, South San Francisco, CA*

MP 711 **Evaluation and Application of Top-Down Mass Spectrometry for Exploring the Low Molecular Weight Proteome of Osteosarcoma Cells**; Liping Yang[1]; Zifeng Song[1]; Claudia S Maier[1]; *[1]Oregon State University, Corvallis, OR*

MP 712 **Top-Down Mass Spectrometry Applications for Detection of N-Terminal Sequence Heterogeneity and PTMs for a Therapeutic Molecule**; Bao Quoc Tran[1]; Shivangi Awasthi[1]; Mohd M Khan[1]; David R Goodlett[1]; Young Ah Goo[1]; *[1]University of Maryland Baltimore*

MP 713 **Targeted Intact Protein Fragmentation in Complex Mixtures Using a Charge State Scheduled Precursor List of Regulated Proteoforms**; Jim Kapron[1]; Rainer Paape[2]; Markus Lubeck[2]; Schmit Pierre-Olivier[3]; *[1]Bruker Ltd, Vancouver, Canada; [2]Bruker Daltonic GmbH, Bremen, Germany; [3]Bruker Daltonique S.A., Wissembourg, bas-rhin*

MP 714 **Investigating Binding Sites of Metal Drugs to Ubiquitin Using Free-Access chemInfo.org Algorithms**; Laure Menin[1]; Ronald F.S. Lee[2]; Luc Patiny[2]; Daniel Ortiz[2]; Paul J. Dyson[2]; *[1]EPFL SB ISIC-GE, Lausanne; [2]EPFL, Lausanne, Switzerland*

MP 715 **Human Proteoform Identification by Top-Down LC-MS/MS Utilizing a 21 Tesla FT-ICR Mass Spectrometer**; Lissa C Anderson[1]; Caroline J DeHart[1]; Nathan K Kaiser[1]; Donald F Smith[1]; Christopher L Hendrickson[1]; *[1]NHMFL, Tallahassee, Fl*

MP 716 **Top-down MS/MS Analysis of Canonical Histone H2A Phosphorylation During the Cell Cycle**; Xibei Dang[1]; Michael E Hoover[2]; Chen Yu[3]; Alan G Marshall[4, 5]; Michael A Freitas[2]; *[1]National High Magnetic Field Laboratory, Tallahassee, FL; [2]Ohio State University, Columbus, OH; [3]University of Illinois at Urbana-Champaign, Urbana-Champaign, IL; [4]National High Magnetic Field Laboratory, Tallahssee, FL; [5]Florida State University, Tallahassee, Florida*

MP 717 **Comprehensive, Quantitative Intact Proteoform Measurements of Patient-Derived Breast Tumor Xenografts Using an Improved Top-Down Proteomics Pipeline**; Tao Liu[1]; Paul D Piehowski[1]; Samuel H Payne[1]; Sangtae Kim[1]; Jungkap Park[1]; Christopher S Wilkins[1]; Carrie D Nicora[1]; Yufeng Shen[1]; Rui Zhao[1]; Anil K Shukla[1]; Ronald J Moore[1]; Sherri R Davies[2]; Shunqiang Li[2]; Reid R Townsend[2]; Matthew J Ellis[3]; Emily S Boja[4]; Henry Rodriguez[4]; Karin D Rodland[1]; Richard D Smith[1]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]Washington University, St Louis, MO; [3]Baylor College of Medicine, Houston, TX; [4]National Cancer Institute, Bethesda, MD*

MP 718 **Top-Down LC/MS Analysis of Myofilament Proteoforms in Dilated Cardiomyopathy**; Yumin Lian[1]; Ziqing Lin[1]; Yi-Chen Chen[1]; Nicole Marie Lane[1]; Takushi Kohmoto[1]; Ying Ge[1]; *[1]University of Wisconsin-Madison, Madison, WI*

MP 719 **YahO Protein as a Calibrant For Top-Down Proteomic Identification of Shiga Toxin Using MALDI-TOF-TOF-MS/MS and Post-Source Decay**; Clifton K. Fagerquist[1]; William James Zaragoza[1]; *[1]USDA/ ARS, Albany, CA*

MP 720 **Label-Free Quantitative Analysis of Mouse Brain Proteoforms Using Top Down Proteomics**; Roderick G. Davis[1]; Kyunggon Kim[1]; Paul M Thomas[1]; Ryan T Fellers[1]; Richard D Leduc[1]; VanNispen J Alexandra[1]; Jonathan Sweedler[2]; Justin Rhodes[2]; Neil L Kelleher[1]; *[1]Northwestern University, Evanston, IL; [2]University of Illinois at Urbana-Champaign, Urbana, IL*

MP 721 **Assessing Organismal and Spatial MBP Proteoform Diversification in Healthy Rats by Top-Down Mass Spectrometry (TDMS)**; Casey E Wing[1]; Micheal Tran[1]; Daniel A Plymire[2]; John Corbett[1, 2]; Steven M Patrie[1, 2]; *[1]University of Texas at Dallas, Richardson, TX; [2]University of Texas Southwestern Medical Center, Dallas, TX*

MP 722 **Top-Down Proteomics can Differentiate Closely Related Pathogenic Enterobacteria**; Mathieu Dupré[1]; Valeria Calvaresi[1]; Christian Malosse[1]; Magalie Duchateau[1]; Dominique Clermont[1]; Julia Chamot-Rooke[1]; *[1]Institut Pasteur, Paris, France*

MP 723 **Analysis of Proteoforms in Membrane Protein Complexes by Top-Down Proteomics**; Hans JCT Wessels[1]; Sergio Guerrero-Castillo[1]; Roel Tans[1]; Schmit Pierre-Olivier[2]; Stuart Pengelley[3]; Alain J Van Gool[1]; *[1]Radboudumc, Nijmegen, Netherlands; [2]Bruker Daltonique S.A., Wissembourg, bas-rhin; [3]Bruker Daltonic GmbH, Bremen, Germany*

MP 724 **Top Down 3D Spatial Mapping of Myelin Basic Protein Proteoforms: Organism and Spatial Diversification and its Potential Impact on Auto Immunity**; Daniel Plymire[1]; John Corbett[1, 2]; Casey Wing[1, 2]; Michael Tran[1, 2]; Steven Patrie[1, 2]; *[1]University of Texas Southwestern Medical Center, Dallas, TX; [2]University of Texas at Dallas, Richardson, TX*

MP 725 **Preparing to Read the Ubiquitin Code: Top-Down Analysis of Polyubiquitin Chains**; Amanda Lee[1]; Lucia Geis-Asteggiante[1]; Emma Dixon[1]; Tanuja Kashyap[1]; Yan Wang[1]; David Fushman[1]; Catherine Fenselau[1]; *[1]University of Maryland, College Park, MD*

MP 726 **Identification of Secretory Virulence Factors in *S. aureus* by Combination of Proteomics Methods**; Santosh Misal[1]; Shital D Ovhal[1]; Jonathan A Karty[1]; James P Reilly[1]; *[1]Indiana University Dept. Chemistry, Bloomington, IN*

MP 727 **Top-Down High Resolution Accurate Mass-Mass Spectrometry for Identification of Clinical Yeast Species**; Joanna Freeke[1]; Azadeh Jamalian[2]; Mansoureh Vatanshenassan[2]; Bert Gerrits van den Ende[2]; Helene L Cardasis[3]; Johan Finell[4]; Ping F. Yip[3]; Scott R. Kronewitter[3]; James Jr L Stephenson[3]; Alexander Y. Cherkassky[3]; J. Benjamin Stielow[1]; Sybren de Hoog[2]; *[1]Thermo Fisher Scientific, Utrecht, Netherlands; [2]CBS-KNAW Fungal Biodiversity Center, Utrecht, Netherlands; [3]Thermo Fisher Scientific, Cambridge, MA; [4]Thermo Fisher Scientific, Vantaa, Finland*

ANTIBODIES & ANTIBODY DRUG CONJUGATES (SEPARATIONS)
001 - 028

TP 001 **A Sensitive Multidimensional Liquid Chromatography Method for the Characterization of Free Drug Impurities in Antibody-drug Conjugates using Mass Spectral Detection**; Robert Birdsall[1]; Sean M McCarthy[2]; Alain Beck[3]; John Gebler[2]; Weibin Chen[2]; *[1]Waters Corporation, Milford, MA; [2]Waters, Milford, MA; [3]Pierre Fabre, St Julien-en-Genevois, France*

TP 002 **Characterization and Spectral Library Building of Glycopeptides in the Tryptic Digest of a Monoclonal Antibody Using 1D and 2D LC-MS/MS**; Qian Dong[1]; Xinjian Yan[2]; Yuxue Liang[2]; Stephen Stein[2]; *[1]NIST, Gaithersburg, MD; [2]NIST, Rockville, MD*

TP 003 **DAR Calculation of Cysteine Linked ADCs by Reversed Phase High Performance Liquid Chromatography Tandem High Resolution mass spectrometry**; Shuai Zuo[1]; Tao Bo[1]; *[1]Agilent Technologies (China) Limited, Beijing, China*

TP 004 **Characterization of Antibody Drug Conjugate: Intact, Fragment and Peptide Mapping using Reversed Phase Columns**; Suresh Babu Cv[1]; Tang Ning[2]; Anne Blackwell[3]; *[1]Agilent Technologies , Bangalore , Karnataka; [2]Agilent Technologies, Santa Clara, CA; [3]Agilent Technologies, Little Falls, DE*

TP 005 **Comparison of Innovator and Biosimilar by Peptide Mapping using HPLC Coupled to Time-of-Flight Mass spectrometry**; Ravindra Gudihal[1]; Ning Tang[2]; *[1]Agilent Technologies India Pvt. Ltd, Bangalore, Karnataka; [2]Agilent Technologies, Santa Clara, CA*

TP 006 **Towards the Complete Characterization of Host Cell Proteins in Biotherapeutics via Affinity Depletions, LC-MS/MS, and Multivariate Analysis**; Jennifer Murphy[1]; James A. Madsen[1]; Victor Farutin[2]; Yan Yin[2]; Stephen Smith[2]; James Anderson[2]; Ishan Capila[2]; *[1]Momenta Pharmaceuticals, Cambridge, MA; [2]Momenta Pharmaceuticals, Cambridge, ma*

TP 007 **Reversed-Phase Separation of Therapeutic Monoclonal Antibodies Using Superficially Porous Column: LC/MS Analysis**; Suresh Babu Cv[1]; Ning Tang[2]; Anne Blackwell[3]; *[1]Agilent Technologies , Bangalore , Karnataka; [2]Agilent Technologies, Santa Clara, CA; [3]Agilent Technologies, Little Falls, DE*

TP 008 **Rapid Automated LC-MS/MS Glycan Analysis for Monoclonal Antibodies**; Bhavana Shah[1]; Jason Richardson[2]; Zhongqi Zhang[2]; *[1]Amgen Inc.,, Thousand Oaks, CA; [2]Amgen, Inc., Thousand Oaks, CA*

TP 009 **Towards the Automated Monoclonal Antibody Sequencing and Characterization from LC-MS data**; Lin He[1]; Mohammad Ziaur Rahman[1]; Ngoc Hieu Tran[2]; Baozhen Shan[1]; Ming Li[2]; *[1]Bioinformatics Solutions Inc., Waterloo, Canada; [2]David R. Cheriton School of Computer Science, University of Waterloo, Waterloo, ON*

TP 010 **Development of a Non-Toxic Antibody Drug Conjugate Mimic to Enable LC-MS Method Development Without Risk**; Kevin Ray[1]; Brian Gau[1]; John Dapron[1]; Nicolas Caffarelli[1]; Jeffrey Turner[1]; *[1]MilliporeSigma, St Louis, MO*

TP 011 **Characterisation of Antibody Conjugates under Denaturing Liquid Chromatography Mass Spectrometry (MS) and Native MS Conditions**; Kersti Karu[1, 2]; Maurício Morais[2]; James R Baker[2]; *[1]UCL Chemistry Mass Spectrometry Facility, London; [2]Department of Chemistry, Christopher Ignold Building, London, UK*

TP 012 **Electrospray-Ionization Time-of-Flight Mass Spectrometry Coupled to Online, Comprehensive Two-Dimensional Liquid Chromatography for the Characterization of Therapeutic Monoclonal Antibodies**; Matthew Sorensen[1]; David Christopher Harmes[1]; Gregory O Staples[2]; Szabolcs Fekete[3, 4]; Davy Guillarme[3, 4]; Alain Beck[5]; Dwight Stoll[1]; *[1]Gustavus Adolphus College, Saint Peter, MN; [2]Agilent Technologies, Santa Clara, CA; [3]University of Geneva, Geneva, Switzerland; [4]University of Lausanne, Geneva, Switzerland; [5]Center for Immunology Pierre Fabre, Saint-Julien-en-Genevois, France*

TP 013 **Native Liquid Chromatography-Mass Spectrometry Applied to the Validation of Drug to Antibody Ratio LC-UV Methods and Antibody Drug Conjugates Development**; Lieza Danan-Leon[1]; Guillaume Tremintin[2]; *[1]stemcentrx, South San Francisco, CA; [2]Bruker Daltonics, Fremont, CA*

TP 014 **Direct Analysis of Intact mAb's and Low Abundant Variants by Advanced LC-MS Approaches**; Xiaomei (Annie) He[1]; Janet Lau; Chen Li; Shiaw-Lin Wu; *[1]BioAnalytix, Cambridge, MA*

TP 015 **Mass Spectrometric Characterization of Half-mAb Separated from Intact Monoclonal Antibody and Fragments using Analytical Size Exclusion Chromatography Column**; Crystal Benner[1]; William Evans[1]; Cesar Zuin[1]; Kyle Root[2]; Kerney Jebrell Glover[3];

Atis Chakrabartl[4]; *[1]tosoh Bioscience LLC, King of Prussia, PA; [2]lehigh University, Bethlem, PA; [3]lehigh University, Bethlehem, PA; [4]Tosoh Bioscience LLC, King of Prussia, PA*

TP 016 **LC-MS Characterization of Proteolytic Cleavage Sites in Therapeutic Monoclonal Antibodies**; Pavel V. Bondarenko[1]; Thomas M Dillon[1]; Gang Xiao[2]; Nicole Ball[1]; Deirdre M Piedmonte[1]; Michael J Treuheit[1]; *[1]Amgen, Inc., Thousand Oaks, CA; [2]Amgen, Inc., Thousand Oaks, CA*

TP 017 **Probing Higher-Order Structural Changes of a Lysine-linked Antibody-Drug Conjugate by Hydrogen-deuterium Exchange Mass Spectrometry (HDXMS)**; Lintao Wang[1]; Alexandru C. Lazar[2]; *[1]ImmunoGen Inc., Waltham, MA; [2]ImmunoGen, Inc., Waltham, MA*

TP 018 **A New Workflow for Characterization of Antibody Mixtures via Slip Flow Chromatography and Ultraviolet Photodissociation for Top-Down Mass Spectrometry**; Luca Fornelli[1]; Philip Compton[1]; Ximo Zhang[2]; Mary Wirth[2]; Neil Kelleher[1]; *[1]Northwestern University, Evanston, IL; [2]Purdue University, West Lafayette, IN*

TP 019 **Glycoform Separation and Characterization of Cetuximab Variants by Middle-up Off-line CE-UV/ESI-MS**; Nassur Said[1]; Michael Biacchi[1]; Rabah Gahoual[1, 2]; Charly Renard[1]; Alain Beck[3]; Yannis-Nicolas Francois[1]; Emmanuelle Leize-wagner[1]; *[1]Laboratoire de Spectrométrie de Masse des Interactions et des Systèmes (LSMIS), CNRS – UMR7140, University of Strasbourg, Strasbourg, France; [2]Division of BioAnalytical Chemistry, AIMMS Research Group BioMolecular Analysis, VU University Amsterdam, Amsterdam, The Netherland; [3]Centre d'Immunologie Pierre Fabre, Saint-Julien-en-Genevois, France*

TP 020 **High-order Structural Interrogation of Antibody-drug Conjugates by a Combination of Intact, Middle-up and Bottom-up Techniques using Sheathless Capillary Electrophoresis-Mass Spectrometry**; Nassur Said[1]; Rabah Gahoual[1, 2]; Laurianne Kuhn[3]; Alain Beck[4]; Yannis-Nicolas Francois[1]; Emmanuelle Leize-wagner[1]; *[1]Laboratoire de Spectrométrie de Masse des Interactions et des Systèmes (LSMIS), CNRS – UMR7140, University of Strasbourg, Strasbourg, France; [2]Division of BioAnalytical Chemistry, AIMMS Research Group BioMolecular Analysis, VU University Amsterdam, Amsterdam, The Netherland; [3]Institut de Biologie Moléculaire et Cellulaire (IBMC), University of Strasbourg, Strasbourg, France; [4]Centre d'Immunologie Pierre-Fabre, St. Julien-en-Genevois, France*

TP 021 **Microchip Capillary Electrophoresis with Integrated ESI-MS for the Detailed Analysis of Intact Biotherapeutic Antibodies and ADCs**; J. Scott Mellors[1]; Erin Anne Redman[2]; J. Michael Ramsey[2]; *[1]908 Devices, Inc., Chapel Hill, NC; [2]University of North Carolina, Chapel Hill, NC*

TP 022 **Capillary Electrophoresis – Mass Spectrometry for Top Down Proteomics**; Andreas Krupke[1]; Shiaw-Min Chen[2]; Achim Karger[2]; Michael Wenz[2]; Daniel Lopez-Ferrer[2]; Aran Paulus[2]; *[1]Thermo Fisher Scientific, South San Francisco, CA; [2]Thermo Fisher Scientific, San Jose, CA*

TP 023 **Intact Immunoglobulin Gamma Analysis by CESI-MS**; Bryan Fonslow[1, 2]; Olga Friese[3]; Ying Zhang[3]; John Yates III[2]; K. Steven Cook[3]; Jason Rouse[4]; *[1]SCIEX, San Diego, CA; [2]The Scripps Research Institute, La Jolla, CA; [3]Pfizer, Chesterfield, MO; [4]Pfizer, Inc. Andover, MA*

TP 024 **Characterization of Monoclonal Antibody Charge Variants using OFFgel Fractionation and Mass Spectrometry**; Alyssa Neill[1]; Yekaterina Kori[2]; Guilong Charles Cheng[1]; Hongcheng Liu[1]; *[1]Alexion Pharmaceuticals Inc., New Haven, CT; [2]University of Massachusetts Amherst, Amherst, Massachusetts*

TP 025 **Bioanalytical Challenges of Next-Generation Antibody-Drug-Conjugates Case Study: Developing a 2nd-Generation Affinity Capture LC-MS to Improve In Vivo Stability Assessment**; Dian Su; *Genentech Inc, South San Francisco, CA*

TP 026 **Novel Microfluidic Chip with In-line Deglycosylation for Rapid Mass Analysis of Reduced Monoclonal Antibodies**; Loredana Serafini[1]; John Corbin[1]; Victoria Smith[1]; Mark Nagel[1]; Leanna Lagpacan[1]; Debi Jin[1]; Andy Gieschen[2]; Caroline S. Chu[2]; Katherine Brendza[1]; *[1]Gilead Sciences, Foster City, CA; [2]Agilent Technologies, Santa Clara, CA*

TP 027 **Multidimensional ionKey/MS for Antibody Drug Conjugate Analysis**; Greg Roman[1]; James P Murphy[1]; *[1]Waters, Milford, MA*

TP 028 **Using Hydrophilic Interaction Chromatography–Mass Spectrometry for Heightened Product Characterization to Overcome Challenges with Hydrophobic Antibodies and Antibody Drug Conjugates**; Jacquelynn Smith[1]; Matthew Lauber[2]; Stephan Koza[2]; Erin Chambers[2]; Jason C Rouse[3]; Olga Friese[4]; *[1]Senior Associate Scientist at Pfizer, Chesterfield, MO; [2]Waters, Milford, MA; [3]Pfizer, Inc. Andover, MA; [4]Pfizer, Chesterfield, MO*

BIOMARKERS: QUANTITATIVE ANALYSIS (PART 1)
029 - 054

TP 029 **Towards Absolute Quantification of Protein Expression in 3D Tissue Culture Samples by MALDI-IMS-MS Imaging**; Rebecca Day[1]; Amanda Harvey[1]; Laura M Cole[1]; Neil Cross[1]; David Smith[1]; Malcolm Clench[1]; *[1]Sheffield Hallam University, Sheffield, United Kingdom*

TP 030 **Double Standards in Proteomics: DOSCATS: Engineered Peptide/Epitope Concatenations for SRM or Western Blotting**; Robert Beynon[1]; Richard J Bennett[1]; Deborah M Simpson[1]; Stephen W Holman[1]; John Colyer[2, 3]; *[1]University of Liverpool, Liverpool, United Kingdom; [2]University of Leeds, Leeds, United Kingdom; [3]Badrilla Ltd., Leeds, UK*

TP 031 **Development of New LC-MS Methodologies to Assess Liver Function in a Clinical Setting using Plasma and Dried Blood Spot**; Lei Guo[1]; Raymond Gonzalez[1]; Kara Pearson[1]; Elizabeth Joshi[2]; Kevin P Bateman[1]; Daniel S Spellman[1]; *[1]Merck & Co., Inc., West Point, PA; [2]Merck & Co, Kenilworth, NJ*

TP 032 **Serial Lectin Affinity Chromatography for Comparative Serum Glycoproteomics on Colon Cancer Biomarker Discovery**; Jinwook Lee[1]; Wonryeon Cho[1]; *[1]wonkwang University, Iksan, Jeonbuk*

TP 033 **Between Good, Fast and Cheap: Method Development for Large-Scale Plasma-Proteome Analysis between the Antagonizing Poles of Sensitivity, Through-put and Costs**; Christoph Stingl[1]; Lennard Dekker[1]; Diana A T Nijholt[1]; Coskun Güzel[1]; Martijn M. van Duijn[1]; Theo M. Luider[1]; *[1]Erasmus Medical Center, Rotterdam, The Netherlands*

TP 034 **Comparative Proteomic Analysis of Kidney Distal Convoluted Tubule and Cortical Collecting Duct Cells following Long-Term Hormonal Stimulation**; Qi Wu[1]; Trairak Pisitkun[2]; Robert Fenton[1]; *[1]Center for Interactions of Proteins in Epithelial Transport, Department of Biomedicine, Aarhus, Denmark; [2]Faculty of Medicine, Chulalongkorn University, Bangkok, Thailand*

TP 035 **Higher Protein Identifications and Coverage May Not Correlate with Higher Numbers of PSMs or Peptides in Quantitative Proteomic Analyses**; Lauren Devine[1]; Tatiana Boronina[1]; Robert N O'Meally[1]; Robert N Cole[1]; *[1]Johns Hopkins University School of Medicine, Baltimore, MD*

TP 036 **Identification of Pathologicalα-Synuclein Forms in Brain Extracts from Patients with Parkinson's Disease by Selected Reaction Monitoring**; Payel Bhattacharjee[1]; Ann Brinkmalm[1]; Annika Öhrfelt[1]; Kaj Blennow[1]; Henrik Zetterberg[1]; *[1]University of Gothenburg, Mölndal, Sweden*

TP 037 **Development of a TFPI (Tissue Factor Pathway Inhibitor) Protein Quantification Assay**; Katherine Wright; *Pfizer, Andover, MA*

TP 038 **A High-throughput Platform for Mass Spectrometric Analysis of Serum Fucosylated Haptoglobin in Hepatocellular Carcinoma**; Jianhui Zhu[1]; Jing Wu[1]; Haidi Yin[1]; Jorge Marrero[2]; David M Lubman[1]; *[1]University of Michigan Medical Center, Ann Arbor, MI; [2]University of Texas Southwestern Medical Center, Dallas, TX*

TP 039 **Development of Plasma Protein Biomarkers for Effects of Radiation Exposure Using Quantitative Mass Spectrometry**; Kate Liu[1]; Dyna Shirasaki[1]; Elizabeth Singer[1]; William McBride[1]; Julian Whitelegge[1]; Joseph A. Loo[1]; *[1]UCLA, Los Angeles, CA*

TP 040 **Phosphoproteomic Analysis of Differential Protein Expression in BRaf-Mutated Melanoma Cells with Acquired Resistance to BRaf, MEK1/2, or ERK1/2 Inhibitors**; Shivangi Awasthi[1]; Jacob Sheenstra[1]; Bao Tran[1]; Young Ah Goo[1]; Paul Shapiro[1]; David R Goodlett[1]; *[1]University of Maryland Baltimore, Baltimore, USA*

TP 041 **Identification of Novel Glycoprotein Biomarkers for Distinguishing Intestinal Inflammation from Fibrosis in Crohn's Disease by LC-MS/MS**; David M Lubman[1]; Jing Wu[1]; Ryan Stidham[1]; Peter Higgins[1]; Henry Appelman[1]; *[1]University of Michigan Medical Center, Ann Arbor, MI*

TP 042 **LC-MS/MS Method for Quantitation of Seven Biomarkers in Human Plasma for the Assessment of Impaired Glucose Tolerance**; Qibo Zhang[1]; Lisa A Ford[1]; Kelli D Goodman[1]; Tiffany A Freed[1]; Deirdre M Hauser[1]; Jessie K Conner[1]; Kate E T Vroom[1]; Klaus-Peter Adam[1]; Michael V Milburn[1]; Douglas R Toal[1]; *[1]Metabolon, Inc., Durham, NC*

TP 043 **A Robust Analytical LC-MS/MS Method to Quantitate Plasma Itraconazole and Hydroxy-Itraconazole in Patients with Solid Tumors**; Claudia Meek[1]; Erling Beck[1]; Richard Leff[2]; *[1]Texas Tech University, Dallas, TX; [2]Texas Tech University Health Sciences Center, Dallas, TX*

TP 044 **Investigation of the Quantitative Properties of Micro Flow LC-MS/MS for Direct Analysis of Frataxin in Human Biopsy**; Qishan Lin [1]; Jinghua Zhu[2]; *[1]University at Albany, Rensselaer , NY; [2]University at Albany, Rensselaer, NY*

TP 045 **Ultra high Performance Liquid Chromatography-Tandem Mass Spectrometry (UHPLC-MS/MS) Platform for Clinical Diagnostics within Diabetes Care**; Linda Ahonen[1]; Sirkku Jäntti[2]; Matej Orešič[1]; Tuulia Hyötyläinen[1]; *[1]Steno Diabetes Center A/S, Gentofte, Denmark; [2]University of Helsinki, Helsinki, Finland*

TP 046 **Quantitative Discovery of the Alterations of the Entire Human Kinome in Human Cells upon Methylglyoxal Treatment**; Weili Miao[1]; Lei Guo[1]; Yongsheng Xiao[1]; Xiaogang Jiang[1]; Yinsheng Wang[1]; *[1]University of California, Riverside, Riverside, CA*

TP 047 **A Comprehensive Investigation towards the Indicative Proteins of Bladder Cancer in Urine: From Surveying Cellular Secretomes to Verifying Urine Proteins**; Jiao Guo; *, Beijing, Beijing*

TP 048 **Development of MS Based Clinical Assays for Measuring Cerebrospinal Fluid Levels of Pre-Synaptic Proteins in Alzheimer's Disease**; Ann Brinkmalm [1]; Gunnar Brinkmalm[1]; Henrik Zetterberg[1, 2]; Kaj Blennow[1]; Annika Öhrfelt[1]; *[1]University of Gothenburg, Mölndal, Sweden; [2]UCL Institute of Neurology, London, UK*

TP 049 **Quantification of Hepcidin-25 in human Cerebrospinal Fluid using LC-MRM**; Jerome Vialaret[1]; Constance Delaby[1]; Pauline Bros[1, 2]; Amandine Moulinier[1]; Vincent Delatour[3]; Audrey Gabelle[4]; Sylvain Lehmann[1]; Christophe HIRTZ[1]; *[1]LBPC, IRMB CHU Montpellier St. Eloi Montpellier, France; [2]Laboratoire National de Métrologie et d'Essais, Paris, France; [3]Laboratoire National de Métrologie et d'Essais, Paris, france; [4]Centre Mémoire Ressources CHRU Montpellier, Montpellier, France*

TP 050 **Measurement of DNA Repair Protein Apurinic/Apyrimidinic Endonuclease 1 (APE1) in Human Tissues by Liquid Chromatography/Tandem Mass Spectrometry with Isotope Dilution**; Pawel Jaruga[1]; Fatos Guldal Kirkali[2]; Prasad T. Reddy[3]; Alessandro Tona[3]; Bryant C. Nelson[3]; Mengxia Li[4]; David M. Wilson, III[5]; Erdem Coskun[6]; Miral Dizdar[6]; *[1]NIST, Gaithersburg, MD; [2]NIH/NCI (National Cancer Institute), Bethesda, MD; [3]NIST, Gaithersburg MD; [4]NIH/NIA/IRP, Baltimore, MD; [5]NIH/NIA (National Institute on Aging), Baltimore, MD; [6]NIST, Rockville, MD*

TP 051 **Phosphoproteome Analysis Reveals Differential Mode of Action of Sorafenib in Wildtype and Mutated FLT3 AML Cells**; Catrin Roolf[1]; Nikolaj Dybowski[2]; Anett Sekora[1]; Stefan Mueller[2]; Gudrun Knuebel[1]; Hugo Murua Escobar[1]; Klaus Godl[2]; Andreas Tebbe[2]; Christian Junghanss[1]; Christoph Schaab[2]; *[1]Rostock, University Medical Center, Department of Hematology/ Oncology/ Palliative Care, Rostock, Germany; [2]Evotec (München) GmbH, Munich, Germany*

TP 052 **Improved Quantification of Rat Plasma NNK and NNAL Using Protein Precipitation and Phospholipid Removal in UFLC-ESI/MS/MS**; Estatira Sepehr[1]; Matthew S Bryant[2]; *[1]National Center for Toxicological Research, FDA, Jefferson, AR; [2]National Center for Toxicological Research - FDA, Jefferson, AR*

TP 053 **Accurate Quantification of Peptide using Multiple Internal Standards in Conjunction with parallel reaction monitoring**; Sebastien Gallien[1]; Bruno Domon[1]; *[1]Luxembourg Clinical Proteomics Center, Strassen, Luxembourg*

TP 054 **Precise MRM-based Quantitation of 200 Proteins from Dried Blood Spots and Single Drops of Blood**; Jingxi Pan[1]; Suping Zhang[2]; Albert Chou[1]; Christoph H. Borchers[3,4]; *[1]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [2]MRM Proteomics, Inc., Victoria, BC, Canada; [3]University of Victoria - Genome BC Proteomics Centre, Victoria, BC; [4]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada*

BIOMOLECULAR STRUCTURE ANALYSIS: CHEMICAL CROSSLINKING AND COVALENT LABELING (CROSS-LINKING)
055 - 075

TP 055 **The Synaptic Vesicle Cycle is Governed by Heterogeneous and Macromolecular Protein Microdomains**; Carla Schmidt; *HALOmem, University of Halle, Halle / Saale*

TP 056 **Structure of α-Synuclein Determined by Structural Proteomics and Constraint-Driven Discrete Molecular Dynamic Modeling**; Nicholas I Brodie[1]; Konstantin I Popov[2]; Evgeniy V Petrotchenko[1]; Nikolay V Dokholyan[2]; Christoph H. Borchers[1, 3]; *[1]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [2]University of North Carolina, School of Medicine, Chapel Hill, NC; [3]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada*

TP 057 **Profiling Yeast Mitochondrial Protein-Protein Interactions in a Whole-Organelle Scale by Cross-Linking Mass Spectrometry**; Chung-Tien Lee[1, 2]; Peter Rehling[2]; Henning Urlaub[1, 2]; *[1]Max Planck Institute for Biophysical Chemistry, Goettingen, Germany; [2]University Medical Center (UMG), Goettingen, Germany*

TP 058 **Transcription Factor-DNA Interaction Studied by Structural Mass Spectrometry**; Lukas Slavata[1, 2]; Michal Rosulek[1, 2]; Daniel Kavan[1, 2]; Alan Kadek[1, 2]; Hynek Mrazek[1,2]; Petr Man[1, 2]; Petr Novak[1, 2]; *[1]Institute of Microbiology CAS, Prague, Czech Republic; [2]Faculty of Science, Charles University in Prague, Prague, Czech Republic*

TP 059 **Assessing the Performance of CID-cleavable cross-linkers and Subsequent Data Analysis Strategies**; Rebecca Beveridge[1]; Karl Mechtler[1]; *[1]Research Institute of Molecular Pathology (IMP), Vienna, Austria*

TP 060 **Improving Cross-linked Peptide Identification in Large Protein Complexes on Quadrupole-Orbitrap and Quadrupole-Orbitrap-Ion Trap Platforms**; Chung-Tien Lee[1]; Olexandr Dybkov[1]; Christof Lenz[1, 2]; Thomas Monecke[3]; Ralf Ficner[3]; Yue Xuan[4]; Henning Urlaub[1, 2]; *[1]Max Planck Institute for Biophysical Chemistry, Goettingen, Germany; [2]University Medical Center (UMG), Goettingen, Germany; [3]Georg August University, Goettingen, Germany; [4]Thermo Fisher Scientific, Bremen, DE*

TP 061 **Optimization of Crosslinked Peptide Analysis on an Orbitrap Fusion Lumos Mass Spectrometer**; Ryan Bomgarden[1]; Erum Raja[1]; Chris Etienne[1]; Fan Liu[2]; Albert J R Heck[2]; Mathias Mueller[3]; Rosa I Viner[4]; *[1]Thermo Fisher Scientific, Rockford, IL; [2]Utrecht University, Utrecht, The Netherlands; [3]Thermo Fisher Scientific, Bremen, DE; [4]Thermo Fisher Scientific, San Jose, CA*

TP 062 **Structural Proteomics Analysis of the Native Tau Protein**; Karl A T Makepeace[1]; Evgeniy V Petrotchenko[1]; Christoph H. Borchers[2, 3]; *[1]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, CANADA; [2]University of Victoria - Genome BC Proteomics Centre, Victoria, BC; [3]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, CANADA*

TP 063 **Evaluation of a Photo-Activatable Unnatural Amino Acid Engineered Into Proteins To Crosslink And Identify interaction partners**; Robert Hettich[1]; Chen Qian[2]; Steven King[2]; Melinda Hauser[2]; Jeffrey Becker[2]; *[1]Oak Ridge National Laboratory, Oak Ridge, TN; [2]University of Tennesse, Knoxville, TN*

TP 064 **Analysis of UV-induced DNA-protein cross-links in a chromatin model by mass spectrometry**; Alexandra Stuetzer[1]; Christin Kappert[1]; Aleksandar Chernev[1]; Wolfgang Fischle[1, 2]; Henning Urlaub[1]; *[1]Max Planck Institute for Biophysical Chemistry, Goettingen, Germany; [2]KAUST, Thuwal, Saudi Arabia*

TP 065 **RNPxl 2 - Protein-RNA Interaction Site Localization from UV Cross-linked Peptide-RNA Oligonucleotides in Proteome Discoverer 2.1**; Timo Sachsenberg[1]; Johannes Veit[1]; Aleksandar Chernev[2]; Kundan Sharma[2]; Romina Hofele[2]; Saadia Qamar[2]; Uzma Zaman[2]; Christin Kappert[2]; Katharina Kramer[3]; Julianus Pfeuffer[4]; Xiao Liang[4]; Knut Reinert[4, 5]; Christof Lenz[2]; Henning Urlaub[2]; Oliver Kohlbacher[1, 6]; *[1]Eberhard Karls University, Tübingen, Germany; [2]Max Planck Institute for Biophysical Chemistry, Göttingen, Germany; [3]Max Planck Institute for Plant Breeding Research, Köln, Germany; [4]Freie Universität Berlin, Berlin, Germany; [5]Max Planck Institute for Molecular Genetics, Berlin, Germany; [6]Max Planck Institute for Developmental Biology, Tübingen, Germany*

TP 066 **Novel Workflow for Characterization of Non-Disulfide Protein Crosslinks in Normal and Cataractous Human Lens**; Ruiqiang Chen[1]; Kristie L. Rose[1]; Zhen Wang[1]; Kevin Schey[1]; *[1]Department of Biochemistry and Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN*

TP 067 **New Methodology for the *in vivo* Identification of Protein Partners using Genetically Encoded Unnatural Amino Acids and Mass Spectrometry**; Mariana Fioramonte[1]; Bing Yang[2]; Ana Gisele C Neves-Ferreira[3]; Lei Wang[2]; Fabio César Gozzo[1]; *[1]University of Campinas, Campinas, Brazil; [2]UCSF, San Francisco, CA; [3]Fiocruz, Rio de Janeiro, RJ*

TP 068 **Systematic Determination of Nuclear Pore Complex Protein Interfaces by XL-MS**; Joseph Glavy[1]; Martin Beck[2]; *[1]Stevens Institute of Tech., Hoboken , NJ; [2]EMBL Heidelberg, Heidelberg, Germany*

TP 069 **Quantitative Cross-linking/LCMS (CX-MS) to Investigate Allosteric Regulation of Phosphodiesterase 6 (PDE6)**; Donna Hogan[1]; Xiongzhuo Gao[1]; Suzanne Matte[1]; Rick Cote[1]; Feixia Chu[1]; *[1]University of New Hampshire, Durham, NH*

TP 070 **Developing a Novel Multiplexed Quantitative Cross-linking Mass Spectrometry Strategy to Define the Structural Dynamics of Cullin-RING Ligase Complex**; Clinton Yu[1]; Haibin Mao[2]; Alex Huszagh[1]; Rosa I Viner[3]; Eric Novitsky[1]; Tonya Second[3]; Scott Rychnovsky[1]; Ning Zheng[2]; Lan Huang[1]; *[1]University of California, Irvine, Irvine, CA; [2]University of Washington, Seattle, WA; [3]Thermo Fisher Scientific, San Jose, CA*

TP 071 **Developing A Novel Acidic Residue Reactive and Sulfoxide-containing MS-cleavable Homobifunctional Cross-linker for Studying Protein-Protein Interactions**; Craig Bryant Gutierrez[1]; Clinton Yu[1]; Alex Huszaugh[1]; Eric Novitsky[1]; Scott Rychnovsky[1]; Lan Huang[1]; *[1]UC-Irvine, Irvine, CA*

TP 072 **Structural Analysis of a Myotoxin-antimytoxin Complex by Cross-linking, Mass Spectrometry and Bioinformatics**; Barbara S. Soares[1]; Surza L. G. Rocha[1]; Diogo B. Lima[2]; Bruno Lomonte[3]; Gilberto B Domont[4]; Jonas Perales[1]; Richard H. Valente[1]; Francisco Gomes-Neto[1]; Ana Gisele Neves-Ferreira[1]; *[1]Oswaldo Cruz Institute, Fiocruz, Rio de Janeiro, Brazil; [2]Carlos Chagas Institute, Fiocruz, Curitiba, Brazil; [3]Clodomiro Picado Institute, University of Costa Rica, San José, Costa Rica; [4]Chemistry Institute, Federal University of Rio de Janeiro, Rio de Janeiro, Brazil*

TP 073 **Photocrosslink Coupled with Mass Spectrometry on a Transmembrane Protein Pump using an Unnatural Amino Acid, Benzoylphenylalanine**; Thao Nguyen[1]; Grzegorz Sabat[2]; Michael Sussman[1]; *[1]UW Madison, Madison, WI; [2]UW-Madison, Madison, WI*

TP 074 ***In vivo* Conformational Dynamics of Hsp90 and Its Interactors**; Juan Chavez[1]; Devin K Schweppe[1]; Jimmy K Eng[1]; James E Bruce[1]; *[1]University of Washington, Seattle, WA*

TP 075 **An Integrated Workflow for Analysis of Proteins and Protein Complexes based on Cross-Linking/Mass Spectrometry with an MS/MS Cleavable Cross-Linker**; Christian Arlt[1]; Michael Goetze[1]; Christian Ihling[1]; Christoph Hage[1]; Mathias Schaefer[2]; Andrea Sinz[1]; *[1]Martin-Luther-Universität, Halle-Wittenberg, Germany; [2]Universität zu Köln, Greinstrasse, Germany*

DATA INDEPENDENT ACQUISITION (SWATH) 076 - 095

TP 076 **Large-scale Quantitative Measurements of Rat Brain Hippocampus Membrane Proteome in Prolonged Simulated Microgravity Model by 2D-SWATH® Mass Spectrometry**; Peibin Qin[1]; Yun Wang[2]; Lihai Guo[1]; Yongqian Zhang[2]; Wenhai Jin[1]; Yulin Deng[2]; *[1]Shanghai AB Sciex Analytical Instrument Trading Co.,Ltd.,China, Beijing, China; [2]School of Life Science,Beijing Institute of Technology,China, Beijing, China*

TP 077 **An Novel Alignment Strategy for SWATH-MS to Generate Comprehensive Proteomics Data Matrices**; Hannes Luc Röst[1, 2]; Yansheng Liu[1]; Giuseppe D'Agostino[3]; Matteo Zanella[3]; Pedro Navarro[4]; George Rosenberger[1]; Ben Collins[1]; Ludovic Gillet[1]; Giuseppe Testa[3]; Lars Malmström[1]; Ruedi Aebersold[1]; *[1]ETH Zurich, Zürich, Switzerland; [2]Stanford University School of Medicine, Palo Alto CA; [3]Department of Experimental Oncology, European Institute of Oncology (Istituto di Ricovero e Cura a Carattere Scientifico, IRCCS), Milan, Italy; [4]Institute for Immunology, University Medical Center of the Johannes Gutenberg University Mainz, Mainz, Germany*

TP 078 **Assessing Proteome Organization by Native SEC Coupled to SWATH-MS**; Moritz Heusel[1]; George Rosenberger[1]; Robin Hafen[1]; Ben C. Collins[1]; Matthias Gstaiger[1]; Ruedi Aebersold[1, 2]; *[1]Institute of Molecular Systems Biology ETH Zurich, Zurich, Switzerland; [2]Faculty of Science, University of Zurich Zurich, Switzerland*

TP 079 **Understanding the Square-Wave Nature of Q1 Isolation for Data Independent SWATH® Acquisition**; Randy J. Arnold[1]; Leroi Desouza[1]; Christie Hunter[2]; Patrick Pribil[1]; *[1]SCIEX, Concord ON, Canada; [2]SCIEX, Redwood City, CA*

TP 080 **Extending the Depth of Coverage in SWATH® Acquisition with Deeper Ion Libraries**; Joerg Dojahn[1]; Nick Morrice[2]; Christie Hunter[3]; *[1]SCIEX, Darmstadt, Germany; [2]SCIEX, Warrington, UK; [3]SCIEX, Redwood City, CA*

TP 081 **The Use of Smaller Q1 Isolation Windows Improves Reproducibility in SWATH Based Protein Quantification Even at Higher Spectral Acquisition Rate**; Dipankar Malakar[1]; Faraz Rashid[1]; Manoj Pillai[1]; *[1]SCIEX, 121 Udyog Vihar Phase IV Gurgaon, India*

TP 082 **Identification and Quantitation of Glycopeptides by SWATH Acquisition**; Chi-Hung Lin[1]; Christoph Krisp[1, 2]; Mark Molloy[1, 3]; *[1]Macquarie University, Sydney, Australia; [2]Australian Proteome Analysis Facility, Sydney, Australia; [3]Australian Proteome Analysis Facility, Sydney, Australia*

TP 083 **Using Scanning SWATH Windows to Improve both Quantitative and Qualitative Data over Conventional SWATH and IDA Methodologies**; Nic Bloomfield[1]; Michael Murphy[1]; Gordana Ivosev[1]; Stephen Tate[1]; *[1]SCIEX, Concord ON, Canada*

TP 084 **Glycopeptide SWATH Analysis – a Workflow for Quantification of Glycopeptides in Complex Samples**; Miloslav Sanda[1]; Nathan Edwards[2]; Radoslav Goldman[1]; *[1]Georgetown University, Lombardi Cancer Center Washington, DC; [2]Georgetown University, Department of Biochemistry and Molecular & Cellular Biology, Washington, DC*

TP 085 **Scrutinization of Library Building for SWATH Analysis**; Katleen Van Steendam[1]; Elisabeth Govaert[1]; Maarten Dhaenens[1]; Liesbeth Vossaert[1]; Dieter Deforce[1]; *[1]Ghent University, Laboratory of Pharmaceutical Biotechnology, Ghent, BELGIUM*

TP 086 **SWATH-MS Proteomics and Chemometrics to Study the Cardiovascular Disease**; Marcello Manfredi[1]; Eleonora Conte[2]; Carmela Chiariello[3]; Elisa Robotti[4]; Elia Ranzato[4]; Simona Martinotti[4]; Eleonora Mazzucco[4]; Fabio Gosetti[4]; Annalisa Castagna[3]; Daniela Cecconi[5]; Oliviero Olivieri[3]; Emilio Marengo[4]; *[1]ISALIT-DISIT, University of Piemonte Orientale, Alessandria, Italy; [2]ISALIT, spin-off DISIT, University of Piemonte Orientale, NOVARA, IT; [3]Department of Medicine, University of Verona, Verona, Italy; [4]DISIT, University of Piemonte Orientale, Alessandria, Italy; [5]Department of Biotechnology, University of Verona, Verona, Italy*

TP 087 **Make Love, Not War: Towards a Comprehensible Workflow for the Integrated Analysis of Transcriptomics and Proteomics Data**; Katleen Van Steendam[1]; Elisabeth Govaert[1]; Liesbeth Vossaert[1]; Maarten Dhaenens[1]; Filip Van Nieuwerburgh[1]; Laura De Clerck[1]; Dieter De Coninck[1]; Dieter Deforce[1]; *[1]Ghent University, Laboratory of Pharmaceutical Biotechnology, Ghent, Belgium*

TP 088 **Single Shot Deep DIA Methods with Optimal Coverage, Reproducibility and Quantification Precision**; Roland Bruderer[1]; David Gomez-Valera[2]; Oliver M Bernhardt[1]; Tejas P Gandhi[1]; Lukas Reiter[1]; *[1]Biognosys AG, Schlieren, Switzerland; [2]Max Planck Institute for Biophysical Chemistry, Goettingen, Germany*

TP 089 **Accelerating Data Independent Acquisition with Microflow Chromatography**; Christie Hunter[1]; Nick Morrice[2]; *[1]SCIEX, Redwood City, CA; [2]SCIEX, Phoenix House Lakeside Drive Warrington Cheshire UK*

TP 090 **Proteome-wide Turnover Analysis Quantifies Genetic Impact in Down Syndrome**; Yansheng Liu[1]; Christelle Borel[2]; Li Li[3]; Torsten Mueller[1]; Paul Boersema[4]; Pierre-Luc Germain[5]; Giuseppe Testa[5]; Andreas Beyer[3]; Stylianos Antonarakis[2]; Ruedi Aebersold[1]; *[1]Department of Biology, Institute of Molecular Systems Biology, ETH Zurich, Zurich, Switzerland; [2]Department of Genetic Medicine and Development, University of Geneva Medical School, and University Hospitals of Geneva, Geneva, Switzerland; [3]University of Cologne, Cologne, Germany; [4]Institute of Biochemistry, Department of Biology, ETH Zurich, Zurich, Switzerland; [5]Department of Experimental Oncology, European Institute of Oncology, Milan, Italy*

TP 091 **Rapid Ion Mobility Deconvolution for High-throughput Analysis of Structural Isomers**; Michael E Pettit[1]; Matthew R Brantley[1]; Touradj Solouki[1]; *[1]Baylor University, Waco, TX*

TP 092 **Phospholipid Analysis Utilising a Novel, Data Independent, Mode of Acquisition on a QTof Instrument with a Scanning Quadrupole Mass Filter**; Jayne Kirk[1]; Steven Lai[2]; Jason Wildgoose[1]; Keith Richardson[1]; Martin Green[1]; Paul Doorbar[1]; Witold Niklewski[1]; Kirsten Craven[1]; Mark Wrona[3]; *[1]Waters Corporation, Wilmslow, UK; [2]Waters Corporation, Beverly, MA; [3]Waters Corporation, Milford, MA*

TP 093 **Data-independent Acquisition (DIA) Reveals Changes in Mouse Cardiac Proteome from SS-31 Drug Intervention**; Ying Sonia Ting[1]; Ying Ann Chiao[1]; Gennifer E Merrihew[1]; Peter Rabinovitch[1]; Michael J MacCoss[1]; *[1]University of Washington, Seattle, WA*

TP 094 **MS1 Based Quantification Optimization on DIA Methods on a Quadrupole-Orbitrap Mass Spectrometer**; Roland Bruderer[1]; Yue Xuan[2]; Oliver M Bernhardt[1]; Tejas Gandhi[1]; Thomas Moehring[2]; Lukas Reiter[1]; *[1]Biognosys AG, Schlieren, Switzerland; [2]Thermo Fisher Scientific, Bremen, DE*

TP 095 **Data-independent Acquisition Mass Spectrometry-Based Proteomics of Thyroid Cancer Allows Comprehensive Identification of Malignancy-Associated Changes**; Juan Martinez-Aguilar[1, 2]; Roderick Clifton-Bligh[3]; Mark Molloy[2, 4]; *[1]National Autonomous University of Mexico, Mexico city, MEXICO; [2]Macquarie University, Sydney, Australia; [3]Kolling Institute of Medical Research, Sydney, Australia; [4]Australian Proteome Analysis Facility, Sydney, Australia*

DIAGNOSTIC CLINICAL CHEMISTRY (GENERAL) 096 - 112

TP 096 **Touch Paper Spray Ambient Mass Spectrometry for Paper-based Immunoassays: Towards On-demand Diagnosis**; Suming Chen[1]; Qiongqiong Wan[1]; Abraham Kwame Badu-Tawiah[1]; *[1]Department of Chemistry and Biochemistry, The Ohio State Univeristy, Columbus, OH*

TP 097 **Real Time and Accelerated Stability Studies of Testosterone Calibrators**; Linda Nagore[1]; Ravi Orugunty[1]; Isil Dilek[1]; Uma Sreenivasan[1]; *[1]Cerilliant Corporation, Round Rock, TX*

TP 098 **Automated Sample Preparation of Whole Blood for Therapeutic Drug Monitoring and Diagnostics by LC-MS using a Commercial Autosampler**; Guenter Boehm[1]; Christian Berchtold[2]; Götz Schlotterbeck[2]; Reto Bolliger[3]; *[1]CTC Analytics AG, Zwingen, BL; [2]Fachhochschule Nordwestschweiz Hochschule für Life Sciences, Muttenz, Switzerland; [3]CTC Analytics AG, Zwingen, Switzerland*

TP 099 **Pharmacotherapy Monitoring and Clinical Diagnosis of Patients with APRT Deficiency Utilizing UPLC-MS/MS Assay**; Unnur Arna Thorsteinsdottir[1, 2]; Finnur Freyr Eiriksson[1, 2]; Hrafnhildur Runolfsdottir[1]; Vidar Edvardsson[3]; Runolfur Palsson[1, 3]; Margret Thorsteinsdottir[1, 2]; *[1]University of Iceland, Reykjavik, Iceland; [2]ArcticMass, Reykjavik, Iceland; [3]The National University Hospital of Iceland, Reykjavik, Iceland*

TP 100 **Quantitative Analysis of Steroids in Serum using Ultra High Performance Liquid Chromatography-Tandem Mass spectrometry**; Heng-Tao Dong[1]; Man-Yu Zhang[1]; Shan-An Chan[2]; *[1]Agilent Technology, Inc. Shanghai, China; [2]Agilent Technology, Inc.Taipei Taiwan, Taiwan*

TP 101 **Breath and Exhaled Breath Condensate Analyzes for Disease Diagnosis and Monitoring of Newborns by Mass Spectrometry**; Vladimir Frankevich[1]; Vitaliy Chagovets[1]; Natalia Starodubtseva[1]; Alexey Kononikhin[1]; Anna Bugrova[1]; Andrey Ryndin[1]; Oleg Ionov[1]; Gennady Sukhikh[1]; *[1]Federal State Budget Institution "Research Center for Obstetrics, Gynecology and Perinatology" Ministry of Healthcare of the Russian Federation, Moscow, RUSSIA*

TP 102 **Using Mass Spectrometry to Identify IgG Fc and Fab Fragments Produced by Plasmin in Patient Serum**; David Barnidge[1]; David Murray[1]; *[1]Mayo Clinic / DLMP, Rochester, MN*

TP 103 **Analysis of Sweat Volatiles using Solid Phase Microextraction in Conjunction with Gas Chromatography – Mass Spectrometry**; Courtney Weston[1]; Changling Qiu[1]; Kevin A. Schug[1]; *[1]The University of Texas, Arlington, TX*

TP 104 **Exploratory Study of NQO1 Expression in Advanced Solid Tumors**; Yuan Tian[1]; Fabiola Cecchi[1]; WEI-LI Liao[1]; David E. Gerber[2]; David A. Boothman[2]; William Hoos[3]; Todd Hembrough[1]; *[1]Nantomics, Rockville, MD; [2]University of Texas Southwestern Medical Center, Dallas, TX; [3]NQ Oncology, INC, Chapel Hill, NC*

TP 105 **Quantification of MET by mass spectrometry for status assessment in prescreening of tumors for targeted therapies**; Kerry Scott[1]; Fabiola Cecchi[1]; Paolo Nuciforo[2]; Wei-Li Liao[1]; *[1]OncoPlex/NantOmics, Rockville, MD; [2]Vall d'Hebron Institute of Oncology, Barcelona, Spain*

TP 106 **Approach to Implementing LC-MS/MS Plasma Metanephrines : Calibrators, Sample Prep, Workflow**; Wai-Yoong Ng[1]; Jinq Shya Yap[2]; Janelle SJ Chin[2]; Chin Pin Yeo[2]; *[1]Singapore General Hospital, Singapore; [2]Singapore General Hospital, Singapore, Singapore*

TP 107 **Identifications of Candidate Breast Cancer-Specific Biomarkers in Fresh Frozen Breast Tissue Sections by the MALDI-imaging Coupled with On-tissue Digestion**; Toyofumi Nakanishi; *Osaka Medical College, Takatsuki, Japan*

TP 108 **Accurate Diagnosis for Prostate Cancer by Measuring the Ratio between Two Types of Prostate Specific Antigens by LDI-TOF MS**; Minyoung Yoo; *Konkuk University, Seoul, South Korea*

TP 109 **LDTD-MS/MS Method for Quantitative Analysis of Four Immunosuppressant Drugs in Whole Blood and Cost Analysis Comparison to LC-MS/MS**; Stephen D Merrigan[1]; Matthew Slawson[2]; Serge Auger[3]; Kamisha L Johnson-Davis[1, 4]; *[1]ARUP Institute for Clinical and Experimental Pathology, Salt Lake City, UT; [2]Utah Public Health Laboratory, Salt Lake City, UT; [3]Phytronix Technologies, Quebec, QC; [4]University of Utah Health Sciences Center, Department of Pathology, Salt Lake City, UT*

TP 110 **Dried Blood Spots, Water-soluble Material and LC-MS based Protein Analysis**; Cecilie Rosting[1]; Trine Grønhaug Halvorsen[1]; Astrid Gjelstad[1]; Christine Østvik Sæ[1]; *[1]School of Pharmacy, University of Oslo, Oslo, Norway*

TP 111 **The Impact of the Antigen-Antibody Interaction on the Tryptic Digestion in Immunocapture Based LC-MS/MS**; Maren Christin Stillesby Levernæs[1]; Trine Grønhaug Halvorsen[1]; Léon Reubsaet[1]; Marianne Nordlund Broughton[2]; *[1]School of Pharmacy, University of Oslo, Oslo, Norway; [2]Radiumhospitalet, Oslo University Hospital, Oslo, Norway*

TP 112 **Analyte Sequestering Transport Particle Chromatography As A Front-End to Mass Spectrometry**; Fred Regnier[1]; ZhiYu Li[2]; JinHee Kim[2]; *[1]Purdue University / Novilytic, Carmel, IN; [2]Novilytic, West Lafayette, IN*

DRUG DISCOVERY/DMPK/ADME (APPLICATIONS) 113 - 129

TP 113 **Evaluation of the Pharmacokinetics of a Novel Anti-Diabetic Agent using Conventional LC/MS/MS**; Kenji Sugawara[1, 2]; Norihide Yokoi[1]; Ritsuko Hoshikawa[1]; Toshiya Matsubara[3]; Susumu Seino[1]; *[1]Division of Molecular and Metabolic Medicine, Kobe University Graduate School of Medicine, Kobe, Japan; [2]Division of Diabetes and Endocrinology, Kobe University Graduate School of Medicine, Kobe, Japan; [3]Shimadzu Corporation, Kyoto, Japan*

TP 114 **Quantification of Bindings of Organometallic Ruthenium Complexes to Protein Thiols by Mass Spectrometry**; Yumiao Han[1, 2]; Yu Lin[1]; Fuyi Wang[1]; *[1]Institute of Chemistry Chinese Academy of Sciences, Beijing, China; [2]University of Pennsylvania, Philadelphia, PA*

TP 115 **Proteome-wide drug dose-response of prostate cancer cell lines exposed to androgen receptor antagonists by microflow-LC SWATH MS analysis**; Ludovic Gillet[1]; Sabine Amon[1]; Yasuo Uchida[1]; Nick Morrice[2]; Christie Hunter[3]; Ruedi Aebersold[1, 4]; *[1]ETH Zurich, Zürich, Switzerland; [2]SCIEX, Phoenix House Lakeside Drive Warrington Cheshire UK, WA1 1RX; [3]SCIEX, Redwood City, CA; [4]University of Zurich, Zurich, Switzerland*

TP 116 **Peptide Metabolism: Identification of Metabolite Structures of GLP-1 Receptor Agonists in Different *in vitro* Systems Using High Resolution Mass Spectrometry**; Andreas Brink[1]; Alessandra Piranha[1, 2]; Yves Siegrist[1]; Aynur Ekiciler[1]; Nicola Thum[3]; Fabien Fontaine[4]; Ismael Zamora[4]; Marcel Gubler[1]; Silke Simon[1]; Nicole Kratochwil[1]; Simone Schadt[1]; *[1]Drug Disposition & Safety, Pharmaceutical Sciences, Pharma Research and Early Development, Roche Innovation Center Basel F. Hoffmann-La Roche Ltd., Basel, Switzerland; [2]Royal Melbourne Institute of Technology, Melbourne, Australia; [3]School of Life Sciences, University of Applied Sciences and Arts Northwestern Switzerland, Basel, Switzerland; [4]Lead Molecular Design, Sant Cugat de Valles, Spain*

TP 117 **Case Study of Stable-Isotopic Dilution for Accurate Mass Spectrometric Pharmacokinetic Quantitation of a Small Intact Protein from *in vivo* Samples**; Phillip Chu[1]; Xinxin Gao[1]; Susan Crowell[1]; Leslie Dickmann[1]; Rami Hannoush[1]; Yichin Liu[1]; John Tran[1]; *[1]Genentech Inc, South San Francisco, CA*

TP 118 **Metabolite Profiling and Covalent Binding of TAK-875 in Human Hepatocytes or Mitochondria**; Wing W Lam[1]; Yong Gong[1]; Rhys Salter[1]; Mark R Player[1]; David C Evans[1]; Monicah Otieno[1]; Heng-Keang Lim[1]; *[1]Janssen Research and Development, Spring House, PA*

TP 119 **High Resolution Accurate Mass Quantitation of Iloperidone and the Hydroxy Iloperidone Metabolite using Full Scan and Selected Ion Monitoring Modes**; David Brant[1]; Keeley Murphy [2]; Jonathan L Josephs[3]; Maciej P Bromirski[4]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, San Jose , CA; [3]Thermo Fisher, San Jose, CA; [4]Thermo Fisher Scientific, Bremen, DE*

TP 120 **Mechanism and Dynamics of SAMT Analog Inactivation of HIV-1 Gag Polyprotein**; Lisa M. Miller Jenkins[1]; Elliott L Paine[1]; Kara M. George Rosenker[2]; Harichandra D Tagad[1]; Michael T Scerba[2]; Lalit Deshmukh[2]; Daniel H Appella[2]; *[1]National Cancer Institute, NIH Bethesda, MD; [2]National Institute of Diabetes and Digestive and Kidney Diseases, NIH, Bethesda, MD*

TP 121 **Development of a Magnetic Microbead Affinity Selection Screening with UHPLC-MS/MS for the Vitamin D Receptor**; Daniel Nosal[1]; Michael D Rush[1]; Jerry J White[1]; Richard B van Breemen[1]; *[1]University of Illinois College of Pharmacy, Chicago, IL*

TP 122 **Implementation of Mass Spectrometry Ligand Binding (MS bind) Assays to Rapidly Identify Molecules for Radioligand Development for New Drug Targets**; Nathan G Hatcher[1]; Rose B Flick[1]; James W Monahan[1]; Gary E Adamson[1]; Nanyan Rena Zhang[1]; Charles M Harrell[1]; Victor N Uebele[1]; *[1]Merck & Co., Inc., West Point, PA*

TP 123 **Further Efforts towards Accurately Determining Unbound Fractions for Highly Plasma Protein Bound Compounds by LC-MS**; Inhou Chu; *Merck & Co, Kenilworth, NJ*

TP 124 ***In vitro* Hepatic Metabolism of Licochalcone A, a Chalcone from the Licorice species Glycyrrhiza inflata.**; Lingyi Huang[1]; Dejan Nikolic[1]; Richard B. van Breemen[1]; *[1]University of Illinois College of Pharmacy, Chicago, IL*

TP 125 **Efficient and Cost-Effective In Vitro Permeability and Transporter Assessment Using the CACOReady 96-well Kit Assay and DiscoveryQuant 3.0**; Jeffrey Clarine[1]; Katherine Andersen[1]; Samuel Sperry[1]; *[1]eFFECTOR Therapeutics, San Diego, CA - California*

TP 126 **Effects of Intestinal Microbiota on the Bioavailability of Aspirin in Rats**; In Sook Kim; Shaheed Ur Rehman; Min Sun Choi; Jong Suk Park; Hyun Kim; Young Seok Ji; Hyeong Jun Kim; So Yeong Yun; *Hanyang University, Ansan-si, Gyeonnggi-do*

TP 127 **A Validated Method for Anatabine Quantification in Human Plasma using High Resolution Parallel Reaction Monitoring Coupled with Chip-Based Nanospray**; Jon M Reed[1, 2]; Prashanthi Vallabhaneni[2]; Rosa Ajoy[2]; Gogce Crynen[2]; Laila Abdullah[2]; James E Evans[2]; Fiona Crawford[1]; *[1]SRQ Bio, Sarasota, FL; [2]Roskamp Institute, Sarasota, FL*

TP 128 **A Multiplex Assay for Direct Analysis of Natural Products in Crude Botanical Extracts**; Geuncheol Gil[1]; Pan Mao[1]; Bharathi Avula[2]; Zulfiqar Ali[2]; Amar G. Chittiboyina[2]; Ikhlas A. Khan[2]; Larry A. Walker[2]; Daojing Wang[1]; *[1]Newomics Inc., Emeryville, CA; [2]National Center for Natural Products Research, School of Pharmacy, The University of Mississippi, University, MS*

TP 129 **Recent Experience on LC-MS/MS Determination of ADC-like Drug Candidates and Corresponding Cytotoxic Agent in Biological Matrices**; Xiongfei Wu[1]; Weimin Hu[1]; Weiqun Cao[1]; Yi Tao[1]; Xinping Fang[1]; Xin Zhang[1]; *[1]WuXi AppTec Co., Shanghai, China*

DRUG METABOLISM: QUALITATIVE AND HIGH THROUGHPUT ANALYSIS
130 - 144

TP 130 **Development of an Automated High Throughput PAMPA Experiment for Permeability Assessment of Small Molecules and Peptides**; Xu Wang[1]; Bernard K Choi[2]; Hui Wan[2]; Chen Shiying[2]; Bahanu Habulihaz[2]; Gino M. Salituro[2]; Lucinda Cohen[2]; *[1]Merck & Co., Rahway, NJ; [2]Merck, Darmstadt, Germany*

TP 131 **Emerging Bioanalytical Tool to Characterize Drug and Drug-products of Biotherapeutics**; Jinal Patel[1]; Mark Cancilla[2]; Xiang Yu[2]; Alina Dindyal-Popescu[1]; Gordon Payne[1]; Eva Duchoslav[3]; Suma Ramagiri[4]; *[1]SCIEX, Concord, ON; [2]Merck & Co., Inc., West Point, PA; [3]SCIEX, Concord , ON; [4]SCIEX, Concord ON, Canada*

TP 132 **Improved Data-Independent Workflow Strategies for Small Molecule Identification Using a High Resolution Q-TOF Mass Spectrometer**; Alina Dindyal-Popescu[1]; Keith Goodman[2]; Eva Duchoslav[3]; Suma Ramagiri[2]; *[1]SCIEX, Concord , ON; [2]SCIEX, Concord ON, Canada; [3]SCIEX, Concord, ON*

TP 133 **A Strategy for the Discovery and Identification of New Natural Product Metabolites by Orbitrap Mass Spectrometer and Multiple Data-Mining Approaches**; Chen Li[1]; Ying Liu[2]; Jiayu Zhang[2]; Siyi Liu[2]; Wei Cai[3]; Jianqiu Lu[2]; *[1]Thermo Fisher Scientific, Shanghai, China; [2]Center of Scientific Experiment, Beijing University of Chinese Medicine, Beijing, China; [3]Hunan University of Medicine, Huaihua, China*

TP 134 **Peptide Screening using Laser Desorption Ionization Mass Spectrometry on Fluorinated Nanopost Array (NAPA) Devices**; Trust Razunguzwa[1]; Nicholas J Morris[2]; Heather Anderson[2]; Matthew J Powell[2]; Marvin S Yu[3]; *[1]Protea Biosciences, Morgantown, WV; [2]Protea Biosciences, Inc. Morgantown, WV; [3]MS2 Array LLC, Pittsburgh, PA*

TP 135 **Metabolic Profiling of Two Novel Topo IIα Catalytic Inhibitors, Fluorescein Hydrazones in rat liver microsomes (RLMs) by LC-MS/MS**; Adnan A Kadi[1]; Nasser S. Al-Shakliah[1]; Youngjoo Kwon[2]; A. F. M. Motiur Rahman[1]; *[1]King Saud University, Riyadh-11451, Saudi Arabia; [2]Ewha Womans University, Seoul, South Korea*

TP 136 **Metabolite Profile Comparison using a HμREL Co-culture Hepatocyte Model vs. a Conventional Hepatocyte Suspension for Low Turnover Drugs**; J. Matthew Hutzler[1]; Richard D. Burton[1]; Xiusheng Miao[1]; Shelby Anderson[1]; Todd Hieronymus[1]; David Heim[1]; Taysir Chamem[1]; *[1]Q2 Solutions, Indianapolis, IN*

TP 137 **Absorption, Distribution and Metabolism of Brodifacoum, a Potent Anticoagulant Rodenticide**; Zane Hauck[1]; Douglas L Feinstein[1]; Richard B van Breemen[1]; *[1]UIC, Chicago, IL*

TP 138 **Chiral Separation and Quantification of Metabolites using Super Critical Fluid Chromatography Coupled with Triple Quadrupole**; Siji Joseph[1]; Syed S Lateef[1]; *[1]Agilent technologies, Bangalore, India*

TP 139 ***In-vitro* Synthesis of Drug Metabolites and Their Screening/Characterization Using Liquid Chromatography-Mass Spectrometry (LC-MS)**; Shubhashis Chakrabarty[1]; Weilin L. L Shelver[1]; Andrew R. R Thompson[1]; David J. J Smith[1]; *[1]USDA-Agricultural Research Service, Biosciences Research Laboratory, Fargo, ND*

TP 140 **Rapid Determination of Pharmacokinetic Profiles of Caffeine and Its Metabolites Collected on Skin by Ambient Mass Spectrometry**; Kun-Da Wu[1]; Hung Su[1]; Sychyi Cheng[1]; JENTAIE SHIEA [1]; *[1]National Sun Yat- Sen University, Kaohsiung, TAIWAN*

TP 141 **Data Robustness of a High-Throughput Autosampler (Apricot Design Dual Arm–ADDA) in DiscoveryADME Sample Analysis**; Xiaotong Li[1]; Yunqiang Su[1]; Chunli Zhu[1]; YI TAO[2]; Xinping Fang[1]; Xin Zhang[1]; *[1]WuXi AppTec Co., Shangha, China; [2]WuXi AppTec Co., Shanghai, CHINA*

TP 142 **Dual-stream UHPLC Separations on a Compact Sample Delivery System Featuring Simplified Software Automation for Increased Throughput in Drug Discovery Bioanalysis**; John Janiszewski[1, 2]; Brendon Kapinos[2]; Wayne Lootsma[3]; Hui Zhang[4]; Julie keefer[5]; Steve Ainley[3]; Mary Piotrowski[5]; *[1]Pfizer Inc., Groton, CT; [2]Pfizer Worldwide Research and Development, Groton, CT; [3]Sound Analytics, Niantic, CT; [4]Pfizer Worldwide Research and Development, Inc Groton, CT; [5]Pfizer, Groton, CT*

TP 143 **Determination of Heavy Metal Contamination in DMSO Solutions used for High Throughput Screening**; John M. Peltier[1]; Nicole White[2]; Melissa Grippo[1]; Jerome Giovanonni[3]; Pascal Bernet[3]; Christian Bergsdorf[3]; Justin Gu[4]; Zhaofu Wang[4]; Adam W Hill[1]; *[1]Novartis Institutes for Biomedical Research, Cambridge, MA; [2]Translational Clinical Oncology, Novartis Institutes for Biomedical Research, Cambridge, MA; [3]Novartis Institutes*

of BioMedical Research, Basel, Switzerland; [4]Novartis Institutes of BioMedical Research, Shanghai, China

TP 144 **Development of a Higher-throughput Metabolic Soft Spot Assay with Integrated Assessment of Glutathione Adduct Formation**; Anthony Paiva[1]; Wilson Shou[1]; Cheryl Klakouski[1]; Tatyana Zvyaga[1]; Benjamin Johnson[1]; Yue-Zhong Shu[2]; Ismael Zamora[3]; *[1]Bristol-Myers Squibb Company, Wallingford, CT; [2]Bristol-Myers Squibb Company, Lawrenceville, NJ; [3]Lead Molecular Design S.L., Sant Cugat de Valles, Spain*

ENERGY: HYDROCARBON AND PETROCHEMICAL (HI RESOLUTION & NOMINAL) 145 - 163

TP 145 **Photoionization as a Soft Ionization Source for Comprehensive Two-dimensional GC (GCxGC) and High-Resolution TOFMS**; Masaaki Ubukata[1]; A. John Dane[1]; Robert B. Cody[1]; Toshiyuki Kato[2]; Masahiro Ito[2]; Bram van der Meer[3]; Junichi Osuga[4]; Jean-François Focant[5]; *[1]JEOL USA, Inc., Peabody, MA; [2]JEOL Ltd., Akishima, Japan; [3]JEOL Europe B. V., Zaventem, Belgium; [4]JEOL Europe SAS, Croissy-Sur-Seine, France; [5]University of Liège, Liège, Belgium*

TP 146 **Investigation of the Partial Oxidation of Propane using a jet-Stirred Reactor and Molecular-Beam Mass Spectrometry**; Dennis Kaczmarek[1]; Patrick Oßwald[2]; Dominik Krüger[2]; Markus Köhler[2]; Tina Kasper[1]; *[1]University of Duisburg-Essen, Duisburg, Germany; [2]Institute of Combustion Technology, German Aerospace Center, Stuttgart, Germany*

TP 147 **Changing the Paradigm in Petroleomics with Comprehensive Two-Dimensional Gas Chromatography- High Resolution Mass Spectrometry**; Joe Binkley[1]; Jonathan D Byer[1]; David E Alonso[1]; Lorne Fell[1]; *[1]LECO Corporation, Saint Joseph, MI*

TP 148 **Analysis of Petroleum Products using Comprehensive Two-Dimensional Gas Chromatography (GC×GC) with Both Time of Flight MS and Flame Ionization Detectors**; Christina Kelly[1]; Joseph E Binkley[1]; Lorne E Fell[1]; Jonathan D Byer[1]; David E Alonso[1]; *[1]LECO Corporation, Saint Joseph, MI*

TP 149 **A New Method for Characterizing Heavy Petrochemical Fractions Based on Thermal Analysis and Laser Photo Ionization Mass Spectrometry**; Ralf Zimmermann[1]; Anne Ulbrich[2]; Thorsten Streibel[3]; Mohammad Saraji-Bozorgzad[4]; Sebastian Wohlfahrt[3]; Michael Fischer[3]; Thomas Denner[5]; Christoph Grimmer[3]; *[1]University of Rostock, Rostock; [2]University of Rostock, Rostock, N/A; [3]University of Rostock, Rostock, Germany; [4]Photonion GmbH, Schwerin, Germany; [5]Netzsch Gerätebau GmbH, Selb, Germany*

TP 150 **Identification of the Byproducts in the Preparation of 2,6-naphthalenedicarboxylic Acid by UPLC-QTOF MS/MS**; Jiwen Li[1]; Liyan Jiang[2]; Junyan Liu[2]; Chuan Wang[2]; *[1]SINOPEC SRIPT, Shanghai, Shanghai; [2]Sinopec Shanghai Research Institute of Petrochemic, Shanghai, China*

TP 151 **High Performance Thin Layer Chromatography (HPTLC) Coupled with DESI-Ion Mobility-Mass Spectrometry: A Novel Approach for Petroleum Characterisation**; Eleanor Riches[1]; Caroline Mangote[2]; Delphine Thuault[2]; Pierre Giusti[2]; Carlos Afonso[3]; Peter Hancock[1]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]TOTAL Refining & Chemicals, Total Research & Technology Gonfreville,, F-76700 Harfleur, France; [3]Normandie Univ, COBRA, UMR6014 and FR3038,Université de Rouen; INSA de Rouen; CNRS, IRCOF,, Rouen, France*

TP 152 **Intrinsic Ion Mobility Peak Width as an Indicator of Isomeric Species Distribution in Petroleum using Ion Mobility - Mass Spectrometry**; Mathilde Farenc[1, 2, 3]; Eleanor Riches[4]; Carlos Afonso[2, 3]; Pierre Giusti[1, 3]; *[1]TOTAL Refining and Chemicals, TRTG Gonfreville l'Orcher, France; [2]Normandie Univ, CNRS UMR 6014 COBRA Mont St Aignan, France; [3]TOTAL RC - CNRS Joint Laboratory C2MC :Complex Matrices Molecular Characterization, -, France; [4]Waters, Wilmslow, United Kingdom*

TP 153 **Petroleomics by Atmospheric Solid Analysis Probe Mass Spectrometry (ASAP-MS)**; Lilian Tose[1]; Michael Murgu[2]; Boniek Gontijo Vaz[3]; Wanderson Romão[1]; *[1]UFES, Vitória, Brazil; [2]waters Corporation, São Paulo, BRAZIL; [3]UFG, Goiânia, Brazil*

TP 154 **Application of Paper Spray Ionization Mass Spectrometry for the Analysis of Weathered Oil**; Donghwi Kim[1]; Purum Kim[2]; Joon Geon An[3]; Un Hyuk Yim[3]; Sangwon Cha[2]; Sunghwan Kim[1]; *[1]Kyungpook National University, Daegu, Republic of Korea; [2]Hankuk Univ. Foreign Studies, Yongin, South Korea; [3]Korea Institute of Ocean Science and Technology, Geoje, South Korea*

TP 155 **UnisprayTM Ion Source Coupled to UHPSFC for the Detection of Oilfield Additives**; Efstathios Andreas Elia[1]; William Durnie[2]; Ed Sparke[3]; John G Langley[1]; *[1]Chemistry, University of Southampton, Southampton, United Kingdom; [2]BP Exploration, Sunbury-on-Thames, Middlesex, United Kingdom; [3]Waters, Wilmslow, United Kingdom*

TP 156 **Insights into Iron Promoted Sugar Conversion to 5-Hydroxymethylfurfural (HMF) and Levulinic Acid (LA) From Tandem Mass Spectrometry**; Yuan Jiang[1]; Linan Yang[1]; Christine M Bohn[1]; Guannan Li[1]; Dong Han[1]; Nathan S Mosier[1]; Jeffrey T Miller[1]; Hilkka I Kenttämaa[1]; Mahdi M Abu-Omar[1]; *[1]Purdue University, West Lafayette, IN*

TP 157 **Untargeted Metabolomic Approach for the Management of Microbiologically Influenced Corrosion in the Oil and Gas Industry**; Vincent Bonifay[1]; Iwona B Beech[1]; Jan A Sunner[1]; *[1]University of Oklahoma, Norman, OK*

TP 158 **A Fast Mass Spectrometric Approach for the Characterization of Aromatic Compounds Present in Crude oil**; Ravikiran Yerabolu[1]; Raghavendhar Kotha[1]; Xueming Dong[1]; John Kong[1]; Bryan Clayton[2]; Hilkka Kenttämaa[1]; *[1]Purdue University-Department of Chemistry, West Lafayette, IN; [2]Pioneer Oil Company, Lawrenceville, IL*

TP 159 **GC-MS and SFC-MS Approaches for the Low –level Detection and Quantification of a New Fuel Marker**; John G Langley[1]; Julie M Herniman[1]; Edward M. J. Wilmot[1]; Anastarsia C. M. Carter[1]; Jim Barker[2, 3]; *[1]University of Southampton, Southampton, United Kingdom; [2]Innospec Inc., Ellesmere Port, United Kingdom; [3]Energy Institute, London, United Kingdom*

TP 160 **Comparison of GC-MS, GC-VUV, and Comprehensive Two-Dimensional GC for the Characterization and Source Identification of Diesel Fuels**; Ling Bai; *University of Texas at Arlington, Arlington, Texas*

TP 161 **Using GC/MSD with High Efficiency Source and Hydrogen Cleaning to Detect Low Level Contaminants in Ethylene and Propylene**; Angela Henry[1]; Bruce Quimby[1]; Badr Astiphan[2]; *[1]Agilent Technologies, Little Falls, DE; [2]Agilent Technologies, Santa Clara, CA*

TP 162 **Can Elusive Structural Features of Heavy Crude Oil Components be Decoded from FT-ICR-MS Data?**; Cristian Blanco-Tirado[1]; Marianny Y Combariza[2]; Cristian Alejandro Blanco-Combariza[2]; *[1]Universidad Industrial de Santander, Bucaramanga, Santander; [2]Universidad Industrial de Santander, Bucaramanga, Santander, Colombia*

TP 163 **Highly Specific Biomarker Determination in Biodegraded Petroleum with Gas Chromatography and Triple Quadrupole Detection using Multiple Reaction Monitoring**; Andrés González[1]; Taylor Motta[1]; Ivama Calles[1]; Sánchez Carlos[1]; Jairo René Martínez[1]; Stashenko Elena[1]; *[1]Universidad Industrial de Santander, Bucaramanga, Santander, Colombia*

ENVIRONMENTAL ANALYSIS: GENERAL (PART 2)
164 - 188

TP 164 **Rapid Exploration of the Mechanism of Action of Forskolin via Untargeted Proteomics and Knowledge-based Pathway Analysis**; Ziad Sahab[1]; Bindesh Shrestha[2]; Lida Parvin[1]; Peter Nemes[1]; Akos Vertes[1]; *[1]George Washington University, Washington, DC; [2]Waters Corporation, Beverly, MA*

TP 165 **Determination fF Aqueous Film Forming Foam (AFFF) Components using a Multivariate Analysis Approach**; Lauren Mullin[1]; Anna Karmann[2]; Gareth Cleland[1]; John Vukovic[1]; Adam Ladak[1]; *[1]Waters, Milford, MA; [2]MTM Research Centre, Örebro University Örebro, Sweden*

TP 166 **Characterization of Fe-rich Multi-element Particles by ICP TOF**; Joel Kimmel[1]; Olga Borovinskaya[1]; Martin Tanner[1]; *[1]TOFWERK, Thun, Switzerland*

TP 167 **Polycyclic Aromatic Hydrocarbon and Metabolite Analysis of Soils Related to Energy Exploration by On-Line SFE/SFC-MS**; Doug D. Carlton[1, 2]; A. Paige Wicker[1]; Kenichiro Tanaka[3]; Erin McAllister[3]; Kevin A Schug[1, 2]; *[1]Department of Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, TX; [2]Affiliate of the Collaborative Laboratories for Environmental Analysis and Remediation, The University of Texas at Arlington, Arlington, TX; [3]Shimadzu Scientific Instruments, Inc., Columbia, MD*

TP 168 **Laser DesorptionSingle Particle Aerosol Mass SpectrometryforDirectAnalysis of Solid Materials**; Mei Liu[1]; Li Xu[1]; Junguo Dong[1]; Zhengxu Huang[2]; Ping Cheng[3]; Zhen Zhou[2]; *[1]School of Environmental and Chemical Engineering, Shanghai University, Shanghai, China; [2]Institute of Atmosphere environment security and Pollution control, Jinan University, GuangZhou, China; [3]School of Environmental and Chemical Engineering, Shanghai University, Shanghai, Shanghai*

TP 169 **Development and Validation of a UPLC-MS/MS Method for Mono(2-ethylhexyl)phthalate, a Metabolite of Di(2-ethylhexyl)phthalate, in Rat Plasma, Amniotic Fluid, and Fetus**; Melanie A. Rehder Silinski[1]; Brenda L. Fletcher[2]; Reshan A. Fernando[2]; Veronica G. Robinson[3]; Paul Foster[3]; Suramya Waidyanatha[3]; *[1]RTI International, Research Triangle Park , NC; [2]RTI International, Research Triangle Park, NC; [3]Division of National Toxicology Program, NIEHS, Research Triangle Park, NC*

TP 170 **An Automated Method for Microcystins Analysis using Two-dimensional Liquid Chromatography-quadrupole Time-of-Flight Mass Spectrometry (2DLC-QTOFMS)**; Xavier Ortiz Almirall[1]; Marie Meyer-Monath[2]; Eva Korenkova[1]; Karl Jobst[1]; Eric Reiner[1]; Karen MacPherson[1]; *[1]Ministry of the Environment and Climate Change of Ontario, Toronto, ON; [2]University of Toronto, Toronto ON, Canada*

TP 171 **Development of an LC-QTOF MS Method for the Non-targeted Analysis of Microcystins**; Marie Meyer-Monath[1,2]; Xavier Ortiz[1]; Eva Korenkova[1]; Ralph Ruffolo[1]; Karl Jobst[1, 3]; Satyendra Bhavsar[1, 2, 4]; Andre Simpson[2]; Eric Reiner[1, 2]; *[1]Ontario Ministry of Environment & Climate Change, Toronto, Canada; [2]University of Toronto, Toronto ON, Canada; [3]McMaster University, Hamilton, Canada; [4]University of Windsor, Windsor, Canada*

TP 172 **Determination of Trace Microcystins in Aqueous Samples by Solid-Supported Liquid Extraction Coupled to Liquid Chromatography-Tandem Mass Spectrometry**; Chang-Lin Hsu[1]; Chung-Yu Chen[1]; Maw-Rong Lee[2]; *[1]National Chung-Hsing University, Taichung, TAIWAN (R.O.C.); [2]National Chung-Hsing University, Taichung, Taichung*

TP 173 **Effect of Analytical Standard Preparation Procedures in the Quantitation of Urinary Monohydroxy-Polycyclic Aromatic Hydrocarbons (OH-PAHs) by Online SPE-HPLC-MS/MS**; Yuesong Wang[1]; Lei Meng[1]; Erin N Pittman[1]; Alisha Etheredge[1]; Kendra Hubbard[1]; Debra A Trinidad[1]; Xiaoyun Ye[1]; Antonia M. Calafat[1]; *[1]CDC, Atlanta, GA*

TP 174 **New 2,4-dinitroanisole (DNAN; Munitions Chemical) (bio)Transformation Products discovered and Bioassayed using High Resolution UPLC-QToFMS**; Leif Abrell[1]; Christopher I. Olivares[1]; Jon Chorover[1]; Reyes Sierra-Alvarez[1]; Jim A. Field[1]; *[1]University of Arizona, Tucson, Arizona*

TP 175 **Investigation of Eicosanoids and Fatty Acids in Pansteatitis-Affected Mozambique Tilapia at Loskop Dam, South Africa**; theresa cantu[1]; John Bowden[2]; Jack McAlhany[3]; Matthew Guillette[4]; hannes botha[5]; Louis J. Guillette[4]; *[1]MUSC, Charleston, SC; [2]National Institute of Standards and Technology, Charleston, SC; [3]college of charleston, charleston, sc; [4]Medical Univ of S Carolina, Charleston, SC; [5]Mpumalanga Tourism and Parks, Pretoria, South Africa*

TP 176 **Analysis of Problematic Cyclic Siloxane Compounds in the Atmosphere of the International Space Station**; Patti Cheng[1]; Vanessa de Vera[1]; Robert Gillispie[1]; Steven Beck[1]; William Wallace[2]; Thomas Limero[2]; *[1]Wyle Science, Technology, and Engineering Group, Houston, TX; [2], Houston, TX*

TP 177 **Accurate Mass Spectral Database: Harnessing the Power of High Performance Mass Spectrometry at Long Last**; Lorne Fell[1]; Viatcheslav Artaev[1]; Kevin McNitt[1]; Steve Robles[1]; Albert Lebedev[2]; *[1]LECO Corporation, Saint Joseph, MI; [2]Moscow State University, Moscow, Russian Federation*

TP 178 **A Method for Real-Time Monitoring of Acrolein in Air using TAGA Mass Spectrometry**; Nicholas Karellas; *Ontario Ministry of the Environment , Toronto, ON*

TP 179 **Mass Spectrometry-based Studies on the Association of Organic Dusts and Respiratory Symptoms**; Brooke Thompson[1]; Paulos Chumala[1]; Shelley Kirychuk[1]; George S. Katselis[1]; *[1]CCHSA/Medicine, College of Medicine, University of Saskatchewan, Saskatoon, SK, Canada*

TP 180 **Monitoring Fugitive Emissions with a Miniature Ion Trap Mass Spectrometer**; Preshious Rearden[1]; Corey Stedwell[1]; Parminder Kaur[1]; Daniel DeBord[1]; *[1]1st Detect Corporation, Webster, TX*

TP 181 **Analytical Strategy to Investigate Naphthenic Acids in Atmospheric Aerosols by Ultrahigh-Performance Liquid Chromatography/Quadrupole Time-of-Flight Mass Spectrometry (UPLC/QTOF-MS)**; Mahmoud Yassine; *Environment and Climate Change Canada, Ottawa, ON*

TP 182 **A Comparison of Thermal- and Valve-based Modulation for the Analysis of Environmental Contaminants by GCxGC-TOF MS**; Tadeusz Gorecki[1]; Matthew Edwards[1, 2]; Haleigh Boswell[1]; Pete Grosshans[3]; *[1]University of Waterloo, Ontario, Canada; [2]Markes International, Cardiff, UK; [3]Markes International Inc, Cincinnati, OH*

TP 183 **High sensitive quantitation method of perfluorinated compounds by an automated online solid extraction LC/MS/MS**; Yoshikane Mitsuha[1]; Jun Watanabe[2]; Kagi Noriko[3]; Minohata Toshikazu[4]; Ogura Tairo[5]; Nakayama Shoji[6]; *[1]IDEA Consultants, Inc., Yaidzu, Japan; [2]Shimadzu Corporation, Kyoto; [3]JASCO International Co., Ltd., Hachioji, Japan; [4]Shimadzu Corporation, Kyoto, Japan; [5]Shimadzu Scientific Instruments, Inc. Columbia.; [6]National Institute for Environmental Studies, Tsukuba, Japan*

TP 184 **A Collaborative EPA Method 625 Update Study using a New Mass Spectrometry Method for Quantification Combined with Stir-bar Sorptive Extraction**; Weier Hao[1]; Andrew Boggess[1]; Edward Pfannkoch[2]; Skip Kingston[1]; *[1]Duquesne University, Pittsburgh, PA; [2]Gerstel, Inc. Linthicum, MD*

TP 185 **Automated Screening of Explosives in Soil Samples by Online SFE-SFC-MS**; William A Hedgepeth [1]; Kenichiro Tanaka[2]; Tairo Ogura[2]; Jonathan Edwardsen[2]; *[1]Shimadzu Scientific Instruments, Inc, Columbia , MD; [2]Shimadzu Scientific Instruments, Inc. Columbia, MD*

TP 186 **Efficiency Screening of Carbon Nanomaterial or Superoxydant in Advanced Water Treatment by Mass Spectrometry Are They Accurate Enough?**; Hugues Preud'homme[1]; Jaber Al-Marri[1]; Pierre Kubiak[1]; Rachid Essehli[1]; *[1]QEERI - HBKU - Qatar Foundation, Doha, QATAR*

TP 187 **Chromatographic Mass Spectrometric Detection of Arsenic Species in Sulfidic Waters – Method Development**; Denzel Bolden[1]; Akeena Harper[1]; Jianye Zhang[1]; *[1]Voorhees College, Denmark, SC*

TP 188 **Fast Detection of Environmental Vapors by Thermal Desorption - Atmospheric Pressure Photoionization - Differential Mobility Analysis - Mass Spectrometry (TD-APPI-DMA-MS)**; Ross David McCulloch[1]; Amo González Mario[1]; *[1]SEADM, Boecillo, Spain*

FAIMS AND DMS
189 - 209

TP 189 **Rapid Separation and Quantification of Hydroxyvitamin D3 Epimers by FAIMS-MS, Eliminating the Need for LC Separation for High-throughput Clinical Analysis**; Lauren Brown[1]; Danielle Toutoungi[1]; Robert Smith[1]; Billy Boyle[1]; *[1]Owlstone Ltd., Cambridge, UK*

TP 190 **Resolution of Isotopologues and Isotopomers by High-Field Ion Mobility Coupled to Mass Spectrometry: Path to Gas-Phase NMR?**; Julia Kaszycki[1]; Matthew A. Baird[1]; Andrew P. Bowman[1]; Alexandre A Shvartsburg[1]; *[1]Wichita State University, Wichita, KS*

TP 191 **Modeling and Characterization of the Ion Transit Time in a FAIMS-MS Interface**; Satendra Prasad[1]; Jean-Jacques Dunyach[1]; Michael W Belford[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

TP 192 **On a Multi-physics Computational Model to Understand Heat Exchange between FAIMS Electrode and Ion Transport Gas**; Satendra Prasad; *Thermo Fisher Scientific, San Jose, CA*

TP 193 **Efficiency of Ion Transmission between FAIMS Electrodes without a Separation Electric Field**; Satendra Prasad[1]; Susan E Abbatiello[2]; Michael W Belford[1]; Jean-Jacques Dunyach[1]; Mary L Blackburn[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Cambridge, USA*

TP 194 **Comparison of Rectangular Waveform FAIMS/MS to Conventional Sum-of-sines Waveform**; Michael Wei[1]; Michael Costanzo[1]; Joaquin Casanova[1]; Jared Boock[1]; Richard A Yost[1]; *[1]University of Florida, Gainesville, Florida*

TP 195 **Glyphosate quantified in Black Tea and Other Food Matrices by Automatically Optimized LC-FAIMS MS/MS**; Bennett Kalafut[1]; Rae Ana Snyder[1]; Claudia Martins[1]; Manish Doshi[1]; Mark Hardman[1]; *[1]Thermo Fisher Scientific, San Jose, California*

TP 196 **Rapid FAIMS at Extreme Fields Inside the Mass Spectrometry Envelope with Applications to Peptide and Protein Analyses**; Alexandre Shvartsburg[1]; Andrew Entwistle[2]; Roger Giles[2]; *[1]Wichita State University, Wichita, KS; [2]Shimadzu Research Laboratory (Europe) Ltd., Manchester, United Kingdom*

TP 197 **Is Differential Mobility Chemically Driven? Evidence and Simulations for Chemical Effects as Primary Separation Factor in DMS**; Walter Wissdorf[1]; Bradley B Schneider[2]; Tom Covey[2]; James Hager[2]; Thorsten Benter[3]; *[1]Bergische Universität Wuppertal, Wuppertal; [2]SCIEX, Concord, ON; [3]Bergische Universität Wuppertal, Wuppertal, Germany*

TP 198 **LESA FAIMS Mass Spectrometry for the Spatial Profiling of Proteins from Tissue**; Rian L. Griffiths[1]; Alex Dexter[1]; Andrew J Creese[1]; Alan M. Race[2]; Josephine Bunch[2, 3]; Helen Cooper[1]; *[1]University of Birmingham, Birmingham, UK; [2]National Physical Laboratory, Teddington, UK; [3]University of Nottingham, Nottingham, UK*

TP 199 **Analysis of Derivatized Glycans using Differential Mobility Spectrometry**; Cathy Lane[1]; Yves J C LeBlanc[2]; J. Larry Campbell[2]; *[1]SCIEX, Phoenix House Lakeside Drive Warrington Cheshire UK, WA1 1RX; [2]SCIEX, Concord, ON*

TP 200 **Improved Quantitative Measurements for Large Scale Proteomic Analyses using Metabolic Labeling and Ion Mobility**; Sibylle Pfammatter[1]; Eric Bonneil[2]; Pierre Thibault[1]; *[1]IRIC-Université de Montréal, Montréal, QC; [2]Universite de montreal, Montreal, QC*

TP 201 **Model FAIMS RF System using Neural Network**; Xiaoqun Zou; *Thermofisher Scientific, San Jose, CA*

TP 202 **Making FAIMS Faster, More Selective, and More Sensitive**; Michael Belford[1]; Satendra Prasad[1]; Jean-Jacques Dunyach[1]; Susan E Abbatiello[1]; Ryan Hermezian[1]; Hoa Pham[1]; Ann Yadlowsky[1]; Alex Zou[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

TP 203 **Selexlon-based Detergent Interference Removal for Shotgun-Lipidomics Analyses**; Cyrus Papan[1]; Julian D Langer[2]; *[1]Sciex, Darmstadt, Hessen; [2]Max-Planck-Institute of Biophysics, Frankfurt Am Main, Germany*

TP 204 **Rapid Analysis of Steroid Metabolites using Field Asymmetric Waveform Ion Mobility Spectrometry Combined with Liquid Chromatography and Mass Spectrometry**; Kayleigh Louise Arthur[1]; Matthew Arran Turner[1]; James Christopher Reynolds[1]; Colin Creaser[1]; *[1]Loughborough University, Loughborough, United Kingdom*

TP 205 **Differential Mobility Spectrometry (DMS) Reveals the Elevation of Urinary Acetylcarnitine in Non-Human Primates (NHP) Exposed to Radiation**; Nicholas B. Vera[1, 2]; Amol Kafle[3]; Evan Pannkuk[4]; Evagelia C. Laiakis[4]; A.J. Fornace, Jr.[4]; Stephen L. Coy[3]; Derek M Erion[1]; Paul Vouros[3]; *[1]Pfizer, Cambridge, MA; [2]Northeastern University, Boston, Massachusetts; [3]Northeastern University, Boston, MA; [4]Georgetown University, Washington, DC*

TP 206 **Characterization of Variables Affecting Internal Energy Deposition inside a Differential Ion Mobility Spectrometer**; Brandon Santiago[1]; Matthew T. Campbell[1]; Gary L. Glish[1]; *[1]The University of North Carolina at Chapel Hill, Chapel Hill, NC*

TP 207 **Analysis of Free Drug in Antibody-Drug Conjugate by Reversed-phase HPLC Coupled with Differential Mobility Mass Spectrometry**; Chunang (Christine) Gu [1]; Marie-France Morissette[2]; Loren Y Olson[3]; Shaokun Pang[3]; Yi Li[2]; Colin Medley[2]; David Russell[2]; *[1]Genentech, South San Francisco, CA; [2]Genentech Inc, South San Francisco, CA; [3]SCIEX, Redwood City, CA*

TP 208 **Optimizing DMS Separations by Comparing Alpha Functions**; Brad Schneider[1]; Erkinjon Nazarov[1]; J.C. Yves Le Blanc[1]; Frank Londry[1]; Thomas Covey[1]; *[1]SCIEX, Concord ON, Canada*

TP 209 **Rapid Ion Trap Mass Analysis of Inorganic Water Clusters Separated by Differential Mobility Spectrometry**; Theresa Evans-Nguyen[1]; Timothy Vazquez[1]; *[1]University of South Florida, Tampa, FL*

FOOD SAFETY (PESTICIDES IN FOOD)
210 - 235

TP 210 **Significant Improvement in GCMS Screening of Pesticides in Scan Mode using a High Efficiency Ion Source and Spectral Deconvolution**; Melissa Churley [1]; Bruce Quimby[2]; *[1]Agilent Technologies, Santa Clara , CA; [2]Agilent Technologies, Little Falls, DE*

TP 211 **A Targeted Quantitative LC-MS/MS Method for 431 Positive and Negative Ion Pesticides in a Single Analysis**; Louis Maljers[1]; Zicheng Yang[2]; *[1]Bruker Daltonics, Fremont, CA; [2]Bruker Daltonics Inc, Fremont, CA*

TP 212 **GC/MS/MS Analysis of Pesticide Residues in Cannabis Using QuEChERS Extraction and Cleanup**; Kathy Stenerson[1]; Craig Aurand[1]; David Bell[1]; Sara Smith[1]; Emily Barrey[1]; Candace Price[1]; *[1]MilliporeSigma, Bellefonte, PA*

TP 213 **Analysis of Pesticides in Spaghetti Sauce by Direct Immersion Solid Phase Microextraction GC/MS**; Kathy Stenerson[1]; Candace Price[1]; Craig Aurand[1]; Dave Bell[1]; Emily Barrey[1]; Sara Smith[1]; *[1]Sigma Aldrich, Bellefonte, PA*

TP 214 **An Optimal Method for the Analysis of Pesticides in a Variety of Matrices**; Jessica Westland[1]; Vivian Chen[2]; *[1]Agilent Technologies, Wilmington, Delaware; [2]AGILENT, Shanghai, China*

TP 215 **Accurately Identify and Quantify A Hundred Pesticides in a Single GC Run**; Jessica Westland[1]; Tom Doherty[2]; Vivian Chen[3]; *[1]Agilent Technologies, Wilmington, Delaware; [2]Agilent Technologies, Santa Clara, CA; [3]Agilent, Shanghai, China*

TP 216 **Maintaining Sensitivity and Reproducibility with the Self Cleaning Ion Source for Pesticides in Food and Feed**; Vivian Chen[1]; Jessica Westland[2]; Elizabeth Almasi[3]; *[1]Agilent, Shanghai, China; [2]Agilent Technologies, Wilmington, Delaware; [3]Agilent Technologies, Santa Clara, CA*

TP 217 **"No Dilute" Just Shoot LC-ESI-MS/MS : Feasibility and Robustness of a Maintenance-Free Source for Applications in Low-level Pesticide Residue Analysis**; Matteo Meglioli[1]; Frank A Kero[2]; Joshua Ye[3]; Craig Young[2]; Sharanya Reddy[2]; *[1]Mosti Mondiale, Villa Ste Catherine, QC; [2]PerkinElmer, Shelton, CT; [3]Ionics Mass Spectrometry Group, Bolton, ON*

TP 218 **Rapid Detection of Pesticides in Honey by C18 Pipette-tip Electrospray Ionization Mass Spectrometry**; Yi-Ching Choi[1]; Tsz-Tsun Ng[1]; Bin Hu[1]; Zhong-Ping Yao[1]; *[1]Department of Applied Biology and Chemical Technology, The Hong Kong Polytechnic University, Hong Kong, China*

TP 219 **A Single LC-MS/MS Method for Confirmation and Quantification of over 400 Pesticides in Complex Matrix without Compromising Data Quality**; Dimple Shah[1]; Eimear McCall[2]; Gareth Cleland[3]; *[1]Waters Corp., Milford, MA; [2]Waters, Wilmslow, United Kingdom; [3]Waters Coorporation, Milford, MA*

TP 220 **Determination of Multiple Pesticides Residues in Imported Tea in UAE Using Liquid and Gas Chromatography Tandem Mass Spectrometry**; Mohammed Meetani[1]; Sarah Ali Almulla[2, 3]; Nasra M. Ibrahim[2]; *[1]United Arab Emirates University, Al-Ain, Abu Dhabi; [2]laboratories Department, Ministry of Environment and Water, Sharjeh, United Arab Emirates; [3]chemistry Department, College of Science, UAE University, Al-Ain, United Arab Emirates*

TP 221 **Multi-residue Analysis of Pesticides in Agricultural Products using QuEChERS and SFC/MS**; Yuka Fujito[1]; Kenichiro Tanaka[2]; Tairo Ogura[2]; Kiyomi Arakawa[1]; Yoshihiro Hayakawa[1]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]Shimadzu Scientific Instruments, Inc. Columbia*

TP 222 **Supercritical Fluid Chromatography/Tandem Mass Spectrometry (SFC-MS/MS) Analysis of Hundreds of Pesticide Residues in Food Safety**; David Baker[1]; Christopher Titman[1]; Jonathan Horner[2]; Neil Loftus[1]; *[1]Shimadzu, Manchester, UK; [2]SAL (Scientific Analysis Laboratories), Cambridge, UK*

TP 223 **Quantitative Analysis of 647 Pesticides (1,929 MRMs) by LC-MS/MS with a Fast 10.5 Minute Cycle Time**; David Baker[1]; Laetitia Fages[2]; Eric Capodanno[2]; Neil Loftus[1]; Simon Ashton[1]; *[1]Shimadzu, Manchester, UK; [2]Phytocontrol, Nimes, France*

TP 224 **Food Residue Screening using Liquid Chromatography Coupled to High Resolution MS/MS (LC-HR-MS/MS) - Multi-Pesticide Identification and Quantitation**; KC Hyland[1]; Paul Winkler[1]; Andre Schreiber[2]; *[1]SCIEX, Redwood City, CA; [2]AB SCIEX, Concord, ON*

TP 225 **Screening of Pesticides in Lipid-rich Food Matrices by using High Resolution GC/Q-TOF and Accurate Mass Pesticide Library**; Kai Chen[1]; Joan Stevens[2]; Hong Chen[1]; Vadim Kalmeyer[1]; Sofia Nieto[1]; *[1]Agilent Technologies, Santa Clara, CA; [2]Agilent Technologies, Wilmington, DE*

TP 226 **Routine Quantitative and Qualitative Methodologies for Food Pesticide Residue Laboratories Using Tandem and High Resolution Accurate Mass (HRAM) LC/MS Instrumentation**; Claudia Martins[1]; Ed George[1]; Dipankar Ghosh[1]; Katerina Bousova[2]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Dreieich, Germany*

TP 227 **Screening for More than 600 Pesticide Residues and Their Identification in Food Samples using a New LCMSMS Library Data Base**; Houssain El Aribi[1]; Salah A. Almaiman[1]; Mustafa A. Gassem[1]; Majed A. Alansari[1]; *[1]Saudi FDA, Riyadh*

TP 228 **Rapid Extraction and Clean-up Kits for the Determination of Pesticide Residues in Food**; Shao Kai Lin; *Taichung, Taichung*

TP 229 **Development of Multi-Pesticides in Avocado using Enhanced Matrix Removal by liquid Chromatography-Tandem Mass Spectrometry with Dynamic MRM and Triggered MRM**; Wen-Yen Lee[1]; Jin-Lan Sun[2]; Chun-Ye Sun[2]; Shan-An Chan[1]; *[1]Agilent, Taipei, Taiwan; [2]Agilent, Shanghai, China*

TP 230 **Rapid Screening and Quantitation of Pesticide Residues in Cannabis by Modified QuEChERS and LC-MS-MS**; Jeff Dahl[1]; Julie Kowalski[2]; Gordon Fagras[3]; *[1]Shimadzu, Columbia, MD; [2]Restek Corporation, Bellefonte, PA; [3]Trace Analytics, Spokane, WA*

TP 231 **Pesticide Analysis in Complex Food Extracts by Multi-transition MRM and Library Searching for Enhanced Residue Confirmation**; David Baker[1]; Christopher Titman[1]; Jonathan Horner[2]; Neil Loftus[1]; *[1]Shimadzu, Manchester, UK; [2]SAL (Scientific Analysis Laboratories), Manchester, UK*

TP 232 **Fast Data Acquisition Speed and High quantitative Performance in the Simultaneous Determination of Mycotoxins, Illegal Dyes and Pesticides in Spices**; Mark Sartain[1]; Thomas Glauner[2]; Craig Marvin[3]; Andre Santos[4]; Anumol Tarun[3]; Jerry Zweigenbaum[3]; *[1]Agilent Technologies, Santa Clara, CA; [2]Agilent Technologies Sales & Services GmbH, Waldbronn, Germany; [3]Agilent Technologies, Wilmington, DE; [4]Agilent Technologies Inc, Barueri, Brazil*

TP 233 **Multi-Residue Pesticides Analysis by LC-MS/MS using the ODS Column and the Biphenyl Column**; Natsuyo Asano[1]; David Baker[2]; Yuki Uno[1]; Atsuhiko Toyama[1]; Jun Watanabe[1]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]Shimadzu, Manchester, UK*

TP 234 **Automated Pressurized Liquid Extraction and Clean Up of Sea Food Samples in the Analysis of Persistent Organic Pollutants (POPs)**; Hamid Shirkhan[1]; Rudolf Addink[1]; *[1]Toxic Report, Watertown, MA*

TP 235 **Fully Automated Online Sample Extraction and Analysis of Mycotoxins in Foods by Online SFE-SFC-MS**; Kenichiro Tanaka[1]; William Hedgepeth[1]; Tairo Ogura[1]; *[1]Shimadzu Scientific Instruments, Inc. Columbia*

FOOD"OMICS" MS CHARACTERIZATION OF FOOD AND NUTRITIONAL SUPPLEMENTS (PART 1)
236 - 250

TP 236 **DLLME-Gas Chromatography-Quadrupole Time-of-Flight Mass Spectrometry for Classification of Botanical Origin of Chinese Honey by Its Volatile and Semi-volatile Compound Profile**; Hui Chen[1]; Linghe Jin[2]; Chunlin Fan[1]; Guofang Pang[1]; Shan Zhou[3]; Wenwen Wang[3]; *[1]Chinese Academy of Inspection and Quarantine, Beijing, China; [2]Shandong Agriculture University, Tai'an, China; [3]Agilent Technologies Company. Ltd, Beijing, China*

TP 237 **Discrimination of Honey of Different Botanical Origins using an Untargeted High-Definition Metabolomic Workflow**; Joanne B. Connolly [1]; Sara Stead[2]; Antonietta Wallace[2]; Delano Turner[2]; *[1]Waters Corporation, Manchester , UK; [2]Waters Corporation, Manchester, UK*

TP 238 **Proteomic and Peptidomic Differences and Similarities between Four Muscle Types from New Zealand Raised Angus Steers**; Stefan Clerens[1, 2]; Ancy Thomas[1]; Jessica Gathercole[1]; Jeffrey E Plowman[1]; Tzer-Yang Yu[1]; Anita J Grosvenor[1]; Stephen R Haines[1]; Peter Dobbie[3]; Kevin Taukiri[3]; Katja Rosenvold[3]; Jolon M Dyer[1]; Santanu Deb-Choudhury[1]; *[1]AgResearch, Lincoln, New Zealand; [2]Biomolecular Interaction Centre, Christchurch, New Zealand; [3]AgResearch, Ruakura, New Zealand*

TP 239 **The Modernisation of Fish Fraud Detection using Rapid Evaporative Ionisation Mass Spectrometry (REIMS)**; Connor Black[1]; Olivier Chevallier[1]; Julia Balog[2]; Sara Stead[3]; Steven D Pringle[4]; Christopher Elliott[1]; Zoltan Takats[5]; *[1]Queens University Belfast, Balfast, UK; [2]Waters WRC, Budapest, Hungary; [3]Waters corp, Manchester, Lanc; [4]Waters, Wilmslow, United Kingdom; [5]Imperial College, London, United Kingdom*

TP 240 **Solid Phase Mesh Enhanced Sorption from Headspace (SPMESH) Coupled to DART-MS/MS for Quantification of Trace-level Odor-active Volatiles in Foodstuffs**; Jillian Jastrzembski; *Cornell University, Ithaca, New York*

TP 241 **Headspace Analysis of E-Cigarette Liquid Flavorings by Vacuum Thermal Desorption**; Eric Knappenberger[1]; Corey Stedwell[1]; J. Daniel DeBord[1]; *[1]1st Detect, Webster, TX*

TP 242 **Direct Analysis of Anthocyanins (a Class of Flavonoid Antioxidants) in Complex Plant Extracts**; Chad C Nelson[1]; Douglas Stevenson[1]; *[1]Nu Skin Enterprises, Provo, UT*

TP 243 **Matrix Effects Limit Accuracy in SPME-GC-MS Analyses of a Grape Mapping Population**; Elizabeth A. Burzynski[1]; Imelda Ryona[2]; Bruce I. Reisch[1]; Gavin L. Sacks[1]; *[1]Cornell University, Ithaca, NY; [2]Q2 Solutions, Ithaca, NY*

TP 244 **HILIC Chromatography Coupled with IMS/MS for Characterization of Phenolic Compounds and Related Pigments in Red Wine** ; Andre De Villiers[1]; Andrew Baker[2]; *[1]Department of Chemistry and Polymer Science, Stellenbosch University, Matieland, South Africa; [2]Waters, Inc., Pleasanton, CA*

TP 245 **Analysis of Pinot Noir Wines by HS-SPME GC/Q-TOF: Correlating Geographical Origin with Volatile Aroma Profiles**; Philip L. Wylie[1]; Anna K. Hjelmeland[2]; Ron C. Runnebaum[2]; Susan E. Ebeler[2]; *[1]Agilent Technologies, Wilmington, DE; [2]University of California-Davis, Davis, CA*

TP 246 **Discrimination of Wine Cultivars and Geographic Origins by Characteristic Components Profiling using UHPLC-ESI/QTOF-MS Combined with Chemometric Analysis**; Nana Liang[1]; Ying Liu[1]; Meiling Lu[2]; Shan Zhou[3]; Jinhua Wang[1]; Zhaohui Zhang[1]; Shen Han[1]; *[1]Beijing Entry-Exit Bureau of Inspection and Quarantine, Beijing, China; [2]2Agilent Technologies (China) Limited, Beijing; [3]Agilent Technologies (China) Limited, Beijing, China*

TP 247 **Unravelling the Color of a Worldwide Rosé Wine Collection by UHPLC-MRM-MS Polyphenol Profiling**; Nicolas Sommerer[1]; Marine Lambert[1]; Arnaud Verbaere[1]; Emmanuelle Meudec[1]; Marie-Agnès Ducasse[2]; Jean-Claude Boulet[1]; Gérard Mazerolles[1]; Gilles Masson[3]; Véronique Cheynier[1]; *[1]INRA, UMR1083 SPO, Montpellier, France; [2]IFV, UMT QUALINNOV, Gruissan, France; [3]IFV, centre du rosé, Vidauban, France*

TP 248 **LC/MS Metabolomic Profiling of an Amber Ale Fermented with Four Different Yeast Strains**; Kearney M Foss[1]; Karen Fortmann[2]; Christine A. Hughey[3]; *[1]James Madison University, Harrisonburg, VA; [2]White Labs, San Diego, CA; [3]James Madison University, Harrisonburg , VA*

TP 249 **Rapid Preparation for Quantitative Analysis of Volatile and Semi-Volatile Compounds in Scotch Using Gas Chromatography Mass Spectrometry**; Yashaswini Nagarajan[1]; Doug D Carlton[1]; Evelyn H Wang[1]; Jillian Melbourne[1]; Kevin A Schug[1]; *[1]Department of Chemistry and Biochemistry, UTA Arlington, tx*

TP 250 **Analysis of the Oligosaccharide and Protein Content of Beer Using Matrix-Assisted Laser Desorption Ionization Time-Of-Flight Mass Spectrometry (MALDI TOFMS)**; Elsa Gorre[1]; Ashley Phetsanthad[1]; Jon Soffer[1]; Kevin G Owens[1]; *[1]Drexel University, Philadelphia, PA*

FORENSICS (PART 1)
251 - 278

TP 251 **Cryogenic-Focusing Fast Gas Chromatography Isotope Ratio Mass Spectrometry for Anti-Doping**; Herbert Tobias[1]; Thomas J Brenna[1]; *[1]Cornell University, Ithaca, NY*

TP 252 **Data Quality Control Measures for Forensic Mass Spectral Libraries**; William E. Wallace[1]; Weihua Ji[1]; Karen W Phinney[2]; Stephen Stein[2]; *[1]National Institute of Standards & Technology, Gaithersburg, MD; [2]National Institute of Standards and Technology, Gaithersburg, MD*

TP 253 **A DART-MS and In-source CID Reverse Library Search Approach for Rapid Screening of Drugs of Abuse**; Frederick Li[1]; Joseph Tice[1]; Stephen Shrader[2]; Brian D Musselman[1]; *[1]IonSense, Inc. Saugus, MA; [2]Shrader Software Solutions, Inc, Grosse Pointe Park, MI*

TP 254 **Forensic Identification of Unknown Compounds in Human Urine Using Complimentary Software with High-Resolution Data and Theoretical Fragmentation Spectra**; Kristine Van Natta[1]; Marta Kozak[1]; Xiaolei Xie[1]; Mindy Gao[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

TP 255 **Rapid Screening of Methylamphetaminein Hair of Drug Addicts using DSA-TOF**; Baohua Shen[1]; Xianyi Zhuo[1]; Jingchao Lin[2]; Chengyuan Cai[2]; Lizhong Yang[2]; Yongming Xie[2]; *[1]Institue of Forensic Science, Ministry of Justice, Shanghai, China; [2]PerkinElmer Management (Shanghai) Co., Ltd, Shanghai, China*

TP 256 **High-throughput LDTD-MS/MS for Quantification of GHB in Hair, Urine and Saliva**; Annie-Claude Bolduc[1]; Réal Paquin[1]; Serge Auger[2]; Alex Birsan[2]; Jean Lacoursière[2]; Pierre Picard[2]; *[1]Université Laval, Quebec, Canada; [2]Phytronix Technologies, Inc. Quebec, Canada*

TP 257 **Tracking the Ages of Latent Fingerprints using Triacylglycerols as an Age Marker**; Kelly O'Neill[1]; Young Jin Lee[2]; *[1]Iowa State University, Ames, IA; [2]Iowa State University, Ames, Iowa*

TP 258 **Detection and Mapping of Proteomic Blood Signatures in Fingerprints for Forensic Analysis**; Lisa Deininger[1]; Ekta Patel[1]; Malcolm R Clench[1]; Vaughn Sears[2]; Chris Sammon[3]; Simona Francese[1]; *[1]Sheffield Hallam University, BMRC Sheffield, United Kingdom; [2]Centre for Applied Science and Technology, Home Office, St Albans, United Kingdom; [3]Sheffield Hallam University, MERI, Sheffield, United Kingdom*

TP 259 **Investigating Environmental Degradation of Trace Explosives with Thermal Desorption DART-MS**; Edward Sisco[1]; Marcela Najarro[1]; Jeffrey Lawrence[1]; Katherine Schilling[2]; *[1]NIST, Rockville, MD; [2]Defense Forensic Science Center, Gillem Enclave, GA*

TP 260 **Metallic Muzzle Discharge Gunshot Residue Analysis By Dart-TOF-MS**; Emily Lennert[1]; Candice Bridge[1]; *[1]National Center for Forensic Science, Orlando, FL*

TP 261 **Laser Ablation Sample Transfer with Vacuum Capture for Forensic Sampling**; Fabrizio Donnarumma[1]; Kermit K Murray[1]; *[1]Louisiana State University, Baton Rouge, LA*

TP 262 **Impact of Energetic Particles on Proteinaceous Specimens**; Christopher Rollman[1]; Mehdi Moini[1]; *[1]George Washington University, Washington, DC*

TP 263 **Species Identification using Bayesian Modeling and Mass Spectrometry**; Jennifer Teubl[1]; Heyi Yang[2]; Donald Siegel[2]; David Fenyo[3]; *[1]NYU Langone Medical Ctr, NY, NY; [2]Office of Chief Med Exam, New York, NY; [3]NYU Langone Medical Center, New York, NY*

TP 264 **Tackling the Sensitivity using an Improved Proteomics Methodology: from Cultural Heritage to Forensic Studies**; Fabrice Bray[1]; Stephanie Devassine[1]; Nicolas Garnier[2]; Christian Rolando[1]; Caroline Tokarski[1]; *[1]USR CNRS 3290 MSAP, Villeneuve d'Ascq, France; [2]SARL Laboratoire Nicolas Garnier, Vic le Comte, France*

TP 265 **In-Depth Analysis of Saliva N-glycans Found in Live Human and Corpse for the Discovery of Post-mortem Interval (PMI) Marker**; Bum Jin Kim[1, 2]; Dong-Gi Lee[3]; Jong-Soon Choi[1, 3]; Hyun Joo An[1, 2]; *[1]GRAST, Chungnam National University, Daejeon, Republic of Korea; [2]AGRS, Chungnam National University, Daejeon, Republic of Korea; [3]Division of Life Science, Korea Basic Science Institute, Daejeon, Republic of Korea*

TP 266 **Postmortem Identification of Metabolizer Type through CYP Quantification and Polymorphism Identification**; Brigitte Desharnais[1, 2]; Pascal Mireault[1]; Cameron D. Skinner[2]; *[1]Laboratoire de sciences judiciaires et de médecine légale, Montréal, QC; [2]Concordia University, Montreal, Canada*

TP 267 **Protein Profiling of Decedent Scalp Hair Segments Exhibiting a Post-Mortem Hair Root Band**; McKay B. Allred[1]; Brian A. Eckenrode[1]; Traci L. Carlson[1]; Jamie N. Fleming[1]; Nicholas R. Vercruysse[1]; Andrew W. Plotner[1]; Hilda S. Castillo[1]; Dawnie W. Steadman[2]; Lee M. Jantz[2]; Kathleen Hauther[2]; Jack Hietpas[1]; JoAnn Buscaglia[1]; Stephen D. Shaw[1]; Mehdi Moini[3]; Joseph Donfack[1]; *[1]FBI Laboratory, Quantico, VA; [2]University of Tennessee, Knoxville, TN; [3]George Washington University, Washington DC*

TP 268 **Quantification of Seven Nerve Agent Compounds by ESI and APCI-MSMS**; Kathleen Housman[1]; Jonathan Oyler[1]; *[1]USA Medical Research Institute of Chemical Defense, Aberdeen Proving Ground, MD*

TP 269 **Validation of a GC/MS/MS Method for the Analysis of Chemical Warfare Agents (CWAs)**; Thomas Rusek[1]; Benjamin L Oyler[2]; Jonathan Oyler[3]; *[1]USAMRICD, ABerdeen Proving Ground, MD; [2]U. Maryland, Baltimore, MD; [3]USAMRICD, Aberdeen Proving Ground, MD*

TP 270 **Rapid and Unambiguous Identification of Ricin in Complex Matrices using a High Throughput, Integrated Immunoaffinity, Proteolysis and Mass Spectrometry Approach**; Bao Quoc Tran[1]; Kathleen J. Housman[2]; Samir V. Deshpande[1]; James D. Wright[3]; Mary M. Wade[3]; Jonathan M Oyler[2]; Raymond F. Sullivan[3]; *[1]Science and Technology Corporation, Belcamp, MD - Maryland; [2]US Army Medical Research Institute for Chemical Defense, Aberdeen Proving Ground, MD - Maryland; [3]US Army Edgewood Chemical and Biological Center, Aberdeen Proving Ground, MD - Maryland*

TP 271 **DART-TOF-MS and ATR-FTIR Analysis of Silicone Based Personal Lubricants**; Lauren Harvey[1]; Candice Bridge[1]; *[1]National Center for Forensic Science, Orlando, FL*

TP 272 **Analytical Validation of a Portable, Ambient Sampling Mass Spectrometer for High Throughput, Forensic Evidence Screening**; Zachary E Lawton[1]; William L Fatigante[1]; Jamie R Wieland[2]; Michael C Gizzi[3]; Herbert Oberacher[4]; Christopher C Mulligan[1]; *[1]Department of Chemistry, Illinois State University, Normal, IL; [2]Department of Technology, Illinois State University, Normal, IL; [3]Department of Criminal Justice Sciences, Illinois State University, Normal, IL; [4]Institute of Legal Medicine, Innsbruck Medial University, Innsbruck, Austria*

TP 273 **Transportable GC/MS for the Rapid Detection and Identification of Suspected Drug Compounds in Field Operations**; Philip Tackett[1]; Mitch Wells[2]; *[1]FLIR Systems, Inc., West Lafayette, Indiana; [2]FLIR Systems, Inc., West Lafayette, IN*

TP 274 **Detection and On-Site Presumptive Testing of a Clandestine Drug Laboratory using a Portable Mass Spectrometer**; Ethan McBride[1]; Phillip Mach[1]; Kenneth C Wright[2]; Guido F Verbeck[1]; *[1]University of North Texas, Denton, TX; [2]Inficon, Syracuse, NY*

TP 275 **Portable MS Systems vs. the Daubert Standard: Anticipating the Admissibility of a New Technology for Forensic Investigation**; Angelica Traub[1]; Zachary E. Lawton[1]; Jamie R. Wieland[2]; Michael C. Gizzi[3]; Christopher C Mulligan[1]; *[1]Department of Chemistry, Illinois State University, Normal, IL; [2]Department of Technology, Illinois State University, Normal, IL; [3]Department of Criminal Justice Sciences, Illinois State University, Normal, IL*

TP 276 **Examining the Legality of using Ambient Sampling, Portable Mass Spectrometers in Criminal Justice Applications**; Alessandra Bruno[1]; Michael C Gizzi[2]; Jamie R Wieland[3]; Christopher C Mulligan[4]; *[1]Illinois State University, Normal, IL; [2]Department of Criminal Justice Sciences, Illinois State University, Normal, IL; [3]Department of Technology, Illinois State University, Normal, IL; [4]Department of Chemistry, Illinois State University, Normal, IL*

TP 277 **Chiral Separation and Quantitation of Cathinone Related Drugs by Gas chromatography Mass spectrometry**; Rashed Alrumaithi[1]; Mohammed Meetani[2]; Saif Eldin Khalil[3]; Khalid Alsumaiti[3]; *[1]Dubai Police, Dubai, Dubai; [2]United Arab Emirates University, Al Ain, United Arab Emirates.; [3]Dubai Police, Dubai, Dubai, United Arab Emirates.*

TP 278 **Improved Sensitivity for the Qualitative and Quantitative Analysis of Active Ricin by MALDI-TOF Mass Spectrometry**; Dongxia Wang[1]; Jakub Baudys[2]; John R Barr[2]; Suzanne R Kalb[2]; *[1]Centers of Disease Control and Prevention (CDC), Atlanta, GA; [2]Centers for Disease Control and Prevention, Atlanta, GA*

GLYCOPROTEINS
279 - 296

TP 279 **A SPEG coupled Mass Spec Approach for Understanding the Glycosylated and Sialylated Proteome of CHO Mutants**; Ozge Can[1, 2]; Deniz Baycin Hizal[3]; A. Emin Atik[2]; R. Serdar Alpan[2]; Sharon Krag[4]; Hui Zhang[5]; Michael Betenbaugh[6]; *[1]Acibadem University, Istanbul, Turkey; [2]Turgut Biotechnology Group, Istanbul, Turkey; [3]Johns Hopkins University, Baltimore, Maryland; [4]Johns Hopkins Bloomberg School of Public Health, Baltimore, MD; [5]Johns Hopkins University School of Medicine, Baltimore, MD; [6]Johns Hopkins University, Baltimore, MD*

TP 280 **Studying the Effect of Glycan and Peptide Backbone Structures on Kinetics of N-glycan Release by PNGase F with MRM Quantization**; Yining Huang[1]; Ron Orlando[2]; *[1]University of Georgia, CCRC, Athens, GA; [2]University of Georgia, CCRC Athens, GA*

TP 281 **Mass Spectrometry-based Quantitative Analysis for Decoding Site-specific Alteration of Sialo-glycoproteome in EGFR-subtype of Non-small Cell Lung Cancers**; Yi-Ju Chen[1]; Yu-Hsien Lin[2, 3]; Yu-Ju Chen[1]; *[1]Institute of Chemistry, Academia Sinica, Taipei City, Nankang; [2]Department of Chemistry, National Taiwan Normal University, Taipei, Taiwan (R.O.C.); [3]Institute of Chemistry, Academia Sinica, Taipei, Taiwan (R.O.C.)*

TP 282 **Features of N-Glycosylation of Immunoglobulins from Two Knockout Pig Models**; Emy Komatsu[1]; Marjorie Buist[1]; Paul Gabriel Lopez[1]; Apolline Salama[2]; David Sachs[3,

[4]; Cesare Galli[5, 6, 7]; Andrea Perota[5]; Sophie Conchon[8]; Jean-Paul Concordet[9]; Jean-Paul Judor[8]; Giovanna Lazzari[6, 7]; Jean-Paul Soulillou[8]; Helene Perreault[1]; *[1]University of Manitoba, Winnipeg, MB; [2]Xenothera, Nantes, France; [3]Massachusetts General Hospital, Boston, MA; [4]Harvard Medical School, Boston, MA; [5]Avantea Laboratorio Di Tecnologie Della Riproduzione, Cremona, Italy; [6]Fondazione Avantea, Cremona, Italy; [7]University of Bologna, Bologna, Italy; [8]Université de Nantes, Nantes, France; [9]Université de Paris-Descartes, Paris, France*

TP 283 **Uncovering Single Glycoprotein Signatures using a One-pot Dual Nanoprobe-based Mass Spectrometry Assay**; Mira Anne C. dela Rosa[1, 2, 3]; Wei-Chun Chen[3]; Yi-Ju Chen[3]; Rofeamor P. Obena[3]; Chih-Hsiang Chang[3]; Rey Y. Capangpangan[3]; Tung-Hung Su[4]; Chi-Ling Chen[4]; Pei-Jer Chen[4]; Yu-Ju Chen[3]; *[1]Department of Chemistry, National Taiwan University, Taipei, Taiwan (R.O.C.); [2]Nano Science and Technology Program, Taiwan International Graduate Program, Academia Sinica, Taipei, TAIWAN (R.O.C.); [3]Institute of Chemistry, Academia Sinica, Taipei, Taiwan (R.O.C.); [4]Graduate Institute of Clinical Medicine, College of Medicine, National Taiwan University, Taipei, Taiwan (R.O.C.)*

TP 284 **Serum N-Glycome and Glycoproteome Analysis for Oral Cancer Patients**; Chuan Fa Chang[1]; Shu-Jie Chang[1]; *[1]National Cheng Kung University, Tainan, TW*

TP 285 **The Comparison of N-glycomics of Membrane Protein with Proteins of Whole Cell Lysate of Breast Cancer Cell Lines**; Parvin Mirzaei[1]; Shiyue Zhou[1]; Rui Zhu[1]; Wenjing Peng[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, Texas*

TP 286 **Characterization of Site-specific N-glycopeptide Isoforms of Alpha-1-acid Glycoprotein from an Interlaboratory Study using LC-MS/MS**; Ju Yeon Lee[1]; Hyun Kyoung Lee[1, 2]; Gun Wook Park[1, 2]; Heeyoun Hwang[1]; Hoi Keun Jeong[1, 2]; Ki Na Yun[1, 3]; Eun Sun Ji[1, 4]; Kwang Hoe Kim[1, 2]; Jun Seok Kim[5]; Jong Won Kim[6]; Sung Ho Yun[7]; Chi-Won Choi[7]; Seung Il Kim[7]; Jong-Sun Lim[8]; Seul-Ki Jeong[8]; Young-Ki Paik[8]; Soo-Youn Lee[9, 10]; Jisook Park[11]; Su Yeon Kim[10]; Young-Jin Choi[1,2]; Yong-In Kim[12]; Jawon Seo[12]; Je-Yoel Cho[12]; Myoung Jin Oh[2]; Nari Seo[2]; Hyun Joo An[2]; Jin Young Kim[1]; Jong Shin Yoo[1, 2]; *[1]Korea Basic Science Institute, Cheongju-Si, Republic of Korea; [2]Chungnam National University, Daejeon, Republic of Korea; [3]Sogang University, Seoul, Republic of Korea; [4]Hannam University, Daejeon, Republic of Korea; [5]Korea Polytechnics, Gyeonggi, Republic of Korea; [6]Osong Medical Innovation Foundation, Cheongju, Republic of Korea; [7]Korea Basic Science Institute, Daejeon, Republic of Korea; [8]Yonsei University, Seoul, Republic of Korea; [9]Sungkyunkwan University, Seoul, Republic of Korea; [10]Samsung Medical Center, Seoul, Republic of Korea; [11]Samsung Biomedical Research Institute, Seoul, Republic of Korea; [12]Seoul National University, Seoul, Republic of Korea*

TP 287 **N-Glycoproteomic Characterization of Recombinant Human Cytomegalovirus Glycoprotein B using Multienzymatic Proteolysis Coupled to LC-MS/MS and CZE-MS/MS**; Nicolas Smargiasso[1]; Johann Far[1]; Catherine Navarre[2]; Gabriel Mazzucchelli[1]; Dominique Baiwir[1]; Marc Boutry[2]; Edwin De Pauw[1]; *[1]University of Liege, Liege, Belgium; [2]University of Louvain, Louvain-la-Neuve, Belgium*

TP 288 **Ultrasensitive Glycoproteomics pairing Liquid Phase Isoelectric Focusing and Data Independent LC-MS reveals Site Specific N-glycosylation Alterations in Gastric Adenocarcinoma**; Josh Smith[1]; Colin Clarke[1]; Stefan Mittermayr[1]; Jonathan Bones[1]; *[1]National Institute of Bioprocessing Research and Training (NIBRT), Dublin, Ireland*

TP 289 **Glycomic Profiling of Human Hyaluronidase 1**; Abby S Gelb[1]; Christine Booth[2]; Melanie A Simpson[2]; Eric D Dodds[2]; *[1]University of Nebraska-Lincoln, Lincoln , NE; [2]University of Nebraska-Lincoln, Lincoln, NE*

TP 290 **The Role of N-Glycosylation in Receptor Tyrosine Kinase (RTK) Signaling**; Kevin B Chandler[1]; Deborah R Leon[1]; Rosana D Meyer[1]; Nader Rahimi[1]; Catherine E Costello[1]; *[1]Boston University School of Medicine, Boston, MA*

TP 291 **MALDI-MS Characterization of Glycan Multivalency in Synthetic Glycan-Protein Conjugates**; Christopher C. Lai[1]; David Farnsworth[1]; Jeffrey C. Gildersleeve[1]; James A. Kelley[2]; *[1]CBL, CCR, NCI-Frederick, NIH, Frederick, MD - Maryland; [2]National Institutes of Health, Frederick, MD*

TP 292 **Glycoproteomic Analysis of HIV Latently Infected Cells and Plasma from Elite Suppressors Identify Important Glycoproteins in virus-host Interaction**; Weiming Yang[1]; Hui Zhang[1]; *[1]Johns Hopkins University School of Medicine, Baltimore, MD*

TP 293 **Revealing the Functions of Glycosylation Genes in Breast Cancer Cell Brain Metastasis with Gene Silencing Coupled to LC-MS/MS Glycomics**; Wenjing Peng[1]; Shiyue Zhou[1]; Xue Dong[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX*

TP 294 **Deciphering Glycomics and Neuroproteomic Alterations in Experimental TBI: Comparative Analysis of Aspirin and Clopidogrel Treatment**; Hisham Bahmad[1]; Rui Zhu[2]; Naify Ramadan[1]; Hussein Abou Abbass[1]; Shiyue Zhou[2]; Xue Dong[2]; Firas Kobeissy[1]; Yehia Mechref[2]; *[1]American University of Beirut, Beirut, Lebanon; [2]Texas Tech University, Lubbock, Texas*

TP 295 **Effect of Aspirin on Platelet Glycoproteins in Presence of Collagen**; Punit Shah[1]; Weiming Yang[1]; Shisheng Sun[1]; Faraday Naudeur[1]; Hui Zhang[1]; *[1]Johns Hopkins University School of Medicine, Baltimore, MD*

TP 296 **Comparative Transcriptomic and Proteomic Analysis of Productively HIV-1-infected and Bystander Monocyte-derived Macrophages during HIV-1 Infection of Uninfected Donors**; Isabel Martinez Ferrando; *Johns Hopkins University School of Medicine, Baltimore, MD*

HIGH MASS ACCURACY/HIGH PERFORMANCE MS METHODS & DEVELOPMENTS
297 - 312

TP 297 **Disulfide Linked Linear Peptides ANP, Insulin, ShK : Automatic Assignment of Exact-Mass ESI-MS/MS Fragment Ion Structures Using the MASSPEC Algorithm**; Marshall M. Siegel [1]; Gary Walker[2]; Serhiy Y Hnatyshyn[3]; Eugene Ciccimaro[3]; Asoka Ranasinghe[3]; *[1]MS Mass Spec Consultants, Fair Lawn , NJ; [2]MS Mass Spec Consultants, Fair Lawn, NJ; [3]Bristol-Myers Squibb, Princeton, NJ*

TP 298 **Optimisation of Two-Dimensional FT-ICR MS for IR-ECD**; Maria Van Agthoven[1]; Federico Floris[2]; Alice Lynch[2]; Christopher Wootton[2]; Lionel Chiron[3]; Mark P Barrow[2]; Marc-André Delsuc[4]; Christian Rolando[5]; Peter B O'Connor[2]; *[1]University of Warwick, Coventry, Midlands; [2]University of Warwick, Coventry, United Kingdom; [3]CASC4DE, Strasbourg, France; [4]IGBMC, Illkirch-Graffenstaden, France; [5]Université Lille 1, Sciences et Technologies Villeneuve d'Ascq, France*

TP 299 **Constructing High Resolution Consensus Spectra for a Peptide Tandem Mass Spectral Library**; Sergey L Sheetlin[1]; Yuri A Mirokhin[1]; Dmitrii V Tchekhovskoi[1]; Xiaoyu Yang[1]; Stephen E Stein[1]; *[1]NIST, Rockville, MD*

TP 300 **Mass Defect-based N,N-Dimethyl Leucine (DiLeu) Labels for quantitative Proteomics and Amine Metabolomics of Pancreatic Cancer Cells**; Ling Hao[1]; Jillian Johnson[2]; Chirstopher Lietz[2]; W.John Kao[2]; Lingjun li[2]; *[1]university of Wisconsin Madison, madison, WI; [2]University of Wisconsin-Madison, Madison, WI*

TP 301 **Using Simultaneous Waveform Averaging and Ion Counting Techniques to Expand the Quantitative Measurement Range in a Time-of-Flight Mass Spectrometer**; Toshinobu Hondo[1, 2]; Yuki Miyada[2]; Yosuke Kawai[3]; Kentaro Terada[3]; Michisato Toyoda[2, 4]; *[1]MS-Cheminformatics, Inabe-gun, Mie; [2]Project Research Center for Fundamental Sciences, Graduate School of Science, Osaka University, Osaka, Japan; [3]Department of Earth and Space Science, Graduate School of Science, Osaka University, Osaka, Japan; [4]Department of Physics, Graduate School of Science, Osaka University, Osaka, Japan*

TP 302 **Computer Modeling of Trapped-Ion Cell Capacitance for Optimization of Ion Image Charge Detection Mass Spectrometry**; Steven C Beu[1]; Nathan K Kaiser[2]; Donald F Smith[2]; Christopher L Hendrickson[2, 3]; *[1]S C Beu Consulting, Austin, TX; [2]Ion Cyclotron Resonance Program, National High Magnetic Field Laboratory, Tallahassee, FL; [3]Department of Chemistry and Biochemistry, Tallahassee, FL*

TP 303 **Static Harmonization of Dynamically Harmonized FT ICR Cell. High Order Contributions to the Electric Field**; Ekaterina Zhdanova[1, 2]; Gleb Vladimirov[2, 3]; Yury Kostyukevich[2, 3]; Eugene Nikolaev[2]; *[1]Moscow Institute of Physics and Technology, Dolgoprudny Moscow Oblast, Russia; [2]Institute for Energy Problems of Chemical Physics, Moscow, Russia; [3]Skolkovo Institute of Science and Technology, Skolkovo Moscow Oblast, Russia*

TP 304 **Setup and Application of Gas-phase APCI Coupled to Ultra-high Resolution Mass Spectrometry for Gas Chromatography and Thermal analysis**; Martin Sklorz[1]; Christopher Paul Rüger[1]; Theo Schwemer[1, 2]; Toni Miersch[1]; Thomas Arthen-Engeland[3]; Ralf Zimmermann[1, 2,4]; *[1]University of Rostock, Analytical Chemistry, Rostock, Germany; [2]HICE - Helmholtz Virtual Institute of Complex Molecular Systems in Environmental Health, Munich, Germany; [3]Bruker Daltonic GmbH, Bremen, Germany; [4]Helmholtz Zentrum München, Cooperation Group "Comprehensive Molecular Analytics", Munich, Germany*

TP 305 **Charge Ordered Parallel Ion aNalysis (CHOPIN) Mass Spectrometry Enhances Global Sequence Coverage, Deep Proteomics and PToMics**; Simon Davis[1]; Philip Charles[1]; Lin He[2]; Benedikt M Kessler[1]; Roman Fischer[1]; *[1]Oxford University, Oxford, United Kingdom; [2]Bioinformatics Solutions Inc., Waterloo, Canada*

TP 306 **Implementation of the All Ion Fragmentation Analysis for Targeted/Untargeted Metabolomic Approaches**; Enrique Sentandreu[1]; Shannon R Sweeney[1]; Jennifer Chiou[1]; Stefano Tiziani[1]; *[1]Dell Pediatric Research Institute, Austin, Tx*

TP 307 **Accurate FT-ICR MS with Fluctuating Ion Sources**; Konstantin O Nagornov[1]; Anton N Kozhinov[1]; Yury O Tsybin[1]; *[1]Spectroswiss Sàrl, Lausanne, Switzerland*

TP 308 **Characterization of a Modified Dynamically Harmonized FT-ICR Cell at High Magnetic Field**; Christopher L Hendrickson[1, 2]; Nathan K Kaiser[1]; Steven C Beu[3]; Greg T Blakney[1]; John P Quinn[1]; Donald J Smith[1]; Alan G Marshall[1, 2]; *[1]Ion Cyclotron Resonance Program, National High Magnetic Field Laboratory, Tallahassee, FL; [2]Department of Chemistry, Florida State University Tallahassee, FL; [3]S C Beu Consulting, Austin, TX*

TP 309 **Boosting FTMS Performance via Advanced Data Acquisition Electronics and Signal Processing**; Yury O Tsybin[1]; Konstantin O Nagornov[1]; Anton N Kozhinov[1]; *[1]Spectroswiss Sàrl, Lausanne, Switzerland*

TP 310 **Implementation of a High-performance FPGA-based Data Acquisition System for FTMS**; Anton Kozhinov[1]; Konstantin Nagornov[1]; Yury Tsybin[1]; *[1]Spectroswiss Sàrl, Lausanne, Switzerland*

TP 311 **Design of Automated Quantitative Optimization Software for Hi-Resolution Analysis**; Eugene F. Ciccimaro[1]; Asoka Ranasinghe[2]; Timothy Olah[2]; Richard Baran[3]; Mark Sanders[3]; Jonathan L Josephs[3]; *[1]Bristol-Myers Squibb, Princeton , NJ; [2]Bristol-Myers Squibb, Princeton, NJ; [3]Thermo Fisher Scientific, San Jose, CA*

TP 312 **9-plex Metabolic Labeling with NeuCode SILAC**; Katherine A Overmyer[1]; Elyse C Freiberger[1]; Stefka Tyanova[2]; Anna E Merrill[1]; William Wood[3]; Marwan Elmasri[3]; Alexander S Hebert[1]; Michael S Westphall[1]; Joel C Bradley[3]; Juergen H Cox[2]; Joshua J Coon[1]; *[1]University of Wisconsin Madison, Madison, WI; [2]Max Planck Institute of Biochemistry, Martinsried, DE; [3]Cambridge Isotope Laboratories, Inc. Tewksbury, MA*

IMAGING MS: DISEASE MARKERS
313 - 344

TP 313 **New Insights into the Microenvironment of Cancerous Tissue by Combined Mass Spectrometry, Microscopy and Multivariate Analysis**; Tina Angerer[1]; John Stephen Fletcher[1]; *[1]University of Gothenburg, Gothenburg, Sweden*

TP 314 **Typing of Colon and Lung Adenocarcinoma using High-throughput Imaging Mass Spectrometry**; Rita Casadonte[1]; Mark Kriegsmann[2]; Rémi Longuespée[1]; Petra Wandernoth[1, 3]; Cristina Mohanu[3]; Tiemo Katzenberger[4]; Daniela Aust[5]; Gustavo Baretton[5]; Jörg Kriegsmann[1, 3, 6]; *[1]Proteopath GmbH, Trier, Germany; [2]University of Heidelberg, Heidelberg, Germany; [3]Molekularpathologie Trier, Trier, Germany; [4]Department of Pathology, Hospital Aschaffenburg, Aschaffenburg, Germany; [5]University of Dresden, Dresden, Germany; [6]Center for Histology, Cytology and Molecular Diagnostics Trier, Trier, Germany*

TP 315 **Desorption Electrospray Ionisation Imaging towards Enhanced Breast Cancer Diagnosis**; Dipa Gurung[1]; James McKenzie[1]; Francesca Rosini[1]; Luisa Doria[1]; Anna Mroz[1]; Rathi Ramakrishnan[1]; Edward R St John[1]; Jeremy K Nicholson[1]; Zoltan Takats[1]; *[1]Imperial College London, South Kensington Campus London, United Kingdom*

TP 316 **MALDI-MS Imaging of Lipid Changes after PI3-K Inhibition in Colorectal Cancer Liver Metastases**; Fiona Henderson[1]; Irma Berrueta Razo[2]; Nicholas Lockyer[2]; Omar Belgacem[3]; Kaye J Williams[4]; Adam McMahon[1]; *[1]Wolfson Molecular Imaging Centre, University of Manchester, Manchester, England; [2]Manchester Institute of Biotechnology, University of Manchester, Manchester, England; [3]Shimadzu, Manchester, England; [4]Stopford Building, University of Manchester, Manchester, England*

TP 317 **Multimodal imaging of lipids in a Zebrafish Melanoma Model by PET and DESI-MS**; Emrys Jones[1]; Fiona Henderson[2]; Anthony Midey[3]; Adam Hurlstone[2]; Duncan Foster[2]; Hannah Johnston[2]; Kaye Williams[2]; Adam W McMahon[2]; Emmanuelle Claude[1]; *[1]Waters Corporation, Wilmslow, UK; [2]Wolfson Molecular Imaging Centre, Manchester, UK; [3]Waters Corporation, Beverly, Massachusetts*

TP 318 **Comparative Mapping of PSA and N-glycan Distributions in FFPE Prostate Cancer Tissues using MALDI-FTICR and Rapid MALDI-TOF Mass Spectrometry Imaging**; Richard R Drake[1]; Peggi M Angel[1]; Hendrik Jan Kobarg[2]; Shannon Cornett[3]; *[1]Medical University of South Carolina, Charleston, SC; [2]SCiLS GmbH, Bremen, Germany; [3]Bruker Daltonic, Billerica, MA*

TP 319 **Imaging Mass Spectrometry Approach for the Diagnosis of Carcinoma of the Cervix**; Rita Casadonte[1]; Rémi Longuespée[1]; Mark Kriegsmann[2]; Michael Becker[3]; Sören-Oliver Deininger[3]; Mike Otto[1]; Jörg Kriegsmann[1, 4]; *[1]Proteopath GmbH, Trier, Germany; [2]University of Heidelberg, Heidelberg, Germany; [3]Bruker Daltonik GmbH, Bremen, Germany; [4]Centre for Histology, Cytology and Molecular Diagnostics, Trier, Germany*

TP 320 **MALDI Imaging a Tool for Clinical Diagnostic – Classification of Prostate Cancer Subgroups**; Birte Beine[1]; Tobias Boskamp[2]; Dimo Dietrich[3]; Hendrik Jan Kobarg[4]; Konrad Steinestel[5]; Piotr Widlak[6]; Barbara Sitek[7]; Helmut Erich Meyer[8]; Corinna Henkel[8]; *[1]ISAS e.V., Dortmund, NRW; [2]Center for Industrial Mathematics, University of Bremen, Bremen, Germany; [3]Institute of Pathology, University Hospital Bonn (AöR), Bonn, Germany; [4]SCiLS GmbH, Bremen, Germany; [5]Gerhard-Domagk-Institute of Pathology, University Hospital Münster (UKM), Münster, Germany; [6]Center for Translational Research and Molecular Biology of Cancer, Maria Sklodowska - Curie Memorial Cancer Center and Institute of Oncology, Gliwice, Poland; [7]Medizinisches Proteom-Center, Ruhr-Universität Bochum, Bochum, Germany; [8]ISAS - e.V., Dortmund, Germany*

TP 321 **Molecular Markers of Serous Ovarian Cancer Aggressiveness and Surgical Outcome by Ambient Ionization Mass Spectrometry Imaging**; Marta Sans Escofet[1]; Kshipra Gharpure[2]; Jialing Zhang[1]; Jinsong Liu[2]; Anil K. Sood[2]; Livia S. Eberlin[1]; *[1]University of Texas at Austin, Austin, TX; [2]the University of Texas M.D Anderson Cancer Center, Houston, TX*

TP 322 **Linking Lipid Metabolism, Hypoxia, Radiation Therapy and Metastasis using DESI Imaging Mass Spectrometry**; Erik J. Soderblom[1]; Kathleen Ashcraft[2]; Matt W. Foster[3]; Emmanuelle Claude[4]; Emrys A Jones[4]; James Langridge[4]; M. Arthur Moseley[3]; Mark Dewhirst[2]; *[1]Proteomics and Metabolomics Shared Resource, Duke University School of Medicine, Durham , NC; [2]Radiation Oncology, Duke University Medical Center, Durham, NC; [3]Proteomics and Metabolomics Shared Resource, Duke University School of Medicine, Durham, NC; [4]Health Sciences, Waters Corp, Manchester, UK*

TP 323 **Elemental Analysis and Imaging of Stroke-affected Brain Tissues by Utilizing Laser Ablation-inductively Coupled Plasma-Mass Spectrometry: Diagnostic Study**; Khalid A. Al-Saad[1]; Mohamed H Ali[2]; MD Fazle Rakib[1]; Eman M Fayyad[1]; Rick Dijkhuizen[3]; Geralda V Tilborg[3]; *[1]Qatar University, Doha, Doha; [2]Qatar Biomedical Research Institute, Doha, Qatar; [3]University Medical Center Utrecht, Utrecht, Netherlands*

TP 324 **Molecular Signature Discovery of Human Chronic Traumatic Encephalopathy Tissues using Mass Spectrometry Imaging**; Bo Yan[1]; Dharmendra B. Goswami[1]; Deborah R Leon[1]; Mark E McComb[1]; Ann C. McKee[1, 2]; Catherine E Costello[1]; *[1]Boston University School of Medicine, Boston, MA; [2]United States Department of Veterans Affairs, VA Boston Healthcare System, Boston, MA*

TP 325 **MALDI Imaging of Neuronal Plasticity: Analysing Fine Adaptations with Large Effects**; Jakob Meier-Credo[1]; Michael Becker[2]; Alice Ly[2]; Shahar Or[1]; Irina Epstein[1]; Thomas Hagedorn[2]; Tamas Dalmay[1]; Johannes J Letzkus[1]; Erin Schuman[1]; Julian Langer[1]; *[1]Max-Planck-Institute for Brain Research, Frankfurt Am Main, Germany; [2]Bruker Daltonik GmbH, Bremen, Germany*

TP 326 **Nanoparticle Matrix Implantation Mass Spectrometry Imaging Discovers and Quantifies Lipid Biomarkers of Traumatic Brain Injury and Tracks Therapeutic Response**; Aurelie Roux[1]; Ludovic Muller[2]; Shelley N Jackson[2]; Jeremy Post; Katherine Baldwin[3]; Barry Hoffer[4]; Carey Balaban[5]; Damon Barbacci[6]; Albert J Schultz[7]; Shawn Gouty[8]; Brian M Cox[8]; Amina S Woods[9]; *[1]All Children's Hospital Johns Hopkins Medicine, Saint Petersburg, FL; [2]NIH/NIDA-IRP, Baltimore, MD; [3]Philadelphia College of Osteopathic Medicine, Philadelphia, PA; [4]University Hospitals of Cleveland, Cleveland, OH; [5]University of Pittsburgh, Pittsburgh, PA; [6]Ionwerks, Gaithersburg, MD; [7]Ionwerks Inc, Houston, TX; [8]Uniformed Services University, Bethesda, MD; [9]NIDA-IRP, NIH Baltimore, MD*

TP 327 **MALDI Mass Spectrometry Imaging in Alzheimer's disease mouse model Het CRND8 (+/-)**;Lyna Sellaml[1]; Marcia Roy[2]; Matthew E Openshaw[1]; Luis Mancera[1]; Omar Belgacem[1]; *[1]Shimadzu, Kratos Manchester, United Kingdom; [2]University of Edinburgh, Edinburgh, UK*

TP 328 **Simultaneous MALDI MS Imaging and Quantitation of Multiple Neurotransmitters In Parkinson's Disease Models**; Elva Fridjonsdottir[1]; Mohammadreza Shariatgorji[1]; Anna Nilsson[1]; Patrik Källback[1]; Xiaoqun Zhang[2]; Per Svenningsson[2]; Per E. Andren[3]; *[1]Uppsala University, Uppsala, Sweden; [2]Karolinska Institutet, Stockholm, Sweden; [3]Uppsala University, Uppsala, SE*

TP 329 **Detection of Ganglioside Lipid Species in the Brain of Mucopolysaccharidosis Type II Mouse by Imaging Mass Spectrometry**; Martin Dufresne[1]; Daniel Guneysu[1]; Martin Marcinkiewicz[2]; Anthony Regina[3]; Michel Demeule[3]; Pierre Chaurand[4]; *[1]Université de Montréal, St-Hyacinthe, QC; [2]Cytochem Inc., Montreal Quebec, Canada; [3]Angiochem Inc., Montréal, QC, Canada; [4]University of Montreal, Montreal, QC*

TP 330 **Studying the Sphingolipid Pathway into Co-morbidity of Depression and Alcoholism by MALDI Imaging FT-ICR Mass Spectrometry**; Christian P Muller[1]; Matthias Witt[2]; Michael L Easterling[3]; Jens Fuchser[2]; Beckmann Janine[2]; Thomas Stockl[1]; Eva Sprenger[1]; Jens Tiesel[1]; Sabine E Huber[1]; Davide Amato[1]; Erich Gulbins[4]; Martin Reichel[1]; Johanes Kornhuber[1]; *[1]Department of Psychiatry and Psychotherapy, Friedrich-Alexander-University of Erlangen-Nuremberg, Erlangen, Germany; [2]Bruker Daltonik GmbH, Bremen, Germany; [3]Bruker Daltonics, Billerica, MA; [4]Department of Molecular Biology, University of Duisburg-Essen, Essen, Germany*

TP 331 **Molecular Mapping of Gangliosides and Related Lipids using Mass Spectrometry Imaging with Ion Mobility Separation**; Bindesh Shrestha[1]; Hernando Olivos[2]; Khaja Muneeruddin[3]; Miguel Sena-Esteves[3]; Scott A Shaffer[3]; *[1]Waters Corp., Beverly, MA; [2]Waters Corporation, Beverly, MA; [3]University of Massachusetts Medical School, Worcester, MA*

TP 332 **Evaluating the Viability of Kidney Transplants using High-speed MALDI-Imaging**; Shane R Ellis[1]; Tim C van Smaalen[2]; Nadine E Mascini[1, 3]; Berta Cillero-Pastor[1]; Tiffany Porta[1]; Benjamin Balluff[1]; Carine J Peutz-Koostra[2]; L.W.E van Heurn[4]; Ron M A Heeren[1]; *[1]M4I, Maastricht University Maastricht, the Netherlands; [2]Maastricht UMC+, Maastricht, Netherlands; [3]FOM Institute AMOLF, Amsterdam, Netherlands; [4]University of Amsterdam, Amsterdam, The Netherlands*

TP 333 **Proteomic Mass Imaging of Kidney from Type 2 Diabetes (T2D) Rat Model**; Hirata Chie[1]; Kuzuhara Yuki[1]; Iwasaki Noriyuki[2]; Kudo Toshiji[2]; Nirasawa Takashi[2]; Masuyama Kei[3]; Kakuda Nobuto[1]; Wakazono Hiroshi[3]; Yanagi Hiroyuki[3]; Masaya Ikegawa[4]; *[1]Doshisha University, Kyotanabe, Japan; [2]Bruker Daltonics K.K., Kanagawa, Japan; [3]Ono Pharmaceutical Co., Ltd., Fukui, Japan; [4]Doshisha University, Kyotanabe City*

TP 334 **Differentiating Macrophages in Atherosclerotic Plaques using Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry Imaging**; Pegah Khamehgir-Silz[1]; Florian Schnitter[2]; Andreas H. Wagner[2]; Sabine Schulz[1]; Markus Hecker[2]; Bernhard Spengler[1]; *[1]Justus Liebig University, Giessen, Germany; [2]Ruprecht-Karls-University, Heidelberg, Germany*

TP 335 **What Can We Learn from the Na+/K+ Ratio in Imaging Mass Spectrometry Experiments?**; Roberto Fernandez[1]; Jone garate[1]; Sergio Lage[1]; Silvia Teres[2]; Pau Gonzalez[3]; Monica Higuera[4]; Alfredo Maqueda[3]; Joan Bestard-Escalas[5]; Daniel H Lopez[5]; Francisca guardiola-serrano[4]; Pablo V Escribá[4]; Javier Rodriguez[3]; Gwendolyn Barceló-Coblijn[5]; Jose A. Fernandez[6]; *[1]Universidad del Pais Vasco, Leioa,*

Spain; [2]Institut européen de chimie et biologie, Pessac, France; [3]National Hospital for Paraplegics, Toledo, Spain; [4]University of the Balearic Islands, Palma Balearic Islands, Spain; [5]Institut d'Investigació Sanitària de Palma, Palma Balearic Islands, Spain; [6]Universidad del Pais Vasco, leioa, Spain

TP 336 **Analysis of Retinal Degeneration in a Leber Congenital Amaurosis Mouse Model Using High Spatial Resolution MALDI-Imaging Mass Spectrometry**; David M. Anderson[1]; Zsolt Ablonczy[2]; Yiannis Koutalos[2]; Nico Verbeeck[3]; Raf Van De Plas[1, 3]; Jeffrey Spraggins[1]; Rosalie K. Crouch[2]; Richard M Caprioli[1]; Kevin L. Schey[1]; *[1]Vanderbilt University MSRC, Nashville, TN; [2]Department of Ophthalmology, Storm Eye Institute, Medical University of South, Charleston, SC; [3]Delft Center for Systems and Control (DCSC), Delft University of Technology, Delft, Netherlands*

TP 337 **Molecular Target Validation in Human Atherosclerosis Based on Mass Spectrometry Imaging and ImmunHistoChemistry Evaluation**; Jonathan Stauber[1]; Gregory Hamm[1]; Sylvia Aldi[2]; Juliette Masure[1]; Kim Holmstrom[3]; Serife Arda[4]; Danielle Van Keulen[5, 6]; David Bonnel[1]; Ivana Bobeldijk-Pastorova[5]; Dennie Tempel[6]; Boye S Nielsen[3]; Michael Gudo[4]; Jan NH Lindeman[7]; Ulf Hedin[2]; Alain van Gool[5]; Eva Hurt Camejo[8]; *[1]ImaBiotech, MS Imaging Dept. Loos, France; [2]Department of Molecular Medicine and Surgery, Karolinska Institutet, Stockholm, Sweden; [3]Bioneer, Hoersholm, Denmark; [4]Morphisto, Frankfurt Am Main, Germany; [5]TNO, Metabolic Health Research Leiden, The Netherland; [6]CardioGenx, Rotterdam, The Netherlands; [7]Leiden University Medical Centre, Leiden, The Netherlands; [8]AstraZeneca R&D, Gothenburg, Sweden*

TP 338 **Simultaneous Detection of N-glycans and Peptides from a Single FFPE Tissue Section by MALDI FT-ICR Imaging Mass Spectrometry**; Peggi Angel[1]; Rita Casadonte[2]; Jörg Kriegsmann[2]; Richard Drake[3]; *[1]Medical University of South Carolina, Charleston, SC; [2]Proteopath GmbH, Trier, Germany; [3]Medical Univ of S Carolina, Charleston, SC*

TP 339 **The Effect of Oxygen on the Lipid Composition of Human Chondrocytes using MALDI Imaging**; Brenda Bakker[1]; Gert Eijkel[2]; Ron Heeren[2]; Marcel Karperien[1]; Janine Post[1]; Berta Cillero-Pastor[2]; *[1]Developmental BioEngineering, University of Twente, Enschede, The Netherlands; [2]The Maastricht Multimodal Molecular Imaging Institute (M4I), Maastricht University, Maastricht, The Netherlands*

TP 340 **Metabolite Profiling of Intestinal Microbiota by Mass Spectrometry Imaging for Biological Understanding of Gastrointestinal Disease**; Gregory Hamm[1]; Juliette Masure[1]; Sylvain Normand[2]; David Bonnel[1]; Mathias Chamaillard[2]; Jonathan Stauber[1]; *[1]ImaBiotech, MS Imaging Dept. Loos, France; [2]Center of Infection and Immunity of Lille (CIIL), Team 7, Inserm U1019, CNRS UMR8204, Lille, France*

TP 341 **Differential Human Pancreatic Lipid and Protein Distributions in Normal and Type 1 Diabetes Revealed by Tissue Imaging Mass Spectrometry**; Boone M Prentice[1]; Rachana Haliyur[1]; Nathaniel J Hart[1]; Audra M Judd[1]; Radhika Aramandla[1]; Marcela Brissova[1]; Jeffrey M Spraggins[1]; Jeremy L Norris[1]; Alvin C Powers[1]; Richard M Caprioli[1]; *[1]Vanderbilt University, Nashville, TN*

TP 342 **Lipid and Metabolite Distribution in Healthy and Diseased Brain Tissue using DESI and High Resolution Mass Spectrometry**; Joseph H Kennedy[1]; Jeff Patrick[1]; Mariam ElNaggar[1]; Justin M Wiseman[1]; *[1]Prosolia, Inc. Indianapolis, IN*

TP 343 **Imaging Mass Spectrometry for the Pathological Studies of Cardiac Allografts**; Terada Megumi[1]; Iwasaki Noriyuki[2]; Kudo Toshiji[2]; Nirasawa Takashi[2]; Bruneval Prtrick[3]; Ishibashi-Ueda Hatsue[4]; Masaya Ikegawa[5]; *[1]Doshisha University, Graduate School of Brain Scie Kyoto, Japan; [2]Bruker Daltonics K.K., Kanagawa, Japan; [3]Georges Pompidou European Hospital, Paris, France; [4]National Cerebral and Cardiovascular Center, Osaka, Japan; [5]Doshisha University, Kyotanabe City*

TP 344 **High Spatial Resolution Lipid Imaging Offers Promising Perspectives in Sustaining Diagnosis of Human Lymphoma**; Yousef El Aalamat[1]; Arndt Asperger[2]; Xian Mao[1]; Wim Waelput[3]; Thomas Tousseyn[4]; Bart De Moor[1]; Etienne Waelkens[5]; *[1]ESAT-STADIUS / iMinds Medical IT, KU Leuven, Leuven, Belgium; [2]shared first author, Bruker Daltonik GmbH,, Bremen, Germany; [3]Dept. of Pathology, UZ-Brussel,, Brussel, Belgium; [4]Dept. Imaging and Pathology, KU Leuven,, Leuven,, Belgium; [5]Dept. Cellular and Molecular Medicine, KU Leuven, Leuven, Belgium*

IMAGING MS: PHARMACEUTICAL APPLICATIONS
345 - 363

TP 345 **Towards Absolute Quantitative MALDI MS Imaging of Drugs**; Patrik Kallback[1]; Theodosia Vallianatou[2]; Anna Nilsson[2]; Mohammadreza Shariatgorji[2]; Per E Andren[2]; *[1]Uppsala University, Uppsala, Uppsala; [2]Uppsala University, Uppsala, Sweden*

TP 346 **Derivatization Strategies for the Quantitation of Triamcinolone Acetonide in Cartilage by using Imaging Mass Spectrometry**; Florian Barré[1]; Bryn Flinders[1]; Joao Garcia[2]; Laura Creemers[2]; Ron M A Heeren[1]; Berta Cillero-Pastor[1]; *[1]M4I Institute - Maastricht University, Maastricht, The Netherlands; [2]Utrecht University, Utrecht, The Netherlands*

TP 347 **3D MALDI Mass Spectrometry Imaging to Empower Drug Distrubution And Quantitation Studies in Solid Tumors**; Silvia Giordano[1]; Lavinia Morosi[1]; Pietro Veglianese[1]; Simonetta Andrea Licandro[1]; Roberta Frapolli[1]; Massimo Zucchetti[1]; Maurizio D'Incalci[1]; Enrico Davoli[1]; *[1]IRCCS Istituto Mario Negri, Milano, Italy*

TP 348 **Study of the Blood Brain Barrier Permeability using a Multimodal Imaging Approach**; David Calligaris[1]; Fa-Ke Lu[1]; Armen Changelian[1]; Isaiah Norton[1]; Brett L Carlson[2]; Jeffrey Agar[3]; William F Elmquist[4]; Daniel MA[2]; Jann N Sarkaria[2]; Nathalie YR Agar[1]; *[1]Department of Neurosurgery, Brigham and Women's Hospital - Harvard Medical School, Boston, MA; [2]Mayo Clinic, Rochester, MN; [3]Barnett Institute of Chemical and Biological Analysis, Northeastern University, Boston, MA; [4]Department of Pharmaceutics, University of Minnesota, Minneapolis, MN*

TP 349 **Comparison of LESA-MS to MALDI-MS for Mouse Whole Body Tissue Profiling: Diclofenac and Major Metabolites**; Walter Korfmacher[1]; Gargey Yagnik[2]; Yongyi Luo[3]; Stacy Ho[2]; Liduo Shen[3]; Terry Wilper[4]; Karen Norton[4]; Eric Solon[5]; Hanlan Liu[2]; Sara Savage[4]; Thomas O'Shea[2]; *[1]Genzyme, Waltham, MA; [2]Genzyme, a Sanofi company Waltham, MA; [3]Sanofi, Waltham, MA; [4]Genzyme, Framingham, MA; [5]QPS, Newark, DE*

TP 350 **Matrix Assisted Laser Desorption/Ionisation Mass Spectrometry Imaging of Therapeutic Oligonucleotides: Application to Antisense Therapy**; C. Logan Mackay[1]; John G Swales[2]; Richard J A Goodwin[2]; *[1]SIRCAMS, Edinburgh, UK; [2]AstraZeneca, Cambridge, UK*

TP 351 **Microinjection and High-throughput Alignment of Cellular Spheroids for MALDI Mass Spectrometry Imaging Analysis**; Jillian Johnson[1]; Fengfei Ma[1]; Weiyuan John Kao[1]; Lingjun Li[1]; *[1]University of Wisconsin-Madison, Madison, WI*

TP 352 **Applications of Single-Probe Device for Ambient Mass Spectrometry Imaging Analysis: Human Corneas and 3D Artificial Tumors**; Xiang Tian[1]; Wei Rao[1]; Ning Pan[1]; Haiqing Yu[1]; Dimitrios Karamichos[2]; Zhibo Yang[1]; *[1]University*

of Oklahoma, Dept. of Chem & Biochem Norman, OK; [2]University of Oklahoma Health Science Center, OKC, OK

TP 353 **Application of Imaging Mass Spectrometry to Assess Ocular Drug Transit**; Kerri Grove[1]; Viral Kansara[2]; Melissa Prentiss[2]; Debby Long[2]; Muneto Mogi[2]; Sean Kim[2]; Patrick Rudewicz[1]; *[1]Novartis Institutes for BioMedical Research, Emeryville, CA; [2]Translational Clinical Oncology, Novartis Institutes for Biomedical Research, Cambridge, MA*

TP 354 **MALDI-FTICR Imaging of the Distribution of Teriflunomide in CNS Tissues in an Experimental Model of Multiple Sclerosis**; Ignacy Rzagalinski[1]; Carola Meier[1]; Nadine Hainz[1]; Thomas Tschernig[1]; Dietrich Volmer[1]; *[1]Saarland University, Saarbrücken, Germany*

TP 355 **Multimodal Mass Spectrometry Imaging for Detection and Early Prediction of Drug Induced Phospholipidosis**; Richard Goodwin[1]; Anna Nilsson[2]; Jennifer Barnes[1]; Julia Sampson[1]; Hui Zhang[3]; John G Swales[1]; Nicole strittmatter[4]; Alan Race[5]; Rory Steven[5]; Logan C Mackay[6]; Josephine Bunch[5]; Per E Andren[2]; *[1]AstraZeneca, Cambridge, UK; [2]Uppsala University, Uppsala, Sweden; [3]AstraZeneca R&D, Mölndal, Sweden; [4]AstraZeneca, Macclesfield, Select State; [5]National Physical Laboratory, Teddington, United Kingdom; [6]University of Edinburgh, Edinburgh, United Kingdom*

TP 356 **The Evaluation of Erythroblast Dynamics in Mice Bone Marrows by MALDI FTICR-MS Imaging which Identifies 57Fe-labeled Heme Isotopic Fine Structure**; Makoto Kihara[1]; Yukari Matsuo-Tezuka[2]; Keigo Yorozu[2]; Mitsue Kurasawa[2]; Hideyuki Yasuno[2]; Yasushi Shimonaka[2]; *[1]Chugai Pharmaceutical Co., Ltd, Kamakura, Japan; [2]Chugai Pharmaceutical Co., Ltd Kamakura, Japan*

TP 357 **Large Scale, Multi-Instrument MALDI-MSI Study into Lipidosis in Inhalation Dosed Rats**; Rory Thomas Steven[1]; Alan Race[1]; Aateka Patel[2]; Lea Ann Dailey[2]; Josephine Bunch[1, 3]; *[1]National Physical Laboratory, Teddington, UK; [2]King's College London, London, UK; [3]University of Nottingham, Nottingham, UK*

TP 358 **MALDI Imaging Mass Spectrometry of Platinum-Based Drugs in Multicellular Tumor Spheroids (MCTS) using Derivatization with Diethyldithiocarbamate (DDTC)**; Xin Liu[1]; Amanda B Hummon[1]; *[1]University of Notre Dame, Notre Dame, Indiana*

TP 359 **Visualization of Small Molecule and Nanoparticle Anticancer Agents in Tissue and Tumor Sections using IR-MALDESI Mass Spectrometry Imaging**; Mark Bokhart[1]; Allison Schorzman[2]; Andrew Lucas[2]; Michael Berens[3]; Harshil Dhruv[3]; William Zamboni[2]; David C Muddiman[1]; *[1]North Carolina State University, Raleigh, NC; [2]UNC - Chapel Hill, Chapel Hill, NC; [3]Translational Genomics Research Institute, Phoenix, AZ*

TP 360 **Tissue Distribution of Compound X and its Metabolites in Jck Mouse Polycystic Kidneys using Mass Spectrometry Imaging (MSI)**; Hanlan Liu[1]; Cristina Silvescu[1]; Mandy Cromwell[2]; Kelly Keefe[2]; Lindsay Quigley[2]; Sirimas Sudsakorn[1]; Sarah Nsereko[1]; Yang Guo[1]; Laurie Smith[3]; Thomas Natoli[3]; Dinesh Bangari[4]; Gregory Hamm[5]; Aurore Tomezyk[5]; Raphael Legouffe[5]; David Bonnel[5]; Jonathan Stauberand[5]; Thomas O'Shea[1]; *[1]Drug Metabolism and Pharmacokinetics, Sanofi, Waltham, MA; [2]Rare Disease Pharmacology, Sanofi, Waltham, MA; [3]Rare Renal Disease Research, Sanofi,, Framingham, MA; [4]Pathology, Sanofi, Framingham, MA; [5]ImaBiotech, MS Imaging Dept. Loos, France*

TP 361 **Visualizing Anti-Retroviral Distribution in Sheep and Human Vaginal Tissue by Imaging Mass Spectrometry**; Michelle Reyzer[1]; Mark Marzinke[2]; Trevelyn Olive[3]; Richard Pyles[3]; Kathleen L Vincent[3]; Manjula Gunawardana[4]; John Moss[4]; Marc M. Baum[4]; Richard M Caprioli[1]; *[1]Vanderbilt University, Nashville, TN; [2]Johns Hopkins University, Baltimore, MD; [3]University of Texas Medical Branch at Galveston, Galveston, TX; [4]Oak Crest Institute of Science, Monrovia, CA*

TP 362 **MALDI IMS in Drug Development: Shedding New Light on Toxicology**; M. Reid Groseclose[1]; Stephen Castellino[1]; *[1]GlaxoSmithKline, Upper Merion, PA*

TP 363 **Complementary Elemental And Molecular Mass Spectrometry Imaging to Investigate 5-aminolevulinic Acid, Protoporphyrin IX and Heme Distribution in Human Brain Tumor**; Sabrina Kröger[1]; Ann-Christin Niehoff[1]; Uwe Karst[1]; *[1]University of Münster, Institute of Inorganic and Analytical Chemistry, Münster*

INFORMATICS: PEPTIDE ID AND QUANTIFICATION
364 - 391

TP 364 **Resolving Complex Glycopeptide Fragmentation Tandem Mass Spectrum**; Aiying Yu[1]; Lauren Zacharias[1]; Rui Zhu[1]; Kerry Wooding[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, Texas*

TP 365 **Recycling Modification Site Information for Improved Glycopeptide Analysis**; Robert Chalkley[1]; Peter R Baker[1]; *[1]UCSF, San Francisco, CA*

TP 366 **Decoding Histone Post-translational Modifications by Bottom-up Mass Spectrometry**; Zuo-Fei Yuan[1]; Simone Sidoli[1]; Shu Lin[1]; Xiaoshi Wang[1]; Natarajan V Bhanu[1]; Benjamin A Garcia[1]; *[1]University of Pennsylvania, Philadelphia, PA*

TP 367 **Peak Annotation of High Resolution Spectra for Constructing Peptide Mass Spectral Libraries**; Xiaoyu Yang[1]; Pedatsur Neta[1]; Yuri Mirokhin[1]; Dmitrii Tchekhovskoi[1]; Yuxue Liang[1]; Zheng Zhang[1]; Sergey Sheetlin[1]; Sanford Markey[1]; Stephen Stein[1]; *[1]NIST, Gaithersburg MD*

TP 368 **A New Hope for Label Free Proteomics: moFF for Open-source, Platform-independent, Automated MS1 Intensity Extraction**; andrea argentini[1, 2, 3]; Kenneth Verheggen[1, 2, 3]; Lennart Martens[1, 2, 3]; *[1]Medical Biotechnology Center, VIB, Gent, Belgium; [2]Department of Biochemistry, Ghent University, Gent, Belgium; [3]Bioinformatics Institute Ghent, Ghent University, Gent, Belgium*

TP 369 **Interconversion of Peptide Spectral Libraries between iTRAQ and TMT Labels**; Zheng Zhang[1]; Xiaoyu Yang[1]; Yuri A Mirokhin[1]; Dmitrii V Tchekhovskoi[1]; Weihua Ji[1]; Sanford P Markey[1]; Jeri Roth[1]; Deniz BaycinHizal[2]; Michael Bowen[2]; Stephen E Stein[1]; *[1]NIST, Rockville, MD; [2]MedImmune, Gaithersburg, MD*

TP 370 **Employing Complementary Ions for Deconvolution of Mixture Tandem Mass Spectra**; Vladimir Gorshkov[1]; Stéphanie Yuki Kolbeck Hotta[1]; Thiago Verano-Braga[1, 2]; Frank Kjeldsen[1]; *[1]University of Southern Denmark, Odense, Denmark; [2]Federal University of Minas Gerais, Belo Horizonte, Brazil*

TP 371 **Combination of MS3/HCD and MS2/CID Improves Peptide IDs in Addition to Reducing the Precursor Interference of TMT-quantitation Experiment**; Wen Yu[1]; Raghothama Chaerkady[1]; Deniz Baycin-Hizal[1]; Mathew Woodward[2]; Michael A Bowen[1]; *[1]MedImmune, Gaithersburg, MD - Maryland; [2]MedImmune, Cambridge, UK*

TP 372 **The Benefits of Recycling – Protein Prospector: the Eco-Friendly Search Engine**; Peter R Baker[1]; Juan A Oses[2]; Robert J Chalkley[2]; *[1]UCSF, Rokietnica; [2]UCSF, San Francisco, CA*

TP 373 **Evaluating Software for Precursor Ion Chromatograms in Label-Free Data-Dependent Acquisition Sets through Differentiation, Quantification, and Clustering**; Yasset Perez-Riverol[1]; Chao Liu[2]; Bridget Calder[3]; Suereta Fortuin[3]; Alexander Giddey[3]; Birgit Schilling[4]; David Lee Tabb[5]; *[1]EMBL-EBI, Hinxton, UK; [2]Institute of Computing Technology, CAS Beijing, CHINA; [3]University of Cape Town, Cape Town, ZA; [4]Buck Institute for Research on Aging, Novato, CA; [5]Stellenbosch University, Liberty, MO*

TP 374 **Identification of Host Cell Protein Impurities using Spectral Libraries**; Meghan Burke[1]; Yuxue Liang[1]; Kelly H. Telu[1]; Jenny Heidbrink Thompson[2]; Chris Larkin[2]; Stephen Stein[1]; *[1]National Institute of Standards and Technology, Gaithersburg, MD; [2]MedImmune, Gaithersburg, MD*

TP 375 **Negative Electron Transfer Dissociation Fragmentation in a Full-Featured Proteomics Search Engine**; Yong J Kil[1]; Wilfred Tang[2]; Nicholas M Riley[3]; Michael S Westphall[3]; Joshua J Coon[3]; Marshall W. Bern[2]; *[1]Protein Metrics, San Carlos, CA; [2]Protein Metrics, Palo Alto, CA; [3]University of Wisconsin Madison, Madison, Wisconsin*

TP 376 **Fast and Comprehensive Peptide Identifications through Index-based Database Search**; Andy Kong[1]; Felipe de Veiga Leprevost[1]; Alexey I Nesvizhskii[1]; *[1]University of Michigan, Ann Arbor, MI*

TP 377 **A Graph-Centric Approach for Metagenome-Guided Peptide Identification in Metaproteomics**; Sujun Li[1]; Yuzhen Ye[1]; Haixu Tang[1]; *[1]Indiana University, Bloomington, IN*

TP 378 **Large Scale Silac Based Quantitative Analysis of Electron Accepter Stressed Azospira Suillum PS using Retention and Drift Time Profiling**; Anthony T Iavarone[1]; Matthew D Youngblut[1]; Emilie Gios[1]; Michael Daly[2]; Hans K Carlson[1]; Ulla N Andersen[1]; Johannes PC Vissers[3]; John D Coates[1]; *[1]UC Berkeley, Berkeley, California; [2]Waters, Inc. Pleasanton, CA; [3]Waters, Wilmslow, United Kingdom*

TP 379 **PGA: an R Package for Identification of Novel Peptides by Customized Database Derived from RNA-Seq**; Bo Wen[1]; Shaohang Xu[1]; Ruo Zhou[1]; Bing Zhang[2]; Wang Xiaojing[2]; Xin Liu[1]; Xun Xu[1]; Siqi Liu[1]; *[1]BGI-Shenzhen, Shenzhen, China; [2]Vanderbilt University School of Medicine, Nashville, TN*

TP 380 **The SysteMHC Atlas Project: toward a First Mass Spectrometry-based Draft of the Human Immunopeptidome**; Witold Wolski[1]; Etienne Caron[2]; Heiko Schuster; Michal Bassani-Sternberg[3]; Lorenz Blum[4]; Christian Panse[5]; Ruedi Aebersold[2]; Ralph Schlapbach[5]; *[1]FGCZ ETH Zurich, Zürich, Not US or Canada; [2]Institute of Molecular Systems Biology ETH Zurich, Zurich, Switzerland; [3]UNIL/CHUV Ludwig Cancer Research Center Lausanne, Switzerland, Lausanne, Switzerland; [4]ETH Zurich, Zürich, Switzerland; [5]FGCZ, Univ Zurich Zurich, Switzerland*

TP 381 **An Approach to Explore Millions of Unidentified MS/MS Peptide Features with Network Modeling and Its Implication for In-depth Proteomics**; Paul E Abraham[1]; John C Cushman[2]; Daniel Jacobson[1]; Robert L Hettich[1]; Richard J Giannone[1]; *[1]Oak Ridge National Laboratory, Oak Ridge, TN; [2]University of Nevada, Reno, Reno, NV*

TP 382 **Should We Care about Peptide Co-elution?** ; Jamie Sherman[1]; Stephen Tate[1]; *[1]SCIEX, Concord ON, Canada*

TP 383 **Solving the "no-enzyme" Problem in MHC-peptide immuno-precipitation Database Searches**; Patrick Murphy[1]; Konda Prathyusha[1]; Clements Derek[1]; Heiko Schuster[2]; Daniel Kowalewski[2]; Brian Erickson[3]; Joao Paulo[3]; Alejandro Cohen[4]; Steven P Gygi[3]; Stefan Stevanovic[2]; Shashi Gujar[1]; Patrick Lee[1]; *[1]Dalhousie University Dept of Microbiology and Immunology, Halifax, Canada; [2]University of Tuebingen, Tuebingen, Germany; [3]Harvard Medical School, Boston, MA; [4]Dalhousie University, Department of Chemistry Halifax, Canada*

TP 384 **New Calibration and Absolute Quantification Features in Skyline**; Nicholas Shulman[1]; Clark Henderson[1]; Birgit Schilling[2]; Will J Thompson[3]; Christopher M Shuford[4]; Andy Hoofnagle[1]; Michael J MacCoss[1]; Brendan MacLean[1]; *[1]University of Washington, Seattle, WA; [2]Buck Institute for Research on Aging, Novato, CA; [3]Duke University, Durham, NC; [4]Center for Esoteric Testing, Burlington, NC*

TP 385 ***De novo* Sequencing of Peptides from High-resolution Bottom-up Tandem Mass Spectra using Top-down Intended Methods**; Kira Vyatkina[1, 2]; Lennard J.M. Dekker[3]; Si Wu[4]; Martijn M. Vanduijn[3]; Xiaowen Liu[5, 6]; Nikola Tolic[7]; Theo M. Luider[3]; Ljiljana Pasa-Tolic[7]; Pavel A. Pevzner[8]; *[1]Saint Petersburg State University, St Peterburg, Russian Federation; [2]Saint Petersburg Academic University, St Petersburg, Russia; [3]Erasmus Medical Center, Rotterdam, The Netherlands; [4]University of Oklahoma, Dept. of Chem & Biochem Norman, OK; [5]Indiana University-Purdue University Indianapolis, Indianapolis, IN; [6]Indiana University School of Medicine, Indianapolis, IN; [7]Pacific Northwest National Laboratory - PNNL, Richland, WA; [8]University of California, San Diego La Jolla, CA*

TP 386 **Advanced XIC-based Label-free Algorithm for High-Resolution Data**; Sung Kyu Robin Park[1]; Rohan Rampuria[2]; Khatereh Motamedchaboki[3]; Jolene Diedrich[2]; Claire Delahunty[2]; John R Yates[2]; *[1]The Scripps Research Institute, San Diego, CA; [2]The Scripps Research Institute, La Jolla, CA; [3]Sanford-Burnham Medical Research Institute, La Jolla, CA*

TP 387 **Pros and Cons of Large Scale MS/MS Clustering - Are We There Yet?**; Benjamin Pullman[1, 2]; Nuno Bandeira[1, 2, 3]; *[1]Center for Computational Mass Spectrometry, University of California San Diego, La Jolla, CA; [2]Computer Science and Engineering, University of California San Diego, La Jolla, CA; [3]Skaggs School of Pharmacy, UC San Diego La Jolla, CA*

TP 388 **Combining RNA-Seq Proteogenomics and Global Post-Translational Modification (G-PTM) Search Strategy to Reveal Human Proteomic Variation**; Anthony J Cesnik[1]; Michael R Shortreed[1]; Gloria M Sheynkman[1]; Brian L Frey[1]; Lloyd M Smith[1]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, WI*

TP 389 **A New Database Format to More Closely Examine Protein Splice Forms**; Aparna Nathan[1]; Waltraud Mair[1]; Jan Muntel[1]; Hendrik Wesseling[1]; Judith Steen[1]; Hanno Steen[1]; *[1]Boston Children's Hospital, Boston, MA*

TP 390 **Challenges and Solutions When using OpenMS LFQProfiler Node in Proteome Discoverer 2.1 for Feature Comparison in Very Large Datasets**; Jana Moerbe Rocker[1]; Lindsay Schambeau[1]; Lewis K Pannell[1]; *[1]University of South Alabama, Mobile, AL*

TP 391 **New Method for Label-free Quantification in the Proteome Discoverer Framework**; David Horn[1]; Torsten Ueckert[2]; Kai Fritzemeier[2]; Carmen Paschke[2]; Katja Tham[2]; Hans Pfaff[2]; Xiaoyue Jiang[3]; Joseph Brown[3]; Iman Mohtashemi[1]; Daniel Lopez Ferrer[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Bremen, DE; [3]Thermo Fisher Scientific, San Jose, CA*

INSTRUMENTATION: GENERAL
392 - 416

TP 392 **Control Software for a Spatially Multiplexed Ion Mobility-Mass Spectrometer**; Babatunde H. Bello[1, 2]; Katrina L. Leaptrot[2, 3]; Jody C. May[2]; John A. McLean[2, 3]; *[1]Department of Mechanical Engineering, Vanderbilt University, Nashville, TN; [2]Department of Chemistry, Vanderbilt University, Nashville, TN; [3]VIIBRE, Vanderbilt University, Nashville, TN*

TP 393 **Real-Time Instrument Control of the Orbitrap Tribrid Mass Spectrometer**; Derek J Bailey[1]; Florian Grosse-Coosmann[2]; Manish Doshi[1]; Qingyu Song[1]; Jesse D Canterbury[1]; Qiming Wan[1]; Michael Senko[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Bremen, DE*

TP 394 **High-Sensitive MCP-based Ion Detector for Time of Flight Mass Spectrometry using Triode Structure**; Masahiro Hayashi[1]; Tetsuya Matsushita[1]; Joji Sakakiyama[1]; Akio Suzuki[1]; Toshiyuki Uchiyama[1]; Yasuhide Naito[2];

[1]Hamamatsu Photonics K.K., Iwata, Japan; [2]GPI, Hamamatsu, Japan

TP 395 **Improved Detection Efficiency of a High Dynamic Range Pulse Counting Detection System**; Bruce Collings[1]; Martian Dima[1]; Pascal Martin[1]; Stephen Bruce Locke[1]; *[1]SCIEX, Concord, ON*

TP 396 **Highly Charge-sensitive Device to Enhance the Direct Detection of Molecular Ions**; Szu-Wei Chou[1]; Yao-Hsin Tseng[1]; Liang-Chun Fan[1]; Yi-Kun Lee[1]; Chun-Yen Cheng[1]; *[1]AcroMass Technologies, Inc. Taipei, Taiwan*

TP 397 **A New Method for Measuring Detector Operating Life Performance**; Toby Shanley[1]; Clifton Chey[1]; Russell Jurek[1]; Kevin L Hunter[1]; Peter Raffin[1]; Daen Ekers[1]; Wayne Sheils[1]; *[1]ETP Ion Detect, Clyde, Australia*

TP 398 **A Method for Controlling Collective Electron Motion in Ion Detectors by Locally Manipulating Magnetic Fields**; Toby Shanley[1]; Russell Jurek[1]; Yair Benari[1]; Dick Stresau[1]; Kevin L Hunter[1]; *[1]ETP Electron Multipliers, Clyde, Australia*

TP 399 **Combined Fast Mode and Polarity Switching for Analysis of a Range of Vitamins and Nutritional Supplements in a Single Injection**; Lisa Cousins[1]; Heather Gamble[1]; Charles Joliffe[1]; Joshua Ye[1]; Jason Cournoyer[2]; *[1]Ionics, Bolton, Canada; [2]PerkinElmer, Waltham, MA*

TP 400 **Evaluation of RF-phase during Photoionization on the Trapping and Ejection of Ions from a 3D Ion Trap**; Laura Bailey[1]; Matthew R. Bell[1]; Nicolas C Polfer[1]; *[1]University of Florida, Gainesville, FL*

TP 401 **Implementation of Ultraviolet Photodissociation using Light Emitting Diodes (LEDs) in an Ion Trap**; Dustin D Holden[1]; Alexander Makarov[2]; Jae C Schwartz[3]; James D Sanders[1]; Eugene Zhuk[3]; Jennifer S Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX; [2]Thermo Fisher Scientific, Bremen, DE; [3]Thermo Fisher Scientific, San Jose, CA*

TP 402 **Improving the Performance of a Wysocki SID Cell for Synapt HDMS**; Mehdi Shirzadeh[1]; David H Russell[1]; *[1]Texas A&M, College Station, TX*

TP 403 **ECD Analysis of Serine Phosphorylated Peptides using EMS Cell**; Valery G. Voinov[1]; Yury V Vasil'ev[1]; Douglas F Barofsky[2]; Joseph Beckman[1]; *[1]Linus Pauling Institute, Oregon State University Corvallis, OR; [2]Oregon State University, Department of Chemistry Corvallis, OR*

TP 404 **Up Front CID in a Laminar Flow Ion Guide for Performance Enhancement in Biological Samples**; Charles Joliffe[1]; Shah Joshua Ye[1]; Heather Gamble[1]; Devanand Pinto[2]; Andrew Leslie[2]; *[1]Ionics, Bolton, Canada; [2]National Research Council of Canada, Halifax, Canada*

TP 405 **Design and Modeling of a Long Distance Low Vacuum Ion Transfer System**; Roman Levin[1, 2]; Evgeny Zhvansky[1,2]; Vasily Eliferov[1, 3]; Igor Popov[1, 2]; Alexey Boldyrev[2]; Gleb Vladimirov[2]; Eugene Nikolaev[2]; *[1]Moscow Institute of Physics and Technology, Dolgoprudny Moscow Oblast, Russia; [2]Institute for Energy Problems of Chemical Physics, Moscow, Russia; [3]Institute for Energy Problems of Chemical Physics, Moscow, Russian Federation*

TP 406 **Efficient Ion Transmission and Desolvation Enabled by Vorticial Flow in DRy Ion Localization and Locomotion (DRILL) MS interface**; Jung Lee[1]; Peter Kottke[1]; Elizabeth S Hecht[2]; David C Muddiman[2]; Nagender Panyala[1]; Matthew Torres[1]; Andrei Fedorov[1]; *[1]Georgia Institute of Technology, Atlanta, GA; [2]NC State University, Raleigh, NC*

TP 407 **A Mass Selective Transfer Line for Injecting Ions in a Uniform Supersonic Flow**; Baptiste Joalland[1]; Ludovic Biennier[1]; Sophie Carles[1]; Alexander Lekkas[2]; Dimitris Papanastasiou[2]; Emmanuel Raptakis[2]; *[1]Institut de Physique de Rennes, CNRS - Université de Rennes 1, Rennes, FR; [2]Fasmatech, Athens, Greece*

TP 408 **Ion Transport through Zirconia Capillaries**; J. A. Jarrell; *Waters Corporation, Milford, MA*

TP 409 **Development of Ultra-High Resolution Biological Target Characterization Mass Spectrometry Instrumentation**; Raul Villacob[1]; Paolo Benigni[1]; Francisco Fernandez-Lima[1]; *[1]Florida International University, Miami, FL*

TP 410 **Coupling Raman Spectroscopy with Laser Desorption-Atmospheric Pressure Chemical Ionization/Mass Spectrometry (LD-APCI/MS) for Polymer Analysis**; Yen-Ting Chen[1]; Siou-Sian Jhang[1]; Jentaie Shiea [1]; *[1]National Sun Yat- Sen University, Kaohsiung, Taiwan*

TP 411 **Thermogravimetric Analyzer Coupled with Atmospheric Pressure Chemical Ionization/Mass Spectrometry (TGA-APCI/MS) to Characterize Polymers in Biodegradable Plastics Materials**; Yao Sheng Zhang[1]; Sheng Hui Chiu[1]; Ming Chen[1]; Siou Sian Jhang[1]; Jentaie Shiea[1]; *[1]National Sun Yat- Sen University, Kaohsiung, Taiwan*

TP 412 **Fully Automated Analysis Platform for the Routine Determination of Immunosuppressants in Whole Blood**; Davide Vecchietti[1]; Maura Brambilla[2]; Daisuke Kawakami[3]; Taku Tsukamoto[3]; Paolo Brambilla[2]; *[1]Shimadzu, Milan, Lombardy; [2]Desio Hospital, Toxicology and Mass spectrometry department, Desio, Italy; [3]Shimadzu Corporation, Kyoto, Japan*

TP 413 **Automated Bottom-up Proteomics Workflow for Liquid AP-MALDI MS/MS Utilising Multiply Charged Ions**; Pavel Ryumin[1]; Jeff Brown[1, 2]; Michael Morris[2]; Rainer Cramer[1]; *[1]University of Reading, Reading, United Kingdom; [2]Waters, Wilmslow, United Kingdom*

TP 414 **A New Conjoined RF Ion Guide for High Efficiency Ion Transmission**; Daniel Kenny[1]; David Gordon[1]; Kevin Giles[1]; *[1]Waters, Wilmslow, United Kingdom*

TP 415 **Performance Monitoring and Quadrupole Maintenance of a First Generation Q Exactive Orbitrap in a Core Facility Setting**; John Leszyk[1]; Scott A Shaffer[1]; *[1]UMass Medical School, Shrewsbury, MA*

TP 416 **Building a Next-Generation Platform for Electron-ion Optics Simulations**; Russell Jurek[1, 2]; Kevin L Hunter[3]; *[1]ETP Ion Detect, Clyde, Australia; [2]ETP Ion Detect, Clyde, Australia; [3]ETP Ion Detect, Clyde, Australia*

INSTRUMENTATION: NEW DEVELOPMENTS IN MASS ANALYZERS
417 - 442

TP 417 **Development and Characterization of an FT-QIT with *in situ* Electron Ionization for Residual and Trace Gas Analysis**; Yessica Brachthaeuser[1]; David Mueller[1]; Hendrik Kersten[1]; Klaus Brockmann[1]; Thorsten Benter[1]; Valerie Derpmann[2]; Alexander Laue[2]; Ruediger Reuter[2]; Michel Aliman[2]; *[1]Bergische Universität Wuppertal, Wuppertal, Germany; [2]Carl Zeiss SMT GmbH, Oberkochen, Germany*

TP 418 **Study of Directional Ion Ejection in an Asymmetric Half-Round Rod Electrode Linear Ion Trap Mass Analyzer**; Zhang Zaiyue[1]; Yuan Guangzhou[1]; Qian Jie[1]; He Yang[1]; Yao Rujiao[1]; Zhang Shuguang[1]; Xiaoxu Li[1]; *[1]Soochow University, Suzhou, China*

TP 419 **Optimization of the Mesh-electrode Linear Ion Trap Performance by Simulations**; Qiankun Dang[1]; Gary Glish[2]; Chuan-Fan Ding[3]; *[1]Fudan University, Shanghai, Shanghai; [2]University of North Carolina at Chapel Hill, Chapel Hill, NC; [3]Fudan University, Shanghai, China*

TP 420 **Improvement of Mass Resolution,Collision Induced Dissociation Efficiency and Low Mass Cutoff by Octopole Field in Linear Ion Trap Mass Analyzer**; Chuan-Fan Ding[1]; Fuxing Xu[2]; Xinhua Dai[3]; Xiang Fang[3]; *[1]Fudan University, Shanghai; [2]Fudan University, Shanghai, China; [3]National Institute of Metrology, Beijing, China*

TP 421 **Design and Analytical Performance Evaluation of a Cooling Cell for a Quadrupole Mass Spectrometer with Enhanced Resolution and Sensitivity**; Tsung-Chi Chen[1]; Philip M Remes[1]; Raman Mathur[1]; Paul H Gregory[1];

Pascual Cardenas[1]; Rexford T Heller[1]; Qingyu Song[1]; Viatcheslav V Kovtoun[1]; Satendra Prasad[1]; Hoa D Truong[1]; Eloy R Wouters[1]; Hans Schweingruber[1]; Eric C Hemenway[1]; Jae C Schwartz[1]; Terry N Olney[1]; Alan E Schoen[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

TP 422 **Effects of Hexapole Electric Fields on the Performance of Linear Ion Trap Mass Analyzer**; Fuxing Xu[1]; Xinhua Dai[2]; Xiang Fang[2]; Yuanyuan Wang[1]; Chuan-fan Ding[1]; *[1]Fudan University, Shanghai, China; [2]National Institute of Metrology,, Beijing, China*

TP 423 **Reducing Space Charge Effects in a Linear Ion Trap by Rhombic Ion Excitation and Ejection**; Lili Hu[1]; Xiaohua Zhang[2]; Yuzhuo Wang[3]; Dan Guo[1]; Wei Xu[1]; *[1]Beijing Institute of Technology, Beijing, China; [2]Fudan University, Shanghai, China; [3]National Institute of Metrology, Beijing, China*

TP 424 **Ion Collision Cross Section Analyses in Quadrupole Ion Traps using Filter Diagonalization Method:A Theoretical Study**; Ting Jiang[1]; He Muyi[1]; Guo Dan[1]; Zhai Yanbing[1]; Xu Wei[1]; *[1]Beijing Institute of Technology, Beijing, China*

TP 425 **Ion Trap Fourier Transform Mass Spectrometer with Induced Current Detection and Arbitrary Storage Waveforms**; Michael W Schmidt[1]; Albrecht Brockhaus[1]; Stefan Butzmann[1]; Michel Aliman[2]; Alexander Laue[2]; *[1]University of Wuppertal, Wuppertal, Germany; [2]Carl Zeiss SMT GmbH, Oberkochen, Germany*

TP 426 **Improved Performance of Ion Trap Mass Spectrometer with Added Octopole and Dodecapole Fields**; Junichi Taniguchi; *Shimadzu Corp., Soraku-gun, Kyoto*

TP 427 **Demonstration of using Isolation Waveform for Beam Type Selected-Reaction-Monitoring on a QqLIT Mass Spectrometer**; Qingyu Song[1]; Jae C Schwartz[1]; Philip M Remes[1]; Dumitresu Dean[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

TP 428 **Advancements in Multi Reflecting High Resolution TOF Mass Spectrometry with Folded Flight Path**; Viatcheslav Artaev[1]; Michael Mason[1]; Peter A Willis[1]; George Tikhonov[1]; Yury Khasin[2]; Anatoly Verenchikov[2]; *[1]LECO Corporation, St Joseph, MI; [2]MSC-CG, Bar, Montenegro*

TP 429 **A Study of Ion Acceleration in tightly Curved Collision Cells**; Felician Muntean[1]; Desmond A Kaplan[1]; *[1]Bruker Daltonics, Inc., Billerica, MA*

TP 430 **Performance of the Orbitrap Fusion Lumos Tribrid in Single-shot Analyses of Human Samples**; Guadalupe Espadas[1, 2]; Eva Borràs[1, 2]; Cristina Chiva[1, 2]; Eduard Sabidó[1, 2]; *[1]Proteomics Unit, Center for Genomic Regulation, Barcelona, Spain; [2]Proteomics Unit, Universitat Pompeu Fabra, Barcelona, Spain*

TP 431 **NTOF Geometry for QqTOF**; Bill Loyd[1]; Robert E. Haufler[2]; *[1]SCIEX, Concord, ON; [2]AB Sciex, Concord, ON*

TP 432 **Optimization of the Performance of Toroidal Ion Trap by Theoretical Simulation**; Haiyang yang[1]; Chengsheng Xu[2]; Chuan-Fan Ding[2]; *[1]Fudan University, Shanghai; [2]Fudan University, Shanghai, China*

TP 433 **A Mathematical and Simulation Study of General Toroidal Ion Trap Mass Spectrometer Devices**; Robert H Jackson[1]; Steve Lammert[2]; Daniel Austin[3]; Karl Warnick[3]; Jessica HIggs[3]; Edgar Lee[2]; *[1]Instrumental Design Physics, LLC, Littleton, MA; [2]PerkinElmer, Inc., American Fork, UT; [3]Brigham Young University, Provo, UT*

TP 434 **Radio Frequency Trapping of Ions in a Pure Toroidal Potential Distribution**; Jessica Higgs[1]; Brae V. Petersen[1]; Steven A. Lammert[2]; Karl F. Warnick[1]; Daniel E. Austin[1]; *[1]Brigham Young University, Provo, UT; [2]PerkinElmer, American Fork, UT*

TP 435 **Simulation of Ion Motion in Non-Ideal Electric Fields Generated by Novel FTICR Mass Analyzers**; Joshua Driver[1]; Andriy Kharchenko[1]; Jon Amster[1]; *[1]Univ of Georgia, Athens, GA*

TP 436 **Cross-field Drift of Ions and Non-Linear ICR Cell Arrays**; Sung-Gun Park[1]; Gordon Anderson[2]; James Bruce[1]; *[1]University of Washington, Seattle, WA; [2]GAA Custom Engineering, LLC, Benton, WA*

TP 437 **Moving Practical Mass Spectrometry Beyond the Molecular Realm**; Roland Jertz[1]; Claudia Kriete[1]; Matthias Witt[1]; Jochen Friedrich[1]; Christopher Thompson[2]; Michael L Easterling[3]; Eugene N Nikolaev[4]; Goekhan Baykut[1]; *[1]Bruker Daltonic GmbH, Bremen, Germany; [2]Bruker Daltonics Inc., Billerica , MA; [3]Bruker Daltonic, Billerica, MA; [4]The Institute for Energy Problems of Chemical Physics Russian Academy of Sciences, Moscow, Russia*

TP 438 **A Timing Control Method to Prevent Ion Overtake in a Multi-turn Time-of-Flight Mass Spectrometer (infiTOF).**; Miki Shinichi[1]; Hirofumi Nagao[1]; Michisato Toyoda[2]; *[1]MSI. Tokyo, INC., Chofu, Tokyo, Japan; [2]Osaka University, Toyonaka, Osaka, Japan*

TP 439 **Improving m/z Resolution in Charge Detection Mass Spectrometry by Reduction of Ion Trap Energy Dependence**; Joanna Hogan[1]; Martin F Jarrold[1]; *[1]Indiana University Dept. Chemistry, Bloomington, IN*

TP 440 **A Novel, Miniaturized Linear Wire Ion Trap Mass Analyzer**; Qinghao Wu[1]; Yuan Tian[1]; Ailin Li[1]; Daniel Austin[1]; Richard N Zare[2]; *[1]Brigham Young University, Provo, Utah; [2]Stanford University, Stanford, CA*

TP 441 **New Analysis of the Bradbury-Nielsen Gates with Space Charge as Applied to Time-of-flight Analyzers**; Robert Jackson; *Instrumental Design Physics, LLC, Littleton, MA*

TP 442 **Addressing the 100 Isotopologue Challenge: Orbitrap Mass Spectrometry as a Means of High-Dimension Clumped and Position-specific Isotope Analysis**; John Eiler[1]; Johannes Schwieters[2]; Dieter Juchelka[2]; Alexander A Makarov[2]; Jens Griep-Raming[2]; *[1]California Institute of Technology, Pasadena, CA; [2]Thermo Fisher Scientific, Bremen, DE*

ION MOBILITY: APPLICATIONS (PROTEINS & PEPTIDES)
443 - 470

TP 443 **CZE-nanoESI-SLIM-IMS-MS Platform for Comprehensive, Ultrasensitive Proteome Analyses**; Roza Wojcik[1]; Ian K Webb[1]; Yehia M Ibrahim[1]; Derek F Hopkins[1]; Spencer A Prost[1]; Randolph V Norheim[1]; Daniel J Orton[1]; Sandilya Garimella[1]; Liulin Deng[1]; Ahmed M Hamid[1]; Ryan T Kelly[1]; Erin Baker[1]; Richard D Smith[1]; *[1]PNNL, Richland, WA*

TP 444 **Separation of Protein Conformers by High Resolution Ion Mobility-Mass Spectrometry**; Urs Rohner[1]; Michael Groessl[1]; Stephan Graf[1]; *[1]TOFWERK, Thun, Switzerland*

TP 445 **Protein Domain Structure Influences the Collision-Induced Ejection of Small Molecule Binders: Implications for the Development of Pharmaceutical Compounds**; Rachel Martini[1]; Joseph Eschweiler[1]; Brandon T Ruotolo[1]; *[1]University of Michigan, Ann Arbor, MI*

TP 446 **Native and Denatured Protein Structural Studies using Ion Mobility MS and Ion Activation Techniques**; Ruwan Kurulugama[1]; George C Stafford[1]; Joseph Eschweiler[2]; Brandon T Ruotolo[2]; John Fjeldsted[1]; *[1]Agilent Technologies, Santa Clara, CA; [2]University of Michigan, Ann Arbor, MI*

TP 447 **MS-based Epitranscriptomics: New Roles for Ion Mobility and Fragmentation Techniques**; Daniele Fabris[1]; Rebecca D'Esposito[2]; Jennifer Lippens[2]; Michael Miller[2]; William McIntyre[2]; Rebecca Rose[2]; *[1]The RNA Institute, University at Albany, Albany, NY; [2]The RNA Institute, University at Albany Albany, NY*

TP 448 **Analysis of Native-Like Protein and Protein Complex Ions using Structures for Lossless Ion Manipulations (SLIM)**; Samuel J. Allen[1]; Rachel M. Eaton[1]; Matthew F. Bush[1]; *[1]University of Washington, Seattle, WA*

TP 449 **Ion Mobility-Mass Spectrometry and Collision Induced Unfolding Rapidly Detect Subtle Differences in Antibody Glycoforms**; Yuwei Tian[1]; Brandon T Ruotolo[1]; *[1]University of Michigan, Ann Arbor, MI*

TP 450 **Ion Mobility Employed as a Second Dimension Separation of Isomeric Glycoforms in Glycopeptides**; Gege Xu[1]; Elisha Goonatilleke[1]; Jasmine Davis[1]; Mariana Barboza[1]; Carlito B Lebrilla[1]; *[1]UC Davis, Davis, CA - California*

TP 451 **Water-Mediated Dimerization of Ubiquitin Ions Captured by Cryogenic Ion Mobility-Mass Spectrometry**; Kelly Servage[1]; David H Russell[2]; *[1]Texas A&M University, College Station, Texas; [2]Texas A&M University, College Station, TX*

TP 452 **Structural Investigation and Binding Site Determination of Huntingtin Protein/Peptide-ligand Complexes by IMS-HDX-MS/MS and Molecular Dynamics Simulations**; Samaneh Ghassabi Kondalaji[1]; Mahdiar Khakinejad[1]; Stephen J Valentine[1]; Justin Legleiter[1]; *[1]West Virginia University, Morgantown, WV*

TP 453 **An LC/ESI-IM-MS/MS Assay for Identification and Quantification of Host Cell Proteins in Therapeutic Monoclonal Antibodies**; Catalin Doneanu[1]; Brad J Williams[2]; Ian Morns[3]; Andrew Borthwick[4]; Jackson Pope[4]; Ying-Qing Yu[5]; Weibin Chen[5]; *[1]Waters Corporation, Milford, MA; [2]Waters Corporation, Beverly, MA; [3]Waters, Necastle upon Tyne, UK; [4]Waters, Necastle upon tyne, UK; [5]Waters, Milford, MA*

TP 454 **Rapid Profiling of Cellular Extracts using Ion Mobility-Mass Spectrometry**; Brett Harper[1]; Brooke Brown[1]; Touradj Solouki[1]; *[1]Baylor University, Waco, TX*

TP 455 **Integrating Ion Mobility Separation into Peptide Mapping for Therapeutic Protein Characterization: Qualitative and Quantitative Aspects**; Ying-Qing Yu [1]; Liuxi Chen[1]; Henry Y Shion[1]; Weibin Chen[1]; *[1]Waters, Milford, MA*

TP 456 **Evaluation of Formulation-Induced Aggregation in Peptide Drug Products by IMS-MS**; Elizabeth E Pierson[1]; Nicholas A Pierson[1]; Paul L Walsh[1]; *[1]Merck Research Laboratories, Rahway, NJ*

TP 457 **Investigation of the Interaction between Antimicrobial Peptides and Lipid Membranes Using Ion Mobility Mass Spectrometry Coupled with Isothermal Titration Calorimetry**; Angi Chen[1]; John W Patrick[1]; David H Russell[1]; *[1]Texas A&M, College Station, TX*

TP 458 **Monitoring Conformational Landscape of Prion Protein**; Guillaume Van der Rest[1]; Human Rezaei[2]; Frederic Halgand[3]; *[1]Universite Paris-Sud, Orsay, France; [2]INRA, Jouy-en-Josas, France; [3]CNRS, Orsay, France*

TP 459 **Structural transitions of Bovine Serum Albumin Studied by IMS–IMS–MS**; Alexander D Jacobs[1]; Joseph D Eschweiler[2]; Sugyan Dixit[2]; Brandon T Ruotolo[2]; David E Clemmer[1]; *[1]Indiana University, Bloomington, IN; [2]University of Michigan, Ann Arbor, MI*

TP 460 **Characterization of Cytochrome c Intramolecular Interactions using nanoESI-HDX-TIMS-MS and Molecular Dynamics**; Juan Camilo Molano[1]; Khoa Pham[1]; Jaroslava Miksovska[1]; Mark E Ridgeway[2]; Melvin Park[2]; Francisco Fernandez-Lima[1]; *[1]Florida International University, Miami, FL; [2]Bruker Daltonic, Billerica, MA*

TP 461 **Effects of Chain Length on the cis/trans Isomerization Mediated Folding of Polyproline Helices**; Daniel W Woodall[1]; Tarick J El-Baba[1]; David E Clemmer[1]; *[1]Indiana University Dept. Chemistry, Bloomington, IN*

TP 462 **Introduction of Hydrophilic Sites: How Physical Modifications Alter the Conformer Preferences of Gramicidin A**; John Patrick[1]; David H Russell[2]; *[1]Texas A&M, college station, TX; [2]Texas A&M University, College Station, TX*

TP 463 **Characterization of Kinetically Trapped Intermediates of Microperoxidase-11 using TIMS-MS/MS and Molecular Modeling**; Jacob Porter[1]; Alyssa Garabedian[1]; Paolo Benigni[1]; Jaroslava Miksovska[1]; Francisco Fernandez-Lima[1]; *[1]Florida International University, Miami, FL*

TP 464 **Proline Influences the Binding of Zinc to Oxytocin**; Daniel R. Fuller[1]; Matthew S. Glover[1]; DoYong Kim[2]; David H. Russell[2]; David E. Clemmer[1]; *[1]Indiana University, Bloomington, IN; [2]Texas A&M University, College Station, TX*

TP 465 **Determination of the Gas-Phase Energy Landscape of Substance P by IMS-IMS-MS**; Chris Conant[1]; David H Russell[2]; David E Clemmer[1]; *[1]Indiana University, Bloomington, IN; [2]Texas A&M, College Station, TX*

TP 466 **Analysis of Ionic Self-Complementary Peptides by Ion Mobility Spectrometry-Mass Spectrometry**; Zhichao Zhang[1]; Daniel R. Fuller[1]; Tarick John El-Baba[1]; David E Clemmer[1]; *[1]Indiana University Dept. Chemistry, Bloomington, IN*

TP 467 **Comparison of Ion Mobility and Capillary Electrophoresis Mass Spectrometry Techniques for Cysteine Connectivity Identification of Peptides Bearing Intra-Molecular Disulfide Bonds**; Philippe Massonnet[1]; Cédric Delvaux[2]; Gregory Upert[3]; Jean R. N. Haler[1]; Jan Jordens[4]; Maarten Honing[4]; Ynze Mengerink[4]; Johann Far[1]; Nicolas Gilles[3]; Loic Quinton[1]; Edwin De Pauw[1]; *[1]University of Liège, Liège, Liège; [2]Laboratory of Mass Spectrometry - ULg, Liege, Belgium; [3]CEA, DSV/iBiTec – S/SIMOPRO, Gif-sur-Yvette, France; [4]DSM Resolve, Geleen, The Netherlands*

TP 468 **Using Gas Phase Conformations to Understand the Role of Solvent in Establishing Biomolecule Structure in Solution**; Tarick El-Baba[1]; Daniel Fuller[1]; DoYong Kim[2]; Dylan Rogers[3]; Faizan Khan[3]; David A Hales[3]; David H Russell[2]; David E Clemmer[1]; *[1]Indiana University Dept. Chemistry, Bloomington, IN; [2]Texas A&M, College Station, TX; [3]Hendrix College, Conway, AR*

TP 469 **Separation of Isomers in Lipidomics and Metabolomics Experiments by High Resolution Ion Mobility-Mass Spectrometry**; Michael Groessl[1]; Stephan Graf[1]; *[1]TOFWERK, Thun, Switzerland*

TP 470 **High Resolution Trapped Ion Mobility Mass Spectrometry Analysis of Isomeric Compounds**; Sven W Meyer[1]; Peter Sander[1]; Alexander Harder[1]; Detlev Suckau[1]; *[1]Bruker Daltonic GmbH, Bremen, Germany*

LC-MS: CHROMATOGRAPHY AND SOFTWARE (PART 2)
471 - 498

TP 471 **Peptide Elution Rate Equation: a Novel Ideal Elution Model to Help Retention Time Prediction**; Wenyuan Lu[1]; Xiaohui Liu[1]; Pengyuan Yang[1]; *[1]Fudan University, Shanghai, China*

TP 472 **Evaluating Effects of Metagenome Database Quality and an Optimized LC/LC-MS/MS Approach for Obtaining Deeper Proteome Coverage of Complex Microbial Communities**; Ramsunder Iyer[1, 2]; Richard J Giannone[2]; Rose S Kantor[3]; Susan T.L Harrison[4]; Robert J Huddy[4]; Jillian F Banfield[5]; Robert L Hettich[2]; *[1]Graduate School of Genome Science and Technology, University of Tennessee, Knoxville, TN; [2]Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN; [3]Department of Plant and Microbial Biology, University of California, Berkeley, CA; [4]Centre for Bioprocess Engineering Research, Department of Chemical Engineering, University of Cape Town, Cape Town, South Africa; [5]Department of Earth and Planetary Sciences, University of California, Berkeley, CA*

TP 473 **Universal Derivatization of Metabolites for Improved Sensitivity in LC-MS**; James Edwards; *Saint Louis University, St Louis, MO*

TP 474 **Optimization of Size Exclusion Chromatography and Atmospheric Pressure Ionization Enabling Characterization of Intact Lignin and Its Degradation Products**; Anastasia Artemyeva[1]; Kubatova Alena[1]; Evguenii I. Kozliak[1]; *[1]University of North Dakota, Grand Forks, ND*

TP 475 **Characterization of Electrochemically Decomposed Lignin Using Liquid Chromatography-High Resolution Mass Spectrometry**; Tobias Dier[1]; Sarah Henrikus[1]; Verlaine Fossog[1]; Rolf Hempelmann[1]; Dietrich A Volmer[1]; *[1]Saarland University, Saarbrücken, Germany*

TP 476 **Deeper Proteomics using Actively Modulated Online HILIC×nRPLC-HRMS**; Andrea Gargano[1, 2]; Martin Samonig[3]; Michael Woldergebriel[2]; Remco Swart[3]; Garry Corthals[4]; Peter Schoenmakers[2]; *[1]VU University Amsterdam, Amsterdam, Netherlands; [2]University of Amsterdam, Amsterdam, The Netherlands; [3]Thermo Fisher Scientific GmbH, Germering, Germany; [4]University of Amsterdam, Amsterdam, NL*

TP 477 **Low-Temperature Mobile Phase for Peptide Trapping at Elevated Separation Temperature Prior to Nano RP-HPLC-MS/MS**; Matthias Schöbinger[1]; Oskar-James Klein[1]; Goran Mitulovic[2]; *[1]Medical University of Vienna, Clinical Institute of Laboratory Medicine, Wien, Austria; [2]Medical University of Vienna, KIMCL, Vienna, No State/Province*

TP 478 **Porous Graphitic Carbon Packed Capillaries for the LC-MSMS Analysis of RNA Modified Nucleosides**; Robert Ross[1]; Peter Sarin[2]; Hannes Drexler[2]; Sebastian Leidel[2]; Patrick A Limbach[1]; *[1]University of Cincinnati, Cincinnati, OH; [2]Max Planck Institute for Molecular Biomedicine, Munster, Deutschland*

TP 479 **Redesign of Peptide Mapping Gradients to Resolve Complex Biological Samples**; Xinli Yang; *Rosalind Franklin University, North Chicago, IL*

TP 480 **LC/MS/MS Method for the Determination of Tricyclic and Tetracyclic Antidepressants in Human Urine**; Amber Awad[1]; Kendra Parker[1]; Lawrence Andrade[2]; *[1]Dominion Diagnostics, N. Kingstown, RI; [2]Dominion Diagnostics, North Kingstown*

TP 481 **A Fast and Sensitive Chiral LC-MS/MS Assay for Ketamine and its Metabolites in Human Plasma**; Michel Coutu[1]; Evgueni Fedorov[1]; Jean-François Larocque[1]; Simon Bourgeois[1]; *[1]Biotrial Bioanalytical Services, Laval, QC*

TP 482 **Proteomics Needs Better Chromatography**; Evgenia Shishkova[1]; Alexander S Hebert[2]; Michael S Westphall[2]; Joshua J Coon[2]; *[1]JJ Coon Research Group, Madison, Wisconsin; [2]University of Wisconsin-Madison, Madison, WI*

TP 483 **A Novel Approach to Studying Thiamine Kinetics: an LC/ESI-MS/MS-based Method for the Analysis of Thiamine and Derivatives in Biological Samples**; Jaeah Kim[1]; Jason Zastre[1]; Michael G Bartlett[1]; *[1]University of Georgia, Athens, GA*

TP 484 **A Functional Group Approach to Determining the Effects of Mobile Phase Modifiers on the Negative Ion ESI Ionization Efficiency**; Melanie Odenkirk[1]; Stephen Lucas[1]; Christine A. Hughey[2]; *[1]James Madison University, Harrisonburg, VA; [2]James Madison University, Harrisonburg , VA*

TP 485 **A Fast LC/MS/MS Method for High Sensitivity Determination of 24 Perfluorocompounds in Textiles**; Jun Xiang Lee[1]; Zhe Sun[1]; Jie Xing[1]; Zhaoqi Zhan[1]; *[1]Shimadzu (Asia Pacific) Pte Ltd, Singapore*

TP 486 **Exploring the Effects of Alternative Dynamic Exclusion Algorithms on Peptide Identification Experiments**; Nina Soltero[1]; Graeme C McAlister[1]; Derek Bailey[1]; Vlad Zabrouskov[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

TP 487 **Targeted Profiling of Oxylipins and Endocannabinoids in Biological Samples using the Nanoflow ionKey/MS system – Method Development and Validation**; Sandra Gouveia-Figueira[1]; Malin Linder Nording[1]; *[1]Umea University, Umea, SE*

TP 488 **The Simultaneous Detection of a Panel of Drugs of Abuse in Post-mortem Hemolyzed Blood Samples (n=40) by LC-ESI-laminar Flow MS/MS**; Sabra Botch-Jones[1]; Raquel LeBlanc[1]; *[1]Boston University School of Medicine, Boston, MA*

TP 489 **UHPLC Optimization Study for Improved LC-MS Performance and Throughput**; Martin Ruehl; *Thermo Fisher Scientific, Germering, Germany*

TP 490 **A Study of the γ-Radiolysis of Di-Dodecyl Di-Octyl Diglycolamide (D3DODGA) using UHPLC-ESI-MS Analysis**; Kristyn M Johnson[1]; Chistopher A Zarzana[1]; Gary S Groenewold[1]; Bruce J Mincher[1]; Andreas Wilden[2]; Holger Schmidt[2]; Giuseppe Modolo[2]; Beatrix Santiago-Schübel[3]; *[1]Idaho National Laboratory, Idaho Falls, ID; [2]Forschungszentrum Jülich GmbH, Institut für Energie- und Klimaforschung- Nukleare Entsorgung und Reaktorsicherheit, Jülich, Germany; [3]Forschungszentrum Jülich GmbH, Zentralinstitut für Engineering, Elektronik und Analytik, Jülich, Germany*

TP 491 **The Use of a HILIC Peptide Retention Prediction Model to Predict the Presence of Modifications in Histones**; Majors Badgett[1]; Barry Boyes[2]; Ron Orlando[1]; *[1]The University of Georgia, Athens, GA; [2]Advanced Materials Technology, Wilmington, DE*

TP 492 **Automation and Remote Visualization of Screening Data**; David M Cox[1]; Burkhard Schaefer[2]; John Gibbons[3]; Viktor Iassinskii[3]; *[1]SCIEX, Concord , ON; [2]BSSN Software, Darmstadt, Germany; [3]SCIEX, Concord, ON*

TP 493 **Long Term Test on a New Four-Channel HPLC**; Pengxiang Yang[1]; BC cha[1]; Terry N Olney[1]; John Brann[2]; Christopher Elicone[2]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Franklin, MA*

TP 494 **New Supercharging Agents for TFA-Based LC-MS of Peptides and Proteins**; Michael Nshanian[1]; Rachel Loo[2]; Joseph A Loo[2]; *[1]University of California Los Angeles, Los Angeles; [2]UCLA, Los Angeles, CA*

TP 495 **Matrix Effects: Do They Differ between SFC/ESI-MS and LC/ESI-MS?**; Alfred Svan[1]; Mikael Hedeland[1, 2]; Torbjörn Arvidsson[1, 3]; Curt E Pettersson[1]; *[1]Uppsala University, Uppsala, Sweden; [2]National Veterinary Institute (SVA) Dept. of Chemistry, Environment and Feed Hygiene, Uppsala, Sweden; [3]Medical Products Agency, Uppsala, Sweden*

TP 496 **Development of a Novel Nano Separation Device for Robust and Accurate Gradient Delivery with Intelligent Diagnostics**; Ole Bjeld Hørning[1]; Stephanie Kaspar-Schoenefeld[2]; Christoph Gebhardt[2]; Peter Aagaard Nielsen[1]; Alexandre Podtelejnikov[1]; Michael Barrett Andersen[1]; Nicolai H Bache[1]; *[1]Bruker Daltonics Scandinavia, Odense, Denmark; [2]Bruker Daltonik GmbH, Bremen, Germany*

TP 497 **HILIC and Mixed-Mode Retention of the FluoroPhenyl Stationary Phase**; Shun-Hsin Liang[1]; Carroll Frances[1]; Sharon Lupo[1]; Ty Kahler[1]; *[1]Restek Corporation, Bellefonte, PA*

TP 498 **Method and Software Workflow for Integrating Paired CE-MS and LC-MS Bottom-up Proteomics Data from SDS-PAGE Pre-fractionated Samples**; Yassene Mohammed[1, 2]; Anthonius A. M. Heemskerk[1]; Dana Ohana[1]; Hans Dalebout[1]; André M Deelder[1]; Oleg Mayboroda[1]; Magnus Palmblad[1]; *[1]LUMC, Center for Proteomics and Metabolomics Leiden, NL; [2]UVic - Genome BC Proteomics Centre, Victoria, Canada*

LIPIDS: ID AND STRUCTURAL ANALYSIS
499 - 518

TP 499 **LipidMatch Software: Identification of Lipids and Their Oxidation Products using Data-Dependent and Data-Independent LC-MS/MS data**; Jeremy Koelmel[1]; Nicholas M. Kroeger[2]; Candice Ulmer[2]; Rainey Patterson[2]; John A Bowden[3]; Timothy J Garrett[2]; Richard A Yost[2]; *[1]University of Florida, Gainesville, Fl; [2]University of Florida, Gainesville, Florida; [3]Hollings Marine Laboratory, National Institute of Standards and Technology, Charleston, SC*

TP 500 **Integrated Software for Data Processing and Analysis in Direct Infusion Ultra-High Resolution / Accurate Mass Spectrometry Based 'Top-Down' Lipidomics Workflows**; Yasuto Yokoi[1]; Yukihiro Fukamachi[1]; David Peake[2]; Reiko Kiyonami[2]; Eileen Ryan[3]; Gavin E Reid[3]; *[1]Mitsui Knowledge Industry Co, Tokyo, Japan; [2]Thermo Fisher Scientific, San Jose, CA; [3]University of Melbourne, Victoria, Australia*

TP 501 **A Lipid Mass Spectral Library for Human Plasma**; Paul D Hutchins[1]; Dain R Brademan[2, 3]; Jason W Russell[2, 4]; Michael S Westphall[2]; Joshua J Coon[2, 3, 5]; *[1]University of Wisconsin Madison, Madison, Wisconsin; [2]Genome Center, University of Wisconsin, Madison, WI; [3]Department of Chemistry, University of Wisconsin, Madison, WI; [4]Morgridge Institute for Research, Madison, WI; [5]Biomolecular Chemistry, University of Wisconsin, Madison, WI*

TP 502 **SimLipid: Software Platform for Automating Shotgun, LC-MS and MALDI-MS Based High-Throughput lipidomics**; Ningombam Sanjib Meitei[1]; Himani Gupta[1]; Arun Apte[2]; *[1]PREMIER Biosoft, Indore, India; [2]PREMIER Biosoft, Palo Alto, CA*

TP 503 **Structural Characterization of Membrane Glycolipids from Marine Sponge-associated Bacteria by Mass Spectrometry**; Benjamin L Oyler[1]; Courtney E Chandler[2]; Fan Zhang[3]; Christopher J Thompson[4]; Jeremy J Wolff[4]; Michael L Easterling[4]; Robert K Ernst[2]; Russell T Hill[3]; David R. Goodlett[2]; *[1]University of Maryland, Baltimore, Whiteford, MD; [2]University of Maryland, Baltimore, Baltimore, MD - Maryland; [3]University of Maryland Center for Environmental Science, Baltimore, MD - Maryland; [4]Bruker Daltonics, Billerica, MA*

TP 504 **Identification and Quantitation of Unsaturated Glycerolipids from Human Plasma using the Paternò-Büchi Reaction and Tandem Mass Spectrometry**; Hilary Brown[1]; Yu Xia[1]; *[1]Purdue University, West Lafayette, IN*

TP 505 **Study and Optimization of online Paternò–Büchi Reactions for Structural Analysis of Unsaturated Lipids using Mass Spectrometry**; Xiaoxiao Ma[1, 2]; Pei Su[1]; Zheng Ouyang[1, 2]; Yu Xia[2]; *[1]Purdue University-Weldon School of Biomedical Engineering, West Lafayette, IN; [2]Purdue University-Department of Chemistry, West Lafayette, IN*

TP 506 **Top-down Structural Elucidation of Gram-negative Bacterial Endotoxins by Tandem Mass Spectrometry**; Mohd M. Khan[1]; Benjamin L Oyler[2]; Kelsey A. Gregg[3]; Robert K. Ernst[3]; Alan S. Cross[4]; David R Goodlett[2]; *[1]University of Maryland School of Pharmacy, Baltimore, MD; [2]Department of Pharmaceutical Sciences, University of Maryland School of Pharmacy, Baltimore, MD; [3]Department of Microbial Pathogenesis, University of Maryland School of Dentistry, Baltimore, MD; [4]Center for Vaccine Development, University of Maryland School of Medicine, Baltimore, MD*

TP 507 **Structural Characterization of Lipid Biomarkers from Staphylococcus aureus following Microextraction for Mass Spectrometric Phenotyping**; Lisa Leung[1]; Benjamin Oyler[2]; Robert Ernst[3]; David R Goodlett[2]; *[1]University of Maryland, Baltimore, MD; [2]University of Maryland School of Pharmacy, Baltimore, MD; [3]University of Maryland Baltimore, Baltimore, MD*

TP 508 **N-Succinylation of L-lysyl-phosphatidylglycerol in Bacillus subtilis**; Paulos Chumala[1]; Metin Atila[1]; George Katselis[1]; Yu Luo[2]; *[1]University of Saskatchewan, Saskatoon, Canada; [2]University of Saskatchewan, Saskatoon, SK*

TP 509 **Systematic Fragmentation of Lipid A Variants by Multiple and Hybrid MS/MS Techniques**; Christopher Martin Crittenden[1]; William Ryan Parker[1]; Jennifer S. Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX*

TP 510 ***In-situ* Characterization of Phospholipids Mixture on Tissue Sections using Wide Ion Gate HE-CID Experiment and ASDF MS/MS Spectra**; Simona Salivo[1]; Yuzo Yamazaki[2]; Peter Quinto Tranchida[1]; Luigi Mondello[1]; Omar Belgacem[3]; *[1]University of Messina, Messina, Italy; [2]Shimadzu Corporation, Kyoto, Japan; [3]Shimadzu, Kratos Manchester, United Kingdom*

TP 511 **Using MS/MS and MSn to Distinguish Cytotoxic J-series Prostaglandin Isomers Produced in Tumorigenic Keratinocytes**; Robert Kobet[1]; Rukiyah T. Van Dross[1]; Allison S. Danell[1]; *[1]East Carolina University, Greenville, NC*

TP 512 **Conformational Atlas of 7 Classes of Sphingolipids and Glycerophospholipids Mapped by Ion Mobility-Mass Spectrometry**; Katrina L. Leaptrot[1]; Jody C. May[1]; James N. Dodds[1]; John A. McLean[1]; *[1]Vanderbilt Dept. of Chemistry, Nashville, TN*

TP 513 **Differentiation of Triacylglycerol Regioisomers Using Differential Ion Mobility Spectrometry**; Jinyuan Wang[1]; Larry J Campbell[2]; Paul RS Baker[1]; *[1]SCIEX, Redwood City, CA; [2]SCIEX, Concord, ON*

TP 514 **Identification of Lipid Metabolites of Docosahexaenoic and Arachidonic Acids in Human Blood Using Stable Isotope Labeled Compounds**; Karl R Kevala[1]; Mark Sanders[2]; Hee-Yong Kim[1]; *[1]National Institutes of Health, Bethesda, MD; [2]Thermo Fisher Scientific, Somerset, NJ*

TP 515 **Identification and Characterization of Sulfolipids Found in Nitzschia palea**; Larry Sallans [1]; Daniel Betz[2]; Stephen F Macha[2]; Edna S. Kaneshiro[2]; *[1]University of Cincinnati, Cincinnati , OH; [2]University of Cincinnati, Cincinnati, OH*

TP 516 **Role of pH and Mobile Phase Modifiers on Untargeted RP LC-MS Analysis of Lipid Extracts**; Elena Sokol[1]; David Peake[2]; *[1]Thermo Fisher Scientific, Hemel Heampstead, United Kingdom; [2]Thermo Fisher Scientific, San Jose, CA*

TP 517 **Identification of Metabolites of Novel Sphingoid Bases in Sphingolipid-depleted Cells using Liquid-Chromatography Electrospray Tandem Mass Spectroscopy**; Brandon M Kenwood[1]; Samuel Kelly[1]; Jingjing Duan[1]; Alfred H Merrill Jr[1]; Cameron Sullards[1]; *[1]Georgia Institute of Technology, Atlanta, GA*

TP 518 **Identification of a Novel Lipid Family Containing a Modified Head Group**; Seetaramanjaneyulu Gundimeda[1]; Arunkumar Padmanaban[2]; *[1]Agilent technologies, bangalore, karnataka; [2]Agilent technologies, Bangalore, India*

METABOLOMICS: SAMPLE PREPARATION
519 - 529

TP 519 **Influence of Sampling Techniques on Human Blood Metabolome Stability during the Long-Term Sample Storage**; Kristaps Klavins[1]; Guido Dallmann[1]; Therese Koal[1]; *[1]Biocrates Life Science AG, Innsbruck, Austria*

TP 520 **Determination of Selectivity Influenced by Liquid-Liquid Extraction in Global Metabolomics using UHPLC-qTOF-MS**; Albert Elmsjö[1]; Mikael Karl Robert Engskog[2]; Jakob Haglöf[1]; Torbjörn Arvidsson[1, 3]; Curt Pettersson[1]; *[1]Department of Medicinal Chemistry; Analytical Pharmaceutical Chemistry, Uppsala University Uppsala, Sweden; [2]Department Medicinal Chemistry; Analytical Pharmaceutical Chemistry, Uppsala University Uppsala, Sweden; [3]Medical Product Agency, Uppsala, Sweden*

TP 521 **Widely Targeted Analysis of Hydrophilic Anionic Metabolites in Mammalian Cells by Ion Chromatography Coupled with High Resolution Mass Spectrometry**; Yoshihiro Izumi[1]; Takahiro Suzuki[2]; Motokazu Kimura[2]; Shigeru Sakamoto[2]; Takeshi Bamba[3]; *[1]Medical Institute of Bioregulation, Kyushu University, Fukuoka, Japan; [2]Thermo Fisher Scientific Japan, Tokyo, Japan; [3]Medical Institute of Bioregulation, Kyushu Univ. Fukuoka, Japan*

TP 522 **Systematic Assessment and Selection of Liquid and Solid-Phase Methods in the Design of Sequential Extraction Protocols for LC-MS Based Metabolomics**; Dmitri Sitnikov[1]; Cian S Morin[1]; Dajana Vuckovic[1]; *[1]Concordia University, Montreal, Canada*

TP 523 **Super-Omics: Liquid-Liquid Extraction for Proteomics, Lipidomics and Metabolomics from a Single Sample, Towards a Method for Biopsies**; Susanne Breitkopf[1]; Min Yuan[1]; Gerburg Wulf[1, 2]; John M Asara[1, 2]; *[1]Beth Israel Deaconess Medical Center, Boston, MA; [2]Harvard Medical School, Boston, MA*

TP 524 **Detection Enhancement of Small Molecules, Lipids and Peptides by Functionalizing Silicon Nanopost Arrays with Fluorous Monolayers**; Heather Anderson[1]; Nicholas Morris[1]; Matthew Powell[1]; Trust T Razunguzwa[1]; *[1]Protea Biosciences, Morgantown, WV*

TP 525 **A Real-time Analysis of Brain Energy Metabolism by Micro-dialysis Linked Ion Chromatography-MS**; Yuki Sugiura; *Keio University, Tokyo*

TP 526 **Characterizing Temporal And Inter-Individual Functional Differences in Infant Gut Microbiome by a Metaproteomics Approach**; Weili Xiong[1]; Michael Morowitz[2]; Jillian Banfield[3]; Robert Hettich[1]; *[1]Oak Ridge National Laboratory, Oak Ridge, TN; [2]University of Pittsburgh, Pittsburgh, PA; [3]University of California, Berkeley, CA*

TP 527 **Custom isotopic N,N-Dimethyl Leucine (iDiLeu) Reagents Enable Absolute Quantification of Amine-containing Metabolites and Its Application to Human Cerebrospinal Fluid**; Pingli Wei[1]; Ling Hao[2]; Jingxin Wang[2]; Xuefei Zhong[1]; Lingjun Li[2]; *[1]University of Wisconsin Madison, Madison, Wisconsin; [2]University of Wisconsin Madison, Madison, WI*

TP 528 **Sub-Minute, Comprehensive Metabolomics Measurements for Disease and Exposure Research**; Xing Zhang[1]; Michelle V Romm[2]; Erika M Zink[3]; Daniel J Orton[3]; Yehia M Ibrahim[3]; Matthew E Monroe[3]; Justin G Teeguarden[3]; Thomas O Metz[3]; Richard D Smith[3]; Nichole A Reisdorph[1]; Erin S Baker[3]; *[1]Anschutz Medical Campus, University of Colorado Denver, Aurora, CO; [2]Agilent Technologies, Santa Clara, CA; [3]Pacific Northwest National Lab, Richland, WA*

TP 529 **Online-SPE-HILIC-ESI-MS Analysis of Redox Cofactors in Chlamydomonas Reinhardtii Algae Cells**; Alexander Schriewer[1]; Heiko Hayen[1]; *[1]Institute of Inorganic and Analytical Chemistry, University of Muenster, Muenster, Germany*

METABOLOMICS: UNTARGETED METABOLITE PROFILING (CELLS/PLANTS)
530 - 557

TP 530 **Rapid Detection of Pathogenic Amoeba in Water Distribution Systems using UPLC-MS**; Zhihao Yu[1]; Haylea Miller[2]; Geoffrey Puzon[2]; Brian H Clowers[1]; *[1]Washington State University, Pullman, WA; [2]CSIRO Land and Water, Perth, Australia*

TP 531 **Metabolomic evaluation of conditions favoring mycotoxin production in isolates of Fusarium fungi**; Mark Busman; *USDA, ARS, NCAUR, BFP, Peoria, IL*

TP 532 **Metabolic Phenotyping of Cell Lines by Rapid Evaporative Ionization Mass spectrometry**; Emrys Jones[1]; Emmanuelle Claude[1]; James Langridge[1]; Fiona Henderson[2]; Adam W McMahon[2]; Zoltan Takats[3]; Steve Pringle[1]; *[1]Waters Corporation, Wilmslow, UK; [2]Wolfson Molecular Imaging Centre, Manchester, UK; [3]Imperial College London, South Kensington Campus London, United Kingdom*

TP 533 **Metabolomic Profiling in Pulmonary Arterial Hypertension Disease Models**; David P Marciano[1]; Caiyun grace Li[1]; Jan k Hennigs[1]; Marlene Rabinovitch[1]; Michael Snyder[1]; *[1]Stanford University School of Medicine, Palo Alto CA, USA*

TP 534 **Non-targeted Metabolite Profiling and Antioxidant Activity of Genetically Diverse Soybean Seeds**; Yongsoo Choi[1]; Jiuliang Xu[2]; Jeong-Sook Shin[1]; Jung-Kyung Moon[3]; *[1]Korea Institute of Science and Technology, Gangneung, South Korea; [2]Korea Institute of Science and Technology, Geagneung, South Korea; [3]National Institute of Crop Science, Cheongju-Si, Chungbuk*

TP 535 **Identification and Chemical Characterization of Marine Natural Products Using UPLC-QTof-MS Coupled to a Novel Informatics Platform**; Roger G. Linington[1]; Kenji L. Kurita[1]; Jimmy Yuk[2]; Kate Yu[2]; Mark Wrona[2]; Giorgis Isaac[2]; *[1]Simon Fraser University, Burnaby, BC, Canada; [2]Waters Corporation, Milford, MA*

TP 536 **Isotopic Ratio Outlier Analysis (IROA) Global Metabolome Interrogation of an Actinomycete Bacterium following Introduction of a Novel Pathway**; Felice de Jong[1]; Taylor A. Lundy[2]; Christopher W W Beecher[1, 3]; Amy L Lane[2]; *[1]IROA Technologies LLC, Bolton, MA; [2]University of North Florida, Jacksonville, FL; [3]University of Florida, Gainesville, FL*

TP 537 **Increasing Arginine Production in C. Glutamicum by Rational Strain Design and Discovery Metabolomics: Linking HRAM QTOF Data to Biology**; Frederik Walter[1]; Marcus Persicke[1]; Aiko Barsch[2]; Christian Ravnsborg[3]; Heiko Neuweger[2]; Matthias Szesny[2]; Nikolas Kessler[2]; Jörn Kalinowski[1]; *[1]Bielefeld University, Bielefeld, Germany; [2]Bruker Daltonics Ltd, Bremen, Germany; [3]Bruker Daltonics, Bremen, Germany*

TP 538 **Metabolite Profiling of Glyphosate Exposed Saccharomyces cerevisiae with REDIchips**; Christopher George[1]; Haddon Goodman[1]; Gregory Boyce[1]; *[1]Protea Biosciences, Morgantown, WV*

TP 539 **Environmental Exposure to Ionizing Radiation Induces Dysbiosis in Gut Microbiome and Fecal Metabolome**; Maryam Goudarzi[1]; Jonathan Jacobs[2]; Tytus Mak[3]; Bo-Hyun Moon[4]; Steve Strawn[4]; Jonathan Braun[2]; David Brenner[5]; Albert Fornace Jr[4]; *[1]Georgetown University, Washington DC, DC; [2]UCLA, Los Angeles, CA; [3]NIST, Rockville, MD; [4]Georgetown University, Washington, DC; [5]Columbia University, New York, NY*

TP 540 **Abiotic Stresses Influence Organic Metabolite Profiles in Soils Hosting Populus Trees and a Microbial Community**; Charles J. Doktycz[1]; Collin M. Timm[1]; Keiji G Asano[1]; David J Weston[1]; Dale A. Pelletier[1]; Greg Hurst[1]; *[1]Oak Ridge National Laboratory, Oak Ridge, TN*

TP 541 **Evaluation of High Speed, High Resolution Data Independent Acquisition for the Analysis of Metabolomic Flux, Kinetics and Pathway**; Loren Y Olson[1]; Baljit Ubhi[1]; *[1]SCIEX, Redwood City, CA*

TP 542 **Untargeted Metabolomics with Fungal Artificial Chromosomes (FAC-MS) Allows Discovery and Facile Dissection of Natural Product Biosynthesis**; Kenneth D Clevenger[1]; Jin Woo Bok[2]; Rosa Ye[3]; Galen P Miley[1]; Thomas Velk[2]; Cynthia Chen[3]; KaHoua Yang[2]; Peng Gao[1]; Matthew Lamprecht[3]; Paul M Thomas[1]; Md Islam[3]; Chengcang C Wu[3]; Nancy P Keller[2]; Neil L Kelleher[1];

[1]Northwestern University, Evanston, IL; [2]University of Wisconsin Madison, Madison, Wisconsin; [3]Intact Genomics, Inc, St. Louis, MO

TP 543 **In vivo Analysis of Metabolites in Single Embryonic Cells in the Developing Frog (Xenopus)Embryo using Microcapillary-Sampling CE-ESI-MS**; Erika Portero[1]; Rosemary M Onjiko[1]; Sally A Moody[1]; Peter Nemes[1]; *[1]The George Washington University, Washington, DC*

TP 544 **Eavesdropping on Marine Microbial Communication: Influence of Quorum Sensing on the Vibrio campbellii Metabolome**; Gregory Ellis[1]; Brian J. Eddie[2]; Arnaldo A. Torres Padua[3]; W. Judson Hervey IV[4]; Gary J. Vora[4]; Dagmar H. Leary[4]; *[1]National Research Council NRL Fellow, Washington, DC; [2]American Society of Engineering Education NRL Fellow, Washington, DC; [3]University of Puerto Rico Mayaguez, Mayaguez, PR; [4]Center for Bio/Molecular Science and Engineering, Naval Research Laboratory, Washington, DC*

TP 545 **Untargeted 2-Sample-Comparison using High-Resolution Data from LC/Ion Mobility Q-TOF Mass Spectrometers via a Novel 4D Molecular Feature Extraction Algorithm**; Frank Kuhlmann[1]; Xiangdong Li[1]; Ed Darland[1]; *[1]Agilent Technologies, Santa Clara, CA*

TP 546 **Metabolic Profiling of Strawberry Leaves Infected by Xanthomonas Fragariae using UPLC/QTOF Mass Spectrometry**; Min-Sun Kim[1]; Geum-Sook Hwang[2]; *[1]Korea Basic Science Institute, Seoul, Republic of Korea; [2]Korea Basic Science Institute, Seoul, Republic of Korea*

TP 547 **Global Metabolomics Approach to Identify Pathways Effected by Glyphosate in Yeast**; Gregory Boyce[1]; Mark Szewc[1]; *[1]Protea Biosciences, Morgantown, WV*

TP 548 **Chemical Profiling of Actaea Species and Commerical Products using UPLC-QTof-MS**; Jimmy Yuk[1]; Maged Sharaf[2]; Kate Yu[1]; Mark Wrona[1]; Giorgis Isaac[1]; *[1]Waters, Milford, MA; [2]American Herbal Products Association, Silver Spring, MD*

TP 549 **Non-targeted Differential Screening using LC-HRAM-MS as a Tool for Evaluating Differences in Chemical Composition between Samples and Sample Groups**; Daniel Arndt[1]; Arno Knorr[1]; Mark Bentley[1]; *[1]Philip Morris International R&D, Neuchâtel, Switzerland*

TP 550 **Non-targeted Differential Screening of Complex Matrices using GC×GC-TOFMS for Comprehensive Characterization of Chemical Composition and Determination of Significant Differences**; Martin Almstetter[1]; Arno Knorr[1]; Quentin Dutertre[1]; Elyette Martin[1]; Antonio Castellon[1]; Pavel Pospisil[1]; Mark Bentley[1]; *[1]Philip Morris International, Neuchâtel, Neuchâtel*

TP 551 **Atmospheric Pressure Gas Chromatography Mass Spectrometry (APGC-MS) Based Metabolomics Profiling of Grape Volatiles**; Manoj Ghaste[1,2]; Giuseppe Astarita[3]; Fulvio Mattivi[2]; Vladimir Shulaev[1]; *[1]University of North Texas, Denton, TX; [2]Fondazione Edmund Mach, San Michele all'Adige TN, Italy; [3]Waters, Milford, MA*

TP 552 **Comparison of Direct Introduction on Orbitrap Fusion and FT-ICR at High-end Resolution for Global Metabolite Screening**; Ulli Martin Hohenester[1,2]; Pierre Barbier Saint Hilaire[1]; Benoit Colsch[1]; Francois Fenaille[1]; Jean-claude Tabet[1]; Christophe Junot[1]; Richard B Cole[2]; *[1]Commissariat à énergie atomique et aux énergies alternatives, Gif Sur Yvette Cedex, Fr; [2]Sorbonne Universités, UPMC Univ Paris 06, Institut Parisien de Chimie Moléculaire, Paris, Fr*

TP 553 **Development of High-Performance Chemical Isotope Labeling LC-MS for Profiling Alcoholic Hydroxyl-Containing Metabolites in Metabolomics**; Shuang Zhao[1]; Liang Li[1]; *[1]Department of Chemistry, University of Alberta, Edmonton, AB, Canada*

TP 554 **Metabolomic Profiling of Food Diets Using Ion Chromatography with High Resolution Orbitrap Mass Spectrometry**; Terri Christison[1]; JUNHUA WANG[2]; Linda Lopez[1]; Ralf Tautenhahn[3]; *[1]Thermo Fisher Scientific Inc, Sunnyvale, CA; [2]Thermo Fisher Scientific Inc, San Jose, CA; [3]Thermo Fisher Scientific, San Jose, CA*

TP 555 **Metabolic Profiling of Bladder Cancer Cell Lines Reveals Molecular Alterations Involved in Methylation and Novel Epigenetic Phenotype**; Feng Jin[1]; Rashmi Krishnapuram[1]; Franklin Gu[1]; Salil Kumar Bhowmik[1]; Suman Maity[1]; Mohan Manikkam[1]; Friedrich-Carl von Rundstedt[1]; Vasanta Putluri[1]; Yair Lotan[2]; Jonathan Levitt[1]; Seth P. Lerner[1]; Cristian Coarfa[1]; Benny Abraham Kaipparettu[1]; Arun Sreekumar[1]; Nagireddy Putluri[1]; *[1]Baylor College of Medicine, Houston, TX; [2]University of Texas Southwestern Medical Center, Dallas, TX*

TP 556 **Metabolomic Signatures in Sera from Early Stage Ovarian Cancer Patients**; David A Gaul[1]; Christina M Jones[1]; Tran Q Long[1]; John F McDonald[1]; Facundo M Fernandez[1]; *[1]Georgia Institute of Technology, Atlanta, GA*

TP 557 **Discovery of Altered Metabolic Pathways in PARPi-Resistant Ovarian Cancer**; Chandra Shekar R Ambati[1]; Sachin Kumar Gupta[1]; Sajna A Vithayathil[1]; Suman Maity[1]; Laising Yen[1]; Benny Abraham Kaipparettu[1]; Cristian Coarfa[1]; Nagireddy Putluri[1]; Vivekananda Shetty[1]; *[1]Baylor College of Medicine, Houston, TX*

NUCLEIC ACIDS
558 - 582

TP 558 **RNA Modification Mapping - Software Development**; Ningxi Yu[1]; Patrick A Limbach[1]; *[1]University of Cincinnati, Cincinnati, Ohio*

TP 559 **Development of a Computational Algorithm to Predict Mobile Phase Additives for Optimal LC-MS Sensitivity of Oligonucleotides**; Babak Basiri[1]; Michael G Bartlett[1]; *[1]University of Georgia, Athens, GA*

TP 560 **A Flow Injection Inductively Coupled Plasma Mass Spectrometry Method for Quantification of Modified Oligonucleotides**; Fanyu Meng[1]; Qiang Tu[2]; Erin Guidry[2]; *[1]Merck & Co., Inc, Rahway, NJ; [2]Merck, Darmstadt, Germany*

TP 561 **Comparison of Q-Tof, Q-Exactive and Triple Quad for Quantitative Bioanalysis of Oligonucleotide Therapeutics**; Yuhuan Ji[1]; Qian Liu[1]; Qian Li[1]; Chengjie Ji[1]; Laixin Wang[1]; *[1]NovaBioAssays, LLC, Woburn, MA*

TP 562 **A Micro-SPE-LC/MS/MS Quantitative Assay for Phosphorodiamidate Morpholino Oligomer (PMOplus®) AVI-7288 in HumanPlasma**; Aihua Liu[1]; Jianbo Zhang[2]; Qian Guo[1]; Bryce Ashby[1]; Scott Reuschel[1]; Jay S. Charleston[2]; Joe Rutkowoski[2]; Min Meng[1]; *[1]Covance, Salt Lake City, UT; [2]Sarepta Therapeutics, Cambirdge, MA*

TP 563 **Determination of a 15-mer Antisense Oligonucleotide in Mouse Plasma by LC-MS/MS**; Lili Xing[1]; Ying Han[1]; Yi Tao[1]; Xinping Fang[1]; Xin Zhang[1]; *[1]WuXi AppTec Co., Shanghai, CHINA*

TP 564 **A Sensitive Liquid Chromatogram/Mass Spectrometry Method for the Determination of a Therapeutic siRNA in Human Plasma**; Pei Li[1]; Dawei Zhou[1]; Xinping Fang[1]; *[1]WuXi AppTec Co., Plainsboro, NJ*

TP 565 **LC-MS/MS-based DNA Adduct Quantification for Assessing the Etiology and Prevention of Skin Cancer**; Yuxiang Cui[1]; Yinsheng Wang[2]; *[1]University of California, Riverside, Riverside, California; [2]University of California, Riverside, Riverside, CA*

TP 566 **Differential Mass Spectrometry Analysis of Transfer RNA by Stable Isotope Labelling**; Mellie Paulines[1]; Patrick A Limbach[1]; *[1]University of Cincinnati, Cincinnati, OH*

TP 567 **Evaluating the Specificity of RNase U2 Variants By Mass Spectrometry**; Beulah Mae Ann Solivio[1]; Ningxi

Yu[2]; Balasubrahmanyam Addepalli[2]; Patrick A Limbach[2]; *[1]University of Cincinnati, Cincinnati , Ohio; [2]University of Cincinnati, Cincinnati, OH*

TP 568 **Screening for Inflammation-induced DNA Adducts with a Comprehensive High Resolution LC-MS3 adductomic Approach**; Andrea Carra[1]; Peter W Villalta[1]; Romel P Dator[1]; Silvia Balbo[1]; *[1]Masonic Cancer Center, University of Minnesota, Minneapolis, MN*

TP 569 **Identification of Isomeric Mono-Methylated Nucleosides in Ribonucleic Acids by Liquid Chromatography – Highly Accurate Tandem Mass Spectrometry**; Hiroshi Nakayama[1]; Yoshio Yamauchi[2]; Masato Taoka[2]; Toshiaki Isobe[2]; *[1]RIKEN Center for Sustainable Resource Science, Wako, Japan; [2]Tokyo Metropolitan University, Tokyo, Japan*

TP 570 **Labeling tRNA Digestion Products using polyA Polymerase and Azido-modified NTPs**; Kayla Borland[1]; Patrick A Limbach[1]; *[1]University of Cincinnati, Cincinnati, OH*

TP 571 **High-Resolution/Accurate-Mass LC-MS3 Screening and SRM Relative Quantitation of DNA Adducts as Biomarkers of Drug Susceptibility**; Alessia Stornetta[1]; Peter W Villalta[2]; Stephen S Hecht[2]; Silvia Balbo[2]; Shana J Sturla[1]; *[1]ETH Zurich, Switzerland, CH; [2]Masonic Cancer Center, University of Minnesota, Minneapolis, MN*

TP 572 **Interaction of Antitumor Metallocenes with Nucleic Acids**; Rahel Patricia Eberle[1]; Stefan Schürch[1]; *[1]University of Bern, Bern, Switzerland*

TP 573 **Characterization of Amino Acid-Linked Platinum Complexes and Their Adducts to RNA Using Tandem Mass Spectrometry Approaches**; M. T. Rodgers[1]; C. C. Hech[1]; L. Hamlow[1]; Y. Zhu[1]; H. Roy[1]; S. Strobehn[1]; B. Kimuntai[1]; X. Bao[1]; C. S. Chow[1]; J. Gao[2]; G. Berden[2]; J. Oomens[2]; *[1]Wayne State University, Detroit, MI; [2]FELIX Facility, Radboud University, Nijmegen, The Netherlands*

TP 574 **Monitoring the Fe(II) Driven Reduction of AMP with Triple Quadrupole Mass Spectrometry**; Jacqueline N Howard[1]; Molly T Soper-Hopper[1]; Jessica C Bowman[1]; Ramanarayanan Krishnamurthy[2]; Loren Dean Williams[1]; Facundo M Fernandez[1]; *[1]Georgia Institute of Technology, Atlanta, USA; [2]The Scripps Research Institute, La Jolla, CA*

TP 575 **RNA-small Molecule Complexes as Models for Salt Bridge and Hydrogen Bond Interactions**; Jovana Vusurovic[1]; Kathrin Breuker[1]; *[1]University of Innsbruck, Innsbruck, Austria*

TP 576 **Comparative Analysis of the Fragmentation of Modified and Unmodified Oligonucleotides**; Ning Li[1, 2]; Babak Basiri[1]; Michael G Bartlett[1]; *[1]University of Georgia, Chemistry Department Athens, GA; [2]Shenyang Pharamaceutical University, Shenyang, Liaoning*

TP 577 **Mapping Eukaryotic mRNA-binding Regions on Proteins using High Resolution Mass Spectrometry**; Meeli Mullari[1]; Nielsen Lund Michael[1]; *[1]Novo Nordisk Foundation Center for Protein Researc, Copenhagen, Denmark*

TP 578 **Förster Resonance Energy Transfer (FRET) Measurements to Probe the Conformation of Gaseous Oligonucleotide Duplexes in the Gas Phase**; Stephen Sciuto[1]; Rebecca A Jockusch[2]; *[1]The University of Toronto, Toronto, ON; [2]University of Toronto, Toronto, Ontario (ON)*

TP 579 **Mass Spectrometry-based Determination of the Complete Chemical Structure of Saccharomyces Cerevisiae Ribosomal RNAs.**; Masato Taoka[1]; Yuko Nobe[1]; Yuka Yamaki[1]; Hideaki Ishikawa[2]; Yoshio Yamauchi[1]; Nobuhiro Takahashi[2]; Hiroshi Nakayama[3]; Toshiaki Isobe[1]; *[1]Department of Chemistry, Tokyo Metropolitan Univ., Tokyo, Japan; [2]Tokyo University of Agriculture and Technology, Tokyo, Japan; [3]RIKEN, Wako, Japan*

TP 580 **Developing Novel Integrated LC-MS Workflows for Oligonucleotide Characterization, High Throughput Mass Confirmation and Impurity Profiling**; HENRY SHION [1]; Robert Birdsall[1]; Joe Fredette[1]; Ying-Qing Yu[1]; *[1]Waters Corporation, Milford, MA*

TP 581 **On-Line Monitoring of Oligonucleotide Manufacturing Using a Compact Mass Spectrometer**; Stilianos G. Roussis[1]; Andrew Rodriguez[2]; Isaiah Cedillo[2]; Josh Brooks[2]; Claus Rentel[2]; *[1]Ionis Pharmaceuticals, Inc., Carlsbad, CA; [2]Ionis Pharmaceuticals, Carlsbad, CA*

TP 582 **Use of Tricationic Ion-Pairing Compounds for the Detection of Nucleotides from Single Cells**; ye guan[1]; Rachel Vowcicefski[1]; Wei Rao[1]; Ning Pan[1]; Anthony Burgett[1]; Zhibo yang[1]; *[1]University of Oklahoma, department of Chemistry & Biochemistry, Norman, OK*

PEPTIDES: PTM IDENTIFICATION
583 - 605

TP 583 **Ultra-sensitive Motif-targeting Approach for Measurement of Tyrosine Phosphorylation Stoichiometry in EGFR**; Yen-Chen Liao[1, 2]; Chia-Feng Tsai[3]; Miao-Hsia Lin[1]; Pei-Yi Lin[1]; Yasushi Ishihama[3]; Yu-Ju Chen[1, 2]; *[1]Institute of Chemistry, Academia Sinica, Taipei, Taiwan (R.O.C); [2]Department of Chemistry, National Taiwan University, Taipei, Taiwan (R.O.C); [3]Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, Japan*

TP 584 **Subphosphoproteome Analysis Strategy to Identify Low-abundance Protein Phosphorylation**; Mingliang Ye[1]; Mingming Dong[1]; Yangyang Bian[1]; Lei Li[2]; Li S.-C. Shawn[2]; Hanfa Zou[1]; *[1]Dalian Institute Chemical Physics, CAS Dalian, China; [2]Western University, London, Canada*

TP 585 **Comprehensive Phosphoproteome Analysis Reveals Acetylation-engaged Enhancement of Thermogenesis in White Adipocytes**; Hsin-Yi Chang[1]; Kosaku Shinoda[2]; Shingo Kajimura[2]; Yasushi Ishihama[1]; *[1]Department of Molecular and Cellular Bioanalysis, Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, Japan; [2]UCSF Diabetes Center and Department of Cell and Tissue Biology, University of California, San Francisco, CA USA*

TP 586 **Identification of Complex Glycosylated and Disulfide-Bonded Peptides Presented by the MHC Class II Processing Pathway in Melanoma**; Stacy Malaker[1]; Michael J Ferracane[2]; Florence R Depontieu[3]; Angela L Zarling[1]; Jeffrey Shabanowitz[1]; Dina L Bai[1]; Engelhard H Victor[1]; Suzanne L Topalian[3]; Donald F Hunt[1]; *[1]University of Virginia, Charlottesville, VA; [2]University of Florida, Gainesville, Florida; [3]Johns Hopkins University School of Medicine, Baltimore, MD*

TP 587 **Development of Rapid LC-MS3 Methodology for In-depth Structural Analysis of Lewis Antigens and Their Sialylated Derivative Isomers using Authentic Standards**; Yaping Lin[1]; Chein-Hung Chen[2]; Fang-Chi Liu[2]; Chia-Lin Wu[2]; Jung-Lee Lin[2]; Chien-Tai Ren[2]; Chung-Yi Wu[2]; Chung-Hsuan Chen[2]; *[1]Academia sinica, Taipei, Taiwan; [2]Academia Sinica, Taipei, Taiwan*

TP 588 **Sialo-glycoproteomic Profiling using Zwitter-Ionic Hydrophilic Interaction Chromatography (ZIC-cHILIC)**; Yu-Hsien Lin[1]; Yi-Ju Chen[1]; Yu-Ju Chen[1]; *[1]Academia Sinica, Taipei, Taiwan*

TP 589 **Proteome Dynamics Reveal Temporal Regulation of O-GlcNAcylation/phosphorylation in Determining Apoptosis of Activated B Cells**; Hsin-Yi Wu[1]; Jung-Lin Wu[2, 3]; Cheng-Tsung Lu[4]; Yi-Ju Chen[5]; Tzong-Yi Lee[4]; Chih-Wei Chien[5]; Yi-Ting Wang[5]; Chun-Cheng Lin[6]; Kay-Hooi Khoo[7]; Yu-Ju Chen[5]; Kuo-I Lin[2]; *[1]Institute of Chemistry, Academia Sinica, Taipei, Taiwan; [2]Genomics Research Center, Academia Sinica, Taipei, Taiwan; [3]Institute and Department of Microbiology and Immunology, National Yang-Ming University, Taipei, Taiwan; [4]Department of Computer Science and Engineering, Yuan Ze University, Taipei, Taiwan; [5]Institute of Chemistry, Academia Sinica, Taipei, TAIWAN (R.O.C.); [6]Department of Chemistry, National Tsing Hua University, Taipei, Taiwan; [7]Institute of Biological Chemistry, Academia Sinica, Taipei, Taiwan*

TP 590 **Efficient Enrichment of SUMOylated Peptides from Alpha-lytic Protease Digest Using K- Ɛ -GG Remnant Immuno-affinity Purification**; Hongbo Gu[1]; Xiaoying Jia[1]; Jian Min Ren[1]; Elizabeth Komives[2]; Matthew P Stokes[1]; *[1]Cell Signaling Technology, Danvers, MA; [2]Department of Chemistry and Biochemistry, UCSD, La Jolla, CA*

TP 591 **An Improved Strategy for In-depth and Site-specific Analysis of the SUMO Proteome.**; Ivo A. Hendriks[1]; Clifford Young[1]; Michael L. Nielsen[1]; *[1]NNF Center for Protein Research, Copenhagen, Denmark*

TP 592 **Ubiquitinated Proteins in MDSC Exosomes Analyzed by High Resolution Tandem Mass Spectrometry**; Katherine Adams[1]; Yan Wang[1]; Suzanne Ostrand-Rosenberg[2]; Catherine Fenselau[1]; *[1]University of Maryland, College Park, MD; [2]University of Maryland, Baltimore County Baltimore, MD*

TP 593 **Low Mass Ions in Peptide CID Spectra are Diagnostic of Lysine Posttranslational Modifications**; Tobias Maile[1]; Tommy K Cheung[1]; Corey Bakalarski[1]; Marie Classon[1]; David Arnott[1]; *[1]Genentech Inc, South San Francisco, CA*

TP 594 **Quantitative Profiling of the Enzymatic Activity of the Protein Lysine Mono-methyltransferase SMYD2 using SILAC-based Proteomics**; Jonathan B Olsen[1]; Xing-Jun CAO[2]; Bomie Han[1]; Lisa Hong Chen[1]; Alexander Horvath[1]; Timothy I Richardson[1]; Robert M Campbell[1]; Benjamin A Garcia[2]; Hannah Nguyen[1]; *[1]Eli Lilly and Company, Indianapolis, IN; [2]University of Pennsylvania, Philadelphia, PA*

TP 595 **Characterizing Post-Translationally Modified Peptides by High-Resolution FAIMS Coupled to Electron Transfer Dissociation**; Matthew Baird[1]; Alexandre A Shvartsburg[1]; *[1]Wichita State University, Wichita, KS*

TP 596 **Innovative Characterization of Hair from pre-Hispanic Andean Mummies using Mass Spectrometry**; Margaux Fresnais[1]; Pascale Richardin[2]; Marcela Sepúlveda[3]; Emmanuelle Leize-Wagner[1]; Armelle Charrié-Duhaut[1]; *[1]Laboratoire de Spectrométrie de Masse des Interactions et des Systèmes (LSMIS), UMR 7140 CNRS-Université de Strasbourg, Strasbourg, France; [2]Centre de Recherche et de Restauration des Musées de France (C2RMF), Paris, France; [3]Laboratorio de Análisis e Investigación Arqueométricas, Instituto de Alta Investigación, University of Tarapacá, Arica, Chile*

TP 597 **Identification and Characterization of Covalent Modification of Catechol Estrogens on Proteins** ; Huei-Chen Liang[1]; Chieh-Ming Fang[1]; Ming-Chun Ku[1]; Shu-Hui Chen[1]; *[1]Chemistry Dept. NCKU, Tainan, Taiwan (R.O.C.)*

TP 598 **Comprehensive Analysis of Post-translational Modifications in Proteins Exposed to Metal Catalyzed Oxidation**; Martin Rykær[1]; Birte Svensson[2]; Kim Henriksen[3]; Per Hägglund[2]; *[1]Technical University of Denmark, Kgs Lyngby, Kgs Lyngby; [2]Technical University of Denmark, Systems biology, KGS Lyngby., DK; [3]Nordic Bioscience A/S, Herlev, DK*

TP 599 **Quantitative Profiling of Prokaryotic Post Translational Modifications**; Charles L Farnsworth[1]; Jian Min Ren[2]; Jake A Namaroff[2]; Xiaoying Jia[1]; Kimberly A Lee[2]; Matthew P Stokes[2]; *[1]Cell Signaling Technology, Danvers, MA; [2]Cell Signaling Technology, Inc. Danvers, MA*

TP 600 **Charged Isotope Tag Improves Identification of Hydrophobic Peptide-Ligand Adducts**; Melissa Budelier[1]; James Janetka[1]; Douglas Covey[1]; Alex Evers[1]; *[1]Washington University in St. Louis, St. Louis, MO*

TP 601 **Alkylamine Ion-pairing Agents for Improved Positive Mode Electrospray Ionization Analysis of Sulfated Peptides**; Phillip McClory[1]; Kristina Hakansson[1]; *[1]University of Michigan, Ann Arbor, MI*

TP 602 **N-Terminal Charged-based Fractional Diagonal Chromatography (ChaFRADIC) to Study Proteolytic Events in Procoagulant Platelets**; Fiorella Andrea Solari[1]; Saskia A. Venne[2]; Nadine J.A. Mattheij[3]; Julia M. Burkhart[2]; Frauke Swieringa[3]; Peter W. Collins[4]; Judith M.E.M Cosemans[3]; Albert Sickmann[2]; Johan W.M. Heemskerk[3]; René P Zahedi[2]; *[1]Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Dortmund, Germany; [2]Leibniz-Institut für Analyt. Wissensch. - ISAS -, Dortmund, Germany; [3]Department of Biochemistry, Cardiovascular Research Institute Maastricht (CARIM) Maastricht University Maastricht, Maastricht, Netherlands; [4]Arthur Bloom Haemophilia Centre, School of Medicine, Cardiff University, Cardiff, United Kingdom*

TP 603 **Utilizing TIMS Mass Spectrometry to Resolve Competitive Isomeric Post-Translational Modifications**; Joshua Silveira[1]; Joe Gomez[2]; Melvin Park[1]; Kristofer Fritz[3]; *[1]Bruker Daltonic, Billerica, MA; [2]University of Colorado, Anschutz Medical Campus, Aurora, CO; [3]University of Colorado, Anschutz Medical Campus, Denver, CO*

TP 604 **System-wide Analysis of the Human Arginine Methylome**; Sara C. Larsen[1]; Kathrine B. Sylvestersen[1]; Andreas Mund[1]; Maria V. Madsen[1]; David Lyon[1]; Jeremy A. Daniel[1]; Lars J. Jensen[1]; Michael L. Nielsen[1]; *[1]NNF Center for Protein Research, Copenhagen, DENMARK*

TP 605 **Method Development for Complete Mutation and Posttranscriptional Modification Characterization of KRAS4b using Recombinant Proteins in Combination with LC-MS/MS**; Zhaojing Meng[1]; William Gillette[1]; Stephen Andrew[1]; Ming Zhou[1]; *[1]Frederick National Laboratory for Cancer Research, Frederick, MD*

PHOSPHOPEPTIDES: QUANTITATIVE ANALYSIS
606 - 623

TP 606 **Multiplexed Targeted Analysis of Post-translational Modifications: Robust and Reproducible Quantitation using isobaric Labels and MS3 Analysis**; Brian Erickson[1]; Robert A Everley[1]; Christopher M Rose[1]; Alison R Erickson[1]; Steven P Gygi[1]; *[1]Harvard Medical School, Boston, MA*

TP 607 **Comparative Phosphoproteomic Analysis of Hippocampal Tissue in a Non-Human Primate Model of Type 1 Diabetes Maintained with Exogenous Insulin**; Fang-Ke Huang[1]; Jose Morales-Corraliza[2, 3]; Paul M. Mathews[2, 3]; Thomas A. Neubert[1]; *[1]Skirball Institute of Biomolecular Medicine, New York University School of Medicine, New York City, NY; [2]Center for Dementia Research, Nathan Kline Institute, Orangeburg, NY; [3]Department of Psychiatry, New York University Langone Medical Center, New York City, NY*

TP 608 **Large-scale Targeted Analysis of Post-translational Modifications by Internal Standard-Triggered Parallel Reaction Monitoring: Application to Determination of Phosphorylation Site Occupancy**; Bruno Domon[1]; Sara Rosati[1]; Adele Bourmaud[1]; Sebastien Gallien[1]; *[1]Luxembourg Clinical Proteomics Center, Strassen, Luxembourg*

TP 609 **Global Phosphoproteomics of Targeted Combinatorial Therapy in Hepatocellular Carcinoma to Identify Molecular Signatures of Effective Therapy**; Joseph Capri[1]; Whitaker Cohn[1]; Thuc Le[1]; Kym F Faull[1]; Julian P Whitelegge[1]; *[1]UCLA, Los Angeles, CA*

TP 610 **Quantitative Analysis of the Cdk-dependent Phosphoproteome in S. Pombe using SILAC and Tandem Mass Tags**; Andrew W Jones[1, 2]; Matthew Swaffer[2]; Jenny T.C Ho[3]; Helen Flynn[1]; Paul Nurse[2]; Gary Woffendin[3]; Madalina Oppermann[3]; Ambrosius P Snijders[1]; *[1]Proteomics Technology Platform, The Francis Crick Institute, London, UK; [2]Cell Cycle Laboratory, The Francis Crick Institute, London, UK; [3]Thermo Fisher Scientific, Hemel Hempstead, Hemel Hempstead, UK*

TP 611 **Phosphoproteome Analysis Reveals Rapid Reprogramming of Signaling Networks of Drug Treated Cancer Cells**; Heiner Koch[1, 2, 3]; Melanie Schoof[1]; Benjamin Ruprecht[1]; Susan Klaeger[1]; Scarlet Beck[4]; Martin Frejno[1, 5]; Mathias Wilhelm[1]; Hannes Hahne[6]; Bernhard Kuster[1, 2, 3, 7]; *[1]Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; [2]German Cancer Consortium (DKTK), Muenchen, Germany; [3]German Cancer Research Center, Heidelberg, Germany; [4]Max Planck Institute for Biochemistry, Martinsried, Germany; [5]Oxford University, Oxford, United Kingdom; [6]OmicScouts GmbH, Freising, Germany; [7]Center for Integrated Protein Science, Munich, Germany*

TP 612 **Effect of Exercise on Skeletal Muscle Phosphoproteome in Obese Insulin Resistant Adults**; Danjun Ma[1]; Lisa Guth[2]; Yue Qi[1]; Michael Caruso[1]; Xiangmin Zhang[1]; Jeffrey Horowitz[2]; Zhengping Yi[1]; *[1]Wayne State University, Detroit, MI; [2]University of Michigan, Ann Arbor, MI*

TP 613 **Quantitative Phosphoproteomic Analysis of Circadian Cycling in Genetically Modified Arabidopsis**; Jae Choi[1]; Jenny Chen[2]; John D Rogers[1]; Dmitri A Nusinow[3]; Bradley S Evans[3]; *[1]Thermo Fisher Scientific, Rockford, IL; [2]Thermo Fisher Scientific, San Jose, CA; [3]Donald Danforth Plant Science Center, St Louis, MO*

TP 614 **Differential Mass Spectrometry Analysis Reveals Differential Hypoxic Response in Ovarian Cancer Cells with Different Metastatic Potential**; Xuemei Zeng[1]; Huang Huang[1]; Xin Huang[1]; Nathan A Yates[1]; *[1]University of Pittsburgh, Pittsburgh, PA*

TP 615 **Rapid Quantitative Phosphoproteome by Tandem Mass Tags**; Haiyan Tan[1]; Bing Bai[2]; Xusheng Wang[2]; Yuxin Li[2]; Ji-Hoon Cho[2]; Tim Shaw[2]; Junmin Peng[2]; *[1]St.Jude Children's Research Hospital, memphis, TN; [2]St Jude Children's Research Hospital, Memphis, TN*

TP 616 **High Throughput Multiplexed Phosphoproteomics Identifies Drivers of Resistance to ALK Inhibitor Treatment in Lung Cancer**; Amanda L. Edwards[1, 2]; Luc Friboulet[1, 2]; Rosa Frias[1, 2]; Kristine Yu[3]; David Ruddy[3]; Jeffrey A. Engelman[1, 2]; Wilhelm Haas[1, 2]; *[1]Massachusetts General Hospital Cancer Center, Charlestown, MA; [2]Harvard Medical School, Boston, MA; [3]Translational Clinical Oncology, Novartis Institutes for Biomedical Research, Cambridge, MA*

TP 617 **Inferring Kinase Network Activity from Activation-loop Phosphopeptides by Data-Independent Acquisition MS**; Sander Piersma[1]; Richard R de Haas[1]; Jaco C Knol[1]; Thang V Pham[1]; Henk MW Verheul[1]; Connie R Jimenez[1]; *[1]VU University medical center, Amsterdam, The Netherlands*

TP 618 **Prediction of Protein Kinase Substrates using Primary Sequence Preference and Quantitative Phosphoproteomics**; Haruna Imamura[1]; Pasrawin Taechawattananant[1]; Omar Wagih[2]; Naoyuki Sugiyama[1]; Pedro Beltrao[2]; Yasushi Ishihama[1]; *[1]Kyoto University, Kyoto, Japan; [2]European Bioinformatics Institute, European Molecular Biology Laboratory, Hinxton, Cambridge, United Kingdom*

TP 619 **Absolute Quantitation of Site-specific Phosphorylation of Insulin Receptor by A Nano UPLC-MS Method**; Zhongping Liao[1]; Kyoung-soo Choi[1]; Jason X Tang[1]; *[1]Eli Lilly and Company, Indianapolis, IN*

TP 620 **Evaluation of Search Engines for Phosphopeptide Identification and Quantitation**; Xiaoyue Jiang[1]; David M Horn[1]; Ryan D Bomgarden[2]; Tara Schroeder[3]; Rosa I Viner[1]; Andreas Huhmer[1]; Steven Danielson[4]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Rockford, IL; [3]Thermo Fisher Scientific, Somerset, NJ; [4]Thermo Fisher, San Jose, CA*

TP 621 **Dimethylated Alanine (DiAla)-assisted Large-scale Protein Phosphorylation Stoichiometry Characterization**; Qing Yu[1]; Yu Feng[2]; Lingjun Li[1]; *[1]University of Wisconsin-Madison, Madison, Wisconsin; [2]University of Wisconsin-Madison, Madison, WI*

TP 622 **High Resolution-Enabled 12-plex DiLeu Tagging for Quantitative Phosphoproteomics Profiling of Vascular Smooth Muscle Cells**; Xiaofang Zhong[1]; Christopher Lietz[1]; Xudong Shi[1]; Amanda Buchberger[1]; Dustin Frost[1]; Craig Kent[1]; Lingjun Li[1]; *[1]University of Wisconsin-Madison, Madison, WI*

TP 623 **Sensitive and Accurate Quantitation of Phosphopeptides using TMT Isobaric Labeling Technique**; Xiaoyue Jiang[1]; Ryan D Bomgarden[2]; Rosa I Viner[1]; Andreas Huhmer[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Rockford, IL*

PROTEINS: COMPLEXES/NON-COVALENT INTERACTIONS
624 - 659

TP 624 **Using Native MS to inform Statistical Thermodynamic Models of Cooperativity**; Melody Pepsi Holmquist[1]; Elihu C Ihms[1]; Vicki H Wysocki[1]; Mark P Foster[1]; *[1]Ohio State University, Columbus, OH*

TP 625 **Native MS analysis of chemically stabilized protein complexes: evidence for non-covalent stabilization of protein-protein interactions**; Roman Subbotin[1]; Dominic Paul B Olinares[1]; Julio C Padovan[1]; Megan Kelley[1]; Zheng Ser[1]; Brian T Chait[1]; *[1]The Rockefeller University, New York, NY*

TP 626 **Probing Nucleotide-dependent Changes in the Oligomeric State of MORC Proteins using Native Mass Spectrometry**; Jonathan Johnston[1]; Linda Yen[2]; Steven E Jacobsen[2]; Alma L Burlingame[1]; *[1]UCSF, San Francisco, CA; [2]UCLA, Los Angeles, CA*

TP 627 **Characterization of a Protein-DNA Complex by Native Mass Spectrometry and Ultraviolet Photodissociation**; Jake Rosenberg[1]; Alyssa Garabedian[2]; Fenfei Leng[2]; Francisco Fernandez-Lima[2]; Jennifer S Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX; [2]Florida International University, Miami, FL*

TP 628 **Investigating the Gas-Phase Conformation of Fibroblast Growth Factor 1 upon Binding of Heparin/HS Using Traveling Wave Ion Mobility Spectrometry (TWIMS)**; Yuejie Zhao[1]; Jon Amster[1]; Arunima Singh[2]; Robert Woods[2]; Yongmei Xu[3]; Jian Liu[3]; Chengli Zong[2]; Geert-Jan Boons[2]; Fuming Zhang[4]; Robert Linhardt[4]; *[1]University of Georgia, Chemistry Department Athens, GA; [2]University of Georgia, CCRC Athens, GA; [3]University of North Carolina, Chapel Hill, NC; [4]Rensselaer Polytechnic University, Troy, NY*

TP 629 **Screening Glycolipids Against Proteins *in vitro* using Picodiscs and Electrospray Ionization Mass Spectrometry**; Jun Li[1]; Xuxin Fan[1]; Elena N Kitova[1]; John S Klassen[1]; *[1]University of Alberta, Edmonton, AB, Canada*

TP 630 **Detecting Protein-Glycolipid Interactions using Glycomicelles and CaR-ESI-MS**; Ling Han[1]; Elena N Kitova[1]; John S Klassen[1]; *[1]University of Alberta, Edmonton, Canada*

TP 631 **Characterization of Heparin Interactions with its Client Proteins: Mapping Minimal Protein-Binding Domains within Glycosaminoglycan Chains using Top-down mass spectrometry**; Yunlong Zhao[1]; Igor A Kaltashov[1]; *[1]University of Massachusetts Amherst, Amherst, MA*

TP 632 **Screening Human Milk Oligosaccharides Against Proteins using Catch-and-Release Electrospray Ionization Mass Spectrometry**; Yajie Chen[1]; Km Shams-Ud-Doha[1]; Elena N Kitova[1]; Lars Bode[2]; John S Klassen[1]; *[1]University of Alberta, Edmonton, Canada; [2]University of California, San Diego La Jolla, CA*

TP 633 **Label Free, LC-MS Based Approaches to Quantitate Small Molecule-Receptor Binding**; Xun Chen; *Merck Research Labs, Kenilworth, NJ*

TP 634 **Label-free Size Exclusion Chromatography Mass Spectrometry for the Characterization of Protein Complex Composition and Stability**; Paola Cavaliere[1]; Nadia Iqbal[1]; Noah E. Dephoure[1]; *[1]Weill Cornell Medical College, New York, NY*

TP 635 **Information-Rich Gas-Phase Analysis of Non-Covalent Protein Complexes and Released Subunits for Primary and Quaternary Structure Analysis**; Deepali Rathore[1]; Forouzan Aboufazeli[1]; Eric D. Dodds[1]; *[1]University of Nebraska-Lincoln, Lincoln, NE*

TP 636 **Study of Noncovalent Interactions of Hydroxylated Polybrominated Diphenyl Ethers with Serum Albumins and Estrogen Receptors Using Ion Mobility Spectrometry-Mass Spectrometry**; Qiang Ma[1]; Liang-Hong Guo[2]; *[1]Chinese Academy of Inspection and Quarantine, Beijing, CHINA; [2]Chinese Academy of Sciences, Beijing, CHINA*

TP 637 **Investigating The Noncovalent Complex Formation of Proteins with Electrolytic Ligands in Gas Phase**; Mehmet Atakay[1]; Haci Mehmet Kayili[1, 2]; Bekir Salih[1]; *[1]Hacettepe University, Department of Chemistry, Ankara, Turkey; [2]Çankırı Karatekin University, Çankiri, Turkey*

TP 638 **Probing the Stability of Noncovalent Interactions Responsible for Covalently Linked Diubiquitin Ion Structure using nESI-TWIMS-MS and CIU**; Nicole Wagner[1]; David H Russell[1]; *[1]Texas A&M University, College Station, TX*

TP 639 **Identification of Grp78/BiP Protein Complexes using Affinity Mass Spectrometry**; Dapeng Chen[1]; Yan Wang[1]; Eva R. Chin[1]; *[1]University of Maryland, College Park, MD*

TP 640 **Comparison of Affinity-Purification Mass Spectrometry Workflow for Charcaterisation of Protein Complexes**; Lu Yu[1]; Mercedes Pardo[2]; Jyoti Choudhary[2]; *[1]Wellcome Trust Sanger Institute, Hinxton, Cambridgeshire; [2]Wellcome Trust Sanger Institute, Cambridge, United Kingdom*

TP 641 **Application of Affinity-purification Mass Spectrometry Based Predictive Mapping for Identification of RBM45 Protein Interactors in Amyotrophic Lateral Sclerosis**; Krystine Garcia[1]; Yang Li[2]; Mahlon Collins[2, 3]; Jiyan An[2]; Rachel Geiser[2]; Tony Tegeler[1]; Kristine Tsantilas[1]; Robert Bowser[2, 3]; Patrick Pirrotte[1]; *[1]TGen, Phoenix, AZ; [2]St. Joseph's Hospital and Medical Center, Phoenix, AZ; [3]University of Pittsburgh School of Medicine, Pitts, PA*

TP 642 **Nanoprobe-based Affinity Mass Spectrometry for Identification of Binding Glycotopes and Protein-Protein Interaction of Galectin-8**; Pin-Rui Su[1]; Chen Yi-Ju[2]; Lin Yu-Hsien[3]; Chen Yu-Ju[2]; *[1]Department of Chemistry, National Taiwan University, Taipei, Taiwan; [2]Institute of Chemistry, Academia Sinica, Taipei, Taiwan; [3]Department of Chemistry, National Taiwan Normal University, Taipei, Taiwan*

TP 643 **Site-specific Characterization of Binding Interfaces in Gaseous HIV-1 RNA-protein Complexes**; Eva-Maria Schneeberger[1]; Kathrin Breuker[1]; *[1]University of Innsbruck, Innsbruck, Austria*

TP 644 **Novel Blue-Native-PAGE and Targeted Mass Spectrometry Strategy Enable robust and Accurate Quantification of the Kinetics of Protein-Ligand Interactions in Plasma**; Shichen Shen[1]; Xiaotao Duan[2]; Bo An[1]; Yang Qu[1]; Joseph Balthasar[1]; Jun Qu[1]; *[1]University at Buffalo, Buffalo, NY; [2]Beijing Proteome Research Center, Beijing, China*

TP 645 **A New Carbene Probe for Efficient Protein Footprinting Allows Mapping of Binding Sites by Mass Spectrometry**; Lucio Manzi[1]; Andrew Barrow[1]; Daniel Scott[1]; Robert Layfield[1]; Timothy Wright[1]; John Moses[1]; Neil Oldham[1]; *[1]University of Nottingham, Nottingham, UK*

TP 646 **Charting the Temporal Landscape of EGF-stimulated EGFR Proteome** ; Yue Chen[1]; Sung Yun Jung[1]; Mei Leng[1]; Jong Min Choi[1]; Antrix Jain[1]; Anna Malovannaya[1]; Yi Wang[1]; Jun Qin[1]; *[1]Baylor College of Medicine, Houston, TX*

TP 647 **Development of a Novel Bioanalytical Platform for Anti-Drug Antibody using Immunocapture-LC/MS**; Lin-Zhi Chen[1]; David Roos[2]; Elsy Philip[2]; *[1]Boehringer Ingelheim Pharmaceuticals, Inc., Ridgefield, CT; [2]Boehringer Ingelheim Pharmaceuticals, Inc, Ridgefield, CT*

TP 648 **Novel Regulators of Alternative NF-kB Pathway Identified through Chemical Proteomics**; Bekim Bajrami[1]; Michelle Ols[1]; John Anderson[1]; Benbo Gao[1]; Brian Lucas[1]; Erik Hett[1]; Alan Buckler[1]; Peter Juhasz[1]; Ru Wei[1]; *[1]Biogen Inc., Cambridge, MA*

TP 649 **Proteomic Analysis Provides Clues about Normal FUS Function and Its Role in ALS**; Jing Chen[1]; Marisa Kamelgarn[1]; Alexandra Arenas[1]; Jianjun Zhai[1]; Haining Zhu[1]; Jozsef Gal[1]; *[1]University of Kentucky, Lexington, KY*

TP 650 **Global Analyses of the Oligomerization, Composition, and Dynamics of Membrane-Associated Protein Complexes**; Zach McBride[1]; Aryal Uma[1]; Chen Donglai[1]; Jun Xie[1]; Daniel Szymanski[1]; *[1]Purdue University, West Lafayette, IN*

TP 651 **Mass Spectrometry Cleavable Cross-linking Approach for Large-scale Identification of Protein-Protein Interactions**; Jayanta Kishor Chakrabarty[1]; Apeksha Bhatt[1]; Saiful M Chowdhury[1]; *[1]University of Texas at Arlington, Arlington, TX*

TP 652 **Relative Abundance Comparative Analysis of ROS-induced Poly(ADP-ribose)-Associated Proteins by LC-MS/MS and Spectral Counting**; Argel Islas-Robles[1, 2]; Frances M Munoz[3]; Serrine S Lau[2]; Terrence J Monks[2]; *[1]University of Arizona, Tucson, AZ; [2]Wayne State University, Detroit, MI; [3]Drexel University, Philadelphia, PA*

TP 653 **Fourier Transform Algorithm for Analysis of Mass Spectra for Heterogeneous Ions with Repeated Subunits**; Sean P Cleary[1]; Jesse W Wilson[1]; Avery M Thompson[1]; James Prell[1]; *[1]University of Oregon, Eugene, OR*

TP 654 **Development of Mass Spectrometry Method for the Unbiased Detection of Cytomegalovirus Proteins in Human Brain Tumor Specimens**; Dhiman Ghosh[1]; Brian P Milless[2]; Philip R Gafken[3]; Charles S Cobbs[1]; *[1]Swedish Neuroscience Institute, Seattle, Washington; [2]Fred Hutchinson Cancer Research Center, Seattle, Washington; [3]Fred Hutchinson Cancer Research Center, Seattle, WA*

TP 655 **Edgotypes and Quantitative Mass Spectrometry**; James Bruce[1]; Juan Chavez[1]; Jimmy K Eng[1]; Arti Navare[1]; Devin Schweppe[1]; Xia Wu[1]; Xuefei Zhong[1]; *[1]University of Washington, Seattle, WA*

TP 656 **Histidine, Arginine's Versatile Cousin**; Amina S Woods[1]; Ludovic Muller[1]; Aurelie Roux[2]; Damon Barbacci[3]; Shelley N Jackson[1]; *[1]NIH/NIDA-IRP, Baltimore, MD; [2]All Children's Hospital Johns Hopkins Medicine, Saint Petersburg, FL; [3]Ionwerks Inc, Houston, TX*

TP 657 **Examination of Aptamer-Protein Complex Structure by Mass Spectrometry**; Guo-Ming Hung[1]; Pang-Hung Hsu[1]; *[1]Department of Bioscience and Biotechnology, National Taiwan Ocean University, Keelung, Taiwan*

TP 658 **Cross-linked PSMs in pepXML: a Common Format for Storing Cross-linked Search Results**; Michael R. Hoopmann[1]; Luis Mendoza[1]; Eric W. Deutsch[1]; David Shteynberg[1]; Robert L Moritz[1]; *[1]Institute for Systems Biology, Seattle, WA*

TP 659 **The Analysis and Identification of STAT3 Interactions and Modifications in the Mitochondria of Cancer Cells**; Daniel Garama[1]; Ching-Seng Ang[2]; Nick Williamson[2]; Daniel Gough[1]; *[1]Hudson Institute of Medical Research, Melbourne, Australia; [2]Bio 21 Institute, Melbourne, Australia*

PROTEOMICS: CLINICAL APPLICATIONS (DEVELOPMENT TOWARD CLINICAL APPLICATION)
660 - 681

TP 660 **Proteomic Profiling of Human Islets Collected from Pancreatic Tissue Sections using Laser Capture Microdissection**; Lina Zhang[1]; Giacomo Lanzoni[2]; Matteo Battarra[2]; Luca Inverardi[2]; Qibin Zhang[3]; *[1], Kannapolis, NC; [2]Diabetes Research Institute, University of Miami, Miami, FL; [3]Department of Chemistry & Biochemistry, University of North Carolina at Greensboro,, Greensboro, NC*

TP 661 **Using Quantitative Proteomics to Profile Changes in Individual Immune Cell Types during an Immune Response**; Allison Galassie[1]; Johannes Goll[2]; Parimal Samir[3]; Travis Jensen[2]; Kristen L Hoek[4]; Leigh M Howard[5]; Tara M Allos[4]; Xinnan Niu[4]; Sebastian Joyce[4, 6]; Kathryn M Edwards[5]; Andrew J Link[4]; *[1]Department of Chemistry, Vanderbilt University, Nashville, TN; [2]The EMMES Corporation, Rockville, MD; [3]Department of Biochemistry, Vanderbilt University School of Medicine, Nashville, TN; [4]Department of Pathology, Microbiology, and Immunology, Vanderbilt University School of Medicine, Nashville, TN; [5]Vanderbilt Vaccine Research Program; Division of Infectious Diseases, Department of Pediatrics, Vanderbilt University School of Medicine, Nashville, TN; [6]Veterans Administration Tennessee Valley Healthcare System, Nashville, TN*

TP 662 **LC-MRM Quantification of Protein Biomarkers in Human Saliva: In Saliva Veritas?**; Jerome Vialaret[1]; Nora Nowak[1]; Audrey Gabelle[2]; Sylvain LEHMANN[1]; Christophe Hirtz[1]; *[1]LBPC, IRMB CHU Montpellier St. Eloi Montpellier, France; [2]Centre Memoire Ressources Recherche Languedoc-Roussillon, CHU Montpellier, Montpellier, France*

TP 663 **Elucidating Cellular Heterogeneity in Tumors: a Combination of Antibody-Based Cellular Pre-Fractionation and Ultrasensitive Proteomics**; Evelyne Maes[1]; Nathalie Cools[2]; Inge Mertens[1, 3]; Dirk Valkenborg[1, 3, 4]; Patrick Pauwels[5]; Geert Baggerman[1, 6]; *[1]VITO, Mol, Belgium; [2]Laboratory of Experimental Hematology, Vaccine & Infectious Disease Institute (VAXINFECTIO), University of Antwerp, Antwerp, Belgium; [3]Center for Proteomics, Antwerp, Belgium; [4]Interuniversity Institute for Biostatistics and Statistical Bioinformatics, Hasselt University, Diepenbeek, Belgium; [5]Pathology Department, University Hospital Antwerp (UZA), Antwerp, Belgium; [6]Center for Proteomics, Antwerp, Belgium*

TP 664 **LC-MS Platform for Identifying Protein Targets of Small-Molecule Binding Relevant to Disease and Metabolism**; Reid O'Brien Johnson[1]; Brett Lomenick[1]; Jing Huang[1]; Joseph A Loo[1]; *[1]UCLA, Los Angeles, CA*

TP 665 **Simple, Robust, Highly Productive Methodology for LC-MS/MS Quantitative Analysis of Laser Capture Microdissected Tissue from FFPE Biopsies Requiring 10,000 Cells**; John P Shapiro[1]; Hannah Komar[1]; Phil Gafken[2]; Philip Hart[1]; Darwin Conwell[1]; Gregory Lesinski[1]; *[1]Ohio State University, Columbus, Ohio; [2]Fred Hutchinson Cancer Research Center, Seattle, WA*

TP 666 **Quantifying Signalling Pathway Activity using iMALDI (immuno-MALDI)**; Robert Popp[1]; Andrew G Chambers[1]; Adriana Aguilar-Mahecha[2]; Oliver Pötz[3]; Mark Basik[2]; Christoph H. Borchers[4, 5, 6]; *[1]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [2]Department of Oncology, McGill University, Montreal, QC, Canada; [3]Natural and Medical Sciences Institute (NMI) at the University of Tübingen, Reutlingen, Germany; [4]University of Victoria - Genome BC Proteomics Centre, Victoria, BC; [5]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada; [6]Segal Cancer Proteomics Center, Lady Davis Institute, McGill University, Montreal, QC, Canada*

TP 667 **Automation of an immuno-MALDI assay for Quantifying Signalling Pathway Activity**; Robert Popp[1]; Björn Fröhlich[1]; Andrew G Chambers[1]; Yassene Mohammed[1, 2]; Adriana Aguilar-Mahecha[3]; Oliver Pötz[4]; Mark Basik[3]; Christoph H. Borchers[1, 5, 6]; *[1]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [2]Center for Proteomics and Metabolomics, Leiden University Medical Center, Leiden, The Netherlands; [3]Department of Oncology, McGill University, Montreal, QC, Canada; [4]Natural and Medical Sciences Institute (NMI) at the University of Tübingen, Reutlingen, Germany; [5]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada; [6]Segal Cancer Proteomics Center, Lady Davis Institute, McGill University, Montreal, QC, Canada*

TP 668 **Can volumetric Absorptive Micro Sampling in the Presence of a Stable-Isotope Labeled Protein Standard Control Pre-Analytical Variability in Proteomics?**; Irene van den Broek[1]; Qin Fu[1]; Kevin Millis[2]; Timothy Eckersley[2]; William W Wood[2]; Michael P Kowalski[3]; Tara R Jones-Roe[3]; Stuart Kushon[4]; Bobby Virasingh[4]; Jennifer E Van Eyk[1]; *[1]Advanced Clinical Biosystems Research Institute, Heart Institute, Cedars Sinai Medical Center, Los Angeles, CA; [2]Cambridge Isotope Laboratories, Inc. Tewksbury, MA; [3]Beckman Coulter Life Sciences, Indianapolis, IN; [4]Neoteryx, Torrance, CA*

TP 669 **Methodological Advances Applied to a Biomarker Study of Complex Samples from a Diseaded Clinical Cohort of Limited Sample Availability**; Stephen Kostel[1]; Patricia Cho[1]; Hui Zhou[1]; John Froehlich[1]; Richard Lee[1]; *[1]Boston Children's Hospital, Harvard Medical School Boston, MA*

TP 670 **Combined Analysis of Nucleic Acids and Protein for Cancer Research**; Jared Isaac[1]; Mazi Mohiuddin[2]; *[1]Thermo Fisher Scientific , Kalamazoo, MI; [2]Thermo Fisher Scientific, San Jose, CA*

TP 671 **Human Plasma Proteome Analysis using Meter-Long Monolithic Silica Columns with Match-between-Runs**; Yi Ting Wang[1]; Chia-Feng Tsai[2]; Kazuhiro Sonomura[1, 3]; Yasushi Ishihama[2]; Fumihiko Matsuda[1]; *[1]Center for Genomic Medicine, Graduate School of Medicine Kyoto University, Kyoto, Japan; [2]Graduate School of Pharmaceutical Sciences Kyoto University, Kyoto, Japan; [3]Life Science Research Center, Technology Research Laboratory, Shimadzu Corporation, Kyoto, Japan*

TP 672 **A Chromosome-Centric Protein-Protein Interaction Profiling of MS-Based Proteome Datasets Derived from Laser-Microdissected Cancerous Cells of Lung Cancer Subtypes**; Kiyonaga Fujii[1]; Hiroyuki Kimura[1]; Hideki Marushima[1]; Rie Tagaya[1]; Hisashi Saji[1]; Noriaki Kurimoto[1]; Sayaka Mikami[2]; Yasuhiko Bando[2]; Noboru Nakayama[1, 2]; Harubumi Kato[3]; Toshihide Nishimura[1, 2]; Haruhiko Nakamura[1]; *[1]St. Marianna University School of Medicine, Meguro-ku, Tokyo; [2]Biosys Technologies, Inc., Tokyo, Japan; [3]Niizashiki Central General Hospital, Saitama, Japan*

TP 673 **High-resolution Quantitative Metaproteomics Pipe-Line: Documenting Effects of Dietary Changes**; Boris Zybaylov[1]; Stephanie Byrum[1]; Galina Glazko[1]; Lisa Orr[1]; Dorothy Kieffer[2]; Sean Adams[1]; Samuel Mackintosh[1]; John Arthur[1]; Brian D. Piccolo[1]; Nosratola D. Vaziri[3]; Shuman Liu[3]; Wei L. Lau[3]; Mahyar Khazaeli[3]; Mary E. Moore[4]; Roy J. Martin[5]; *[1]University of Arkansas for Medical Sciences, Little Rock, AR; [2]University of California, Davis, Davis, CA; [3]Division of Nephrology, University of California, Irvine, Irvine, CA; [4]Dept. of Food Science and Technology, University of California, Davis, Davis, CA; [5]Obesity & Metabolism Research Unit, USDA, Davis, CA*

TP 674 **Investigation of Neutrophilic Proteins/Peptides in Periprosthetic Tissue by MALDI Imaging Mass Spectrometry**; Rémi Longuespée[1]; Rita Casadonte[1]; Mark

Kriegsmann[2]; Mike Otto[1, 3]; Sascha Gravius[4]; Thomas Randau[4]; Soeren-Oliver Deininger[5]; Edwin De Pauw[6]; Jörg Kriegsmann[1, 3]; *[1]Proteopath GmbH, Trier, Germany; [2]University of Heidelberg, Heidelberg, Germany; [3]Center for Histology Cytology and Molecular Diagnostics, Trier, Germany; [4]University Bonn, Bonn, Germany; [5]Bruker Daltonik, Bremen, Germany; [6]University of Liege, GIGA-Proteomics Liege, Belgium*

TP 675 **Generation of High Quality MALDI-TOF Serum Mass Spectra to Detect Hepatocellular Carcinoma in High-Risk Patients**; Nicholas F Dupuis[1]; Maximillian Steers[1]; Alex A Nickel[1]; Gary P Pestano[1]; *[1]Biodesix, Inc., Boulder, Colorado [CO]*

TP 676 **Correlating Apolipoprotein Proteoform Profiles to Cardiovascular Disease Risk Factors: a Translational Top-Down Proteomics Approach to Pathophysiology**; Henrique dos Santos Seckler[1]; Kyunggon Kim[1]; Luca Fornelli[1]; Paul M Thomas[1]; Philip Compton[1]; John T Wilkins[2]; Neil L Kelleher[1]; *[1]Northwestern University, Evanston, IL; [2]Northwestern Feinberg School of Medicine, Chicago, IL*

TP 677 **Application of Tissue Surrogate for Variance Calibration in Mass Spectrometry Based Amyloidosis Diagnosis**; Han-Yin Yang[1]; Andrew N Hoofnagle[1]; Michael J MacCoss[1]; *[1]University of Washington, Seattle, WA*

TP 678 **Quantitative Analysis of Protein Composition in Amyloid Plaques from FFPE Specimens using Parallel Reaction Monitoring (PRM)**; Maria Stella Ritorto[1]; Oana Madalina Mereuta[1]; Janine Pichardo[1]; Ahmet Dogan[1]; *[1]Memorial Sloan Kettering Cancer Center, New York, NY*

TP 679 **Analysis of Native Proteolytic BNP Variants: Simultaneous Separation of Multiple Samples using Capillary Electrophoresis-Mass Spectrometry with Multi-Segment Injection**; Shenyan Zhang[1]; Koen Raedschelders[1]; Jennifer Van Eyk[1]; *[1]Barbra Streisand Women's Heart Center, Heart Institute, Cedars-Sinai Medical Center, Los Angeles, CA - California*

TP 680 **Implementation of siKALIP to Identify the Substrates of CDKL5, a Kinase Linked to Severe Neurodevelopmental Disorders**; Justine Arrington[1]; Juan Sebastian Paez Paez[2]; Weiguo Andy Tao[1]; *[1]Purdue University, West Lafayette, IN; [2]National University of Colombia, Bogota, Colombia*

TP 681 **Dried Blood Spots as a Simple Sample Collection Tool for Personalized Medicine**; Jeffrey J. Jones[1]; Ryan Benz[1]; Phong Cun[1]; William Smith[1]; John Blume[1]; *[1]Applied Proteomics Inc., San Diego, CA*

PROTEOMICS: INFECTIOUS DISEASES
682 - 702

TP 682 **Characterization of the Host Proteome within Virion Particles of Sindbis Virus**; Andrew Kilianski[1]; Amanda Piper[2]; Vancini Ricardo[2]; Raquel Hernandez[2]; Trevor Glaros[1]; *[1]ECBC, Apg, MD; [2]North Carolina State University, Raleigh, North Carolina*

TP 683 **Mass Spectrometric Analysis of the Human Pathogen Cryptosporidium parvum**; John Robert Haserick[1]; Deborah R Leon[1]; Yi Pu[1, 2]; John Crawford Samuelson[1, 3]; Catherine E Costello[1]; *[1]Boston University School of Medicine, Boston, MA; [2]Boston University, Boston, MA; [3]Boston University School of Dental Medicine, Boston, MA*

TP 684 **The Detection of a Clinically Relevant ß-lactamase, CTX-M-15, Using MALDI-TOF MS**; Jonathan B. Thacker[1]; Brad S. Pierce[1]; Kevin A. Schug[1]; *[1]University of Texas at Arlington, Arlington, TX*

TP 685 **Pseudomonas aeruginosa Develops Ciprofloxacin Resistance from Low to High Level with Distinctive Proteome Changes**; Jianhe Peng[1]; Jeffrey Hill[2]; *[1]Experimental Therapeutics Centre, A-STAR,Singapore, Singapore, Singapore; [2]Experimental Therapeutics Centre, A-STAR, Singapore, Singapore*

TP 686 **Proteomics Analysis of Chlamydia trachomatis: Virulence-Plasmid Mediated Protein Expression Changes**; Christopher C R Grant[1]; Stuart McCorrister[1]; Michael Patton[2]; Harlan Caldwell[2]; Garrett R Westmacott[1]; Grant McClarty[1]; *[1]National Microbiology Laboratory, Public Health Agency of Canada, Winnipeg, Canada; [2]Chlamydial Diseases Section, Laboratory of Clinical Infectious Diseases NIAID, NIH, Bethesda, MD - Maryland*

TP 687 **Mass Spectrometry Based Studies on Irreversible Inhibition of Recombinant Mycobacterium Tuberculosisshikimate Kinase by the Marine Sponge Metabolite Ilimaquinone**; Angela Calderon[1]; Johayra Simithy[2]; Douglas Goodwin[2]; Mark T Hamann[3]; *[1]Auburn University, Auburn, AL; [2]Auburn University, Auburn, Alabama; [3]Medical University of South Carolina, Charleston, SC*

TP 688 **Determination of Hepatitis B Virus Infection by Means of Targeted Proteomics Strategy**; Hsing-Fen Tsai[1]; He-Hsuan Hsiao[1]; *[1]NCHU, Department of Chemistry, Taichung, Taiwan*

TP 689 **A Key Retromer Trafficking Interactome of Toxoplasma Gondii Brought to Light by Comprehensive Proteomic Analyses**; Benoît Westermann[1]; Lamba Omar Sangaré[2]; Agnes Hovasse[1]; Tchilabalo Dilezitoko Alayi[1]; Stan Tomavo[2]; Alain Van Dorsselaer[1]; Christine Schaeffer-Reiss[1]; *[1]IPHC, UdS CNRS UMR 7178 Strasbourg, FRANCE; [2]CNRS UMR 8204, Lille, France*

TP 690 **Proteomic Deciphering of Cystic Echinococcosis using Laser Microdissection-based Microproteomics and MALDI Imaging**; Rémi Longuespée[1]; Rita Casadonte[1]; Mark Kriegsmann[2]; Gabriel Mazzucchelli[3]; Edwin De Pauw[4]; Michael Becker[5]; Jörg Kriegsmann[1, 6]; *[1]Proteopath GmbH, Trier, Germany; [2]University of Heidelberg, Heidelberg, Germany; [3]University of Liege, GIGA-Proteomics Liege, Belgium; [4]Université de Liège, Liège, Belgium; [5]Bruker Daltonik GmbH, Bremen, Germany; [6]Center for Histology Cytology and Molecular Diagnostics, Trier, Germany*

TP 691 **Plasma Proteomic Changes Induced by Salmonella Typhimurium Lipopolysaccharides in an Avian Model of Inflammation** ; Balamurugan Packialakshmi[1]; Rohana Liyanage[1]; Jackson O Lay, Jr[1]; Sarbjeet K Makkar[1]; Narayan Rath[2]; *[1]University of Arkansas, Fayetteville, AR; [2]PPPSRU, USDA-ARS Fayetteville, AR*

TP 692 **Top Down Proteomic Profiling of a Hypervirulent Clinical Isolate of Acinetobacter baumannii**; Zack Li[1]; Kelly Fulton[1]; Rhonda Kuo Lee[1]; Howard H Xu[2]; Patricia Massel[1]; Susan Twine[1]; Wangxue Chen[1]; *[1]National Research Council Canada, Ottawa, Canada; [2]California State University, Los Angeles, Los Angeles, CA - California*

TP 693 **Evolutionary Dynamics of Pseudomonas aeruginosa Revealed by Population Proteome Analysis**; Xia Wu[1]; Katherine B Hisert[1]; Jayanthi Garudathri[1]; Benjamin J Staudinger[1]; Jimmy K Eng[1]; Colin Manoil[1]; Pradeep K Singh[1]; James E Bruce[1]; *[1]University of Washington, Seattle, WA*

TP 694 **A Plasmodium Vivax Trophozoite-schizont Stage Transition Proteome**; D. C. Anderson[1]; Stacey A. Lapp[2]; John Barnwell[3]; Mary R. Galinski[4]; *[1]SRI International, Harrisonburg, VA; [2]Emory Vaccine Center, Yerkes National Primate Research Center, Emory University, Atlanta, GA; [3]Malaria Branch, Division of Parasitic Diseases, Centers for Disease Control and Prevention, Atlanta, GA; [4]Emory Vaccine Center, Yerkes National Primate Research Center, Emory University; Department of Medicine, Division of Infectious Diseases, Emory University School of Medicine, Atlanta, GA*

TP 695 **Bridging Virology with Proteomics to Define Mechanisms of Cellular Immune Signaling upon Herpesvirus Infection**; Krystal K Lum[1]; Benjamin A Diner[1]; Joseph W Boerma[1]; Ileana M. Cristea[1]; *[1]Princeton University, Princeton, NJ*

TP 696 **Identifying Host Factors Associated with Replicating Viral DNA**; Emigdio D Reyes[1, 2]; Katarzyna Julia Kulej[1, 2]; Daphne C Avgousti[1, 2]; Lisa Akhtar[3]; Daniel Bricker[2]; Neha Pancholi[1, 2]; Sarah A. Koniski[2]; Benjamin A Garcia[4]; Matthew D Weitzman[1, 2]; *[1]Department of Pathology and Laboratory Medicine, University of Pennsylvania Perelman School of Medicine, Philadelphia, PA; [2]Division of Cancer Pathobiology, The Children's Hospital of Philadelphia, Philadelphia, PA; [3]Department of Pediatrics, Division of Infectious Diseases, The Children's Hospital of Philadelphia, Philadelphia, PA; [4]Epigenetics program, Department of Biochemistry and Biophysics, University of Pennsylvania Perelman School of Medicine, Philadelphia, PA*

TP 697 **Protein-protein Interaction Network of Toll-like Receptor 4 in Macrophages with Exposure to their Agonists and External Factors**; Abu Hena M Kamal[1]; Jayanta Kishor Chakrabarty[1]; Saiful M Chowdhury[1]; *[1]University of Texas at Arlington, Arlington, TX*

TP 698 **Engineering Novel Trypsin Cleavage Sites Improves Proteome Detection and PTM Recovery**; Cristal Reyna[1]; Patricia A Champion[2]; Matthew M Champion[2]; *[1]University of Notre Dame, South Bend, Indiana; [2]University of Notre Dame, Notre Dame, Indiana*

TP 699 **Understanding Virus Mechanisms by Means of Native Mass Spectrometry**; Boris Krichel[1]; Sven Falke[2]; Johannes Heidemann[1]; Julia Lockhauserbäumer[1]; Rolf Hilgenfeld[3]; Mathhew Dunne[4]; Rob Meijers[5]; Lars Redecke[3]; Charlotte Utrecht[1, 6]; *[1]Heinrich Pette Institute - Leibniz Institute for Experimental Virology, Hamburg, Germany; [2]University of Hamburg, Hamburg, Germany; [3]University of Lübeck, Lübeck, Germany; [4]ETH Zürich, Zürich, Switzerland; [5]EMBL Hamburg c/o DESY, Hamburg, Germany; [6]European XFEL, Hamburg, Hamburg*

TP 700 **Cracking the Code on N-Terminal Protein Acetylation in Mycobacterium tuberculosis**; Cristal Reyna[1]; Patricia Champion[1]; Matthew Champion[1, 2]; *[1]University of Notre Dame, Notre Dame, IN; [2]The Center For Rare And Neglected Diseases, Notre Dame, IN*

TP 701 **Proteomic Analysis of the Secretome of Dengue Virus-infected Vero Cells: Characterization of the Overexpressed Viral Non-structural Protein 1 (NS1)**; Chen-Ching Wu[1]; Chun-Hao Huang[2]; Shyh- Horng Chiou[2]; *[1]Kaohsiung Medical University, Kaohsiung City, Taiwan; [2]Quantitative Proteomics Center and Graduate Institute of Medicine, Kaohsiung, TAIWAN (R.O.C.)*

TP 702 **iTRAQ Proteomic and Protein Microarray Analysis of Potential Biomarkers OipA, BabA, and SabA in Helicobacter Pylori-related Gastric Cancer**; Yu-Lin Su[1]; Jyh-Chin Yang[2]; Lu-Ping Chow[1]; *[1]Institute of Biochemistry and Molecular Biology, College of Medicine, National Taiwan University, Taipei, Taiwan (R.O.C.); [2]Department of Internal Medicine, Hospital and College of Medicine, National Taiwan University, Taipei, Taiwan (R.O.C.)*

PROTEOMICS: QUANTITATIVE (APPLICATION BIOLOGICAL RESEARCH)
703 - 727

TP 703 **Environmental Stress Induced Proteins Changes in Green Algae by Quantitative Proteomics**; Yan Gao[1]; Teck Kwang Lim[2]; Qingsong Lin[2]; SAM LI[1]; *[1]Department of Chemistry, National University of Singapore, Singapore, Singapore; [2]Department of Biological Sciences, National University of Singapore, Singapore, Singapore*

TP 704 **Proteins Associated with Olfactory Receptor Nuclear Foci**; Martin Escamilla Del Arenal[1]; Fiona Clowney[1]; Shujuan Tao[1]; David Chen[1]; Lewis M. Brown[2]; Stavros Lomvardas[1]; *[1]Columbia University, New York, NY; [2]Columbia University, New York , NY*

TP 705 **Quantitative Proteomic Approach Reveals Landscape of the Regulatory Elements for Lysine 2-Hydroxyisobutyrylation Pathway**; He Huang[1]; Kyle Delaney[1]; Shankang Qi[1]; Okwang Kwon[1]; Yingming Zhao[1]; *[1]The University of Chicago, Chicago, IL*

TP 706 **Proteomics-based Comparison of Ionic and Nano Silver at Cytotoxic Concentrations**; Suresh Narayanasamy[1]; Samanthi I Wickramasekara[2]; Eric Sussman[2]; *[1]U.S. Food and Drug Administration, Silver Spring, MD; [2]U.S. Food and Drug Administration, Silver Spring, MD*

TP 707 **Quantitative Proteomic Analysis of PP2A-associated Proteins in BR Signaling Regulation Pathway**; Chao Liu[1]; Shuo-Lei Bu[2]; Hao Chi[1]; Zhi-Yong Wang[3]; Si-Min He[1]; *[1]ICT, CAS, Beijing, China; [2]Hebei Normal University, ShiJiaZhuang, China; [3]Department of Plant Biology, Carnegie Institution for Science, Stanford, USA*

TP 708 **Insights from Redox Proteomics: Focus on S-glutathionylation Stoichiometry and Redox Status of Protein Cysteines**; Jicheng Duan[1]; Matthew J Gaffrey[2]; Hannah J. Hatchell[2]; Rosalie Chu[2]; Richard D Smith[2]; Brian D Thrall[2]; Wei-jun Qian[2]; *[1]Pacific Northwest National Laboratory, Richland, Washington; [2]Pacific Northwest National Laboratory, Richland, WA*

TP 709 **An In-depth Proteome Foryeast Meiosis**; Guo Yueshuai[1]; wen Fuping[2]; Hu Yang[2]; Wang Yuanting[2]; Wang Qian[2]; Yu Haiyan[2]; Tang Chaoming[2]; Sha Jiahao[1]; Guo Xuejiang[1]; Li Wei[2]; *[1]Nanjing Medical University, Nanjing, China; [2]Institute of Zoology, Chinese Academy of Sciences, beijing, china*

TP 710 **Rootstock Influences Protein Profile at Different Stages of Berry Development in Grape, as Revealed by Whole Proteome Analysis using HRMS**; Smita Maske[1]; Anuradha Upadhyay[1]; Satisha Jogaiah[1]; Akanksha Singh[2]; Dipankar Malakar[3]; Manoj Pillai[3]; Kaushik Banerjee[1]; *[1]ICAR-National Research Centre for Grapes, Pune, Maharashtra India; [2]SCIEX, Gurgaon, Haryana; [3]SCIEX, Gurgaon, Haryana India*

TP 711 **Proteome-wide Quantitative Profiling of Mis-Incorporation of Selenocysteine into Proteins by LC-MS Based Shotgun Proteomics**; Chunlin Hao; *The Hong Kong University of Science and Technology, Hong Kong SAR, HK*

TP 712 **A Mesenchymal Stem Cells differentiation study by using SILAC and Sequence-specific DNA Affinity Purification Approaches**; Michele Puglia[1]; Inigo Barrio-Hernandez[1]; Blagoy Blagoev[1]; *[1]University of Southern Denmark, Odense, Denmark*

TP 713 **The Impact of Deyolking on Quantitative Proteomics in Zebrafish Embryos**; Fatima Rahlouni[1]; Vladimir Shulaev[2]; Laszlo Prokai[1]; *[1]University of North Texas Health Science Center, Fort Worth, TX; [2]University of North Texas, Denton, TX*

TP 714 **Investigation of Murine Neural Progenitor Cell to NG2 Cell Differentiation by TMT based Quantitative Proteomics**; Carmen Schoor[1]; Alireza Dehghani[1]; Volkmar Gieselmann[1]; Dominic Winter[1]; *[1]University of Bonn, Bonn, Germany*

TP 715 **Proteomics- and Physiology-based Studies in Deciphering Epithelial Crosstalk Mechanism(s) Using Rhodnius prolixus as Experimental Model**; Noman Hassan[1]; George Katselis[2]; Juan Ianowski[2]; *[1]University of Saskatchewan, Saskatoon, SK; [2]University of Saskatchewan, Saskatoon, Canada*

TP 716 **Age Dependent Protein Expression in Drosophila Models of Neurodegeneration**; Chris Brown[1]; Jonathan C Trinidad[1]; David E Clemmer[1]; *[1]Indiana University Dept. Chemistry, Bloomington, IN*

TP 717 **Quantitative Proteome Profiling of Marinobacter sp. CP1 enriched from Microbial Fuel Cell Biocathode MCL**; W. Judson Hervey, IV[1]; Zheng Wang[1]; Brian J. Eddie[1]; Anthony P. Malanoski[1]; Baochuan Lin[1]; Sarah M. Strycharz-Glaven[1]; *[1]Naval Research Laboratory, Center for Bio/ Molecular Science & Engineering, Washington, DC*

TP 718 **Novel Top-down Quantitative LC/MS Strategy Reveals New Insights into Molecular Heterogeneity In Skeletal Muscle**; Ziqing Lin[1]; Liming Wei[1, 2]; Yutong Jin[1]; Wenxuan Cai[1]; Zachery Gregorich[1]; Gary M Diffee[1]; Ying Ge[1]; *[1]University of Wisconsin-Madison, Madison, WI; [2]Fudan University, Shanghai, China*

TP 719 **Combined Discovery- and Targeted-based Proteomic Analysis of Tumor-Associated Antigen Peptides Derived from MAGE Proteins**; Darshit Shah[1]; Xunbao Duan[2]; MacDonald Douglas[2]; Robert Salzler[2]; *[1]Regeneron Pharmaceuticals Inc., Tarrytown, NY; [2]Regeneron Pharmaceuticals, Tarrytown, NY*

TP 720 **Fast MS/MS Data Acquisition without Dynamic Exclusion Enables Precise and Accurate Quantification of Proteome**; Yichu Shan; *, dalian, liaoning*

TP 721 **A Comparison of Isobaric Labeling with MS1-XIC Quantitation using a Two-Proteome Model**; David Mccaskill[1]; Trent Oman[1]; Tao Xu[1]; Jeffrey R Gilbert[1]; *[1]Dow AgroSciences, Indianapolis, IN*

TP 722 **Application of Mass Spectrometry Profiling to Establish Brusatol as an Inhibitor of Global Protein Synthesis**; Taylur Ma[1]; Steffan Vartanian[2]; James Lee[2]; Peter M Haverty[2]; Donald S Kirkpatrick[2]; Kebing Yu[2]; David Stokoe[2]; *[1]Genentech, Inc., South San Francisco, CA; [2]Genentech Inc, South San Francisco, CA*

TP 723 **Proteomics Profiling of Parental and mAb-producing CHO-derived Cell Lines to Facilitate Optimization of mAb Production**; Yee Jiun Kok[1]; Ally Lau[1]; Daniel Ng[1]; Lu Zheng[1]; Yuansheng Yang[1]; Xuezhi Bi[1]; *[1]Bioprocessing Technology Institute, Singapore*

TP 724 **Quantitative Analysis of Chromatin Proteome Remodeling Mediated by SWI/SNF Complexes**; Zhiping Wu[1]; Eun-Ah Cho[2]; Haiyan Tan[3]; Haifeng Yang[2]; Junmin Peng[3]; *[1]ST. Jude, Memphis, TN; [2]Thomas Jefferson University, Philadelphia, PA; [3]St. Jude Children's Reseach Hospital, Memphis, TN*

TP 725 **Use of Variant Proteomics to Inform Genomic Searches for Novel Targets in Glioma**; Ekaterina Mostovenko[1]; Melinda Rezeli[2]; Akos Vegvari[1]; Gyorgy Marko-Varga[2]; Yanhong Liu[3]; E. Susan Amirian[3]; Melissa L Bondy[3]; Carol L Nilsson[1]; *[1]UTMB Galveston, Galveston, TX; [2]Lund University, Lund, Sweden; [3]Dan L. Duncan Cancer Center, Houston, TX*

TP 726 **Determining Isotope Enrichment in Heavy Water Labeling**; Jayant Avva[1]; Kwangwon Lee[2]; Takhar Kasumov[3]; Rovshan Sadygov[1]; *[1]University of Texas Medical Branch at Galveston, Galveston, TX; [2]Northeast Ohio Medical University, Rootstown, OH; [3]Northeast Ohio Medical University, Rootstown, OH*

TP 727 **Quantitative MS Investigation of the Effect of Amyloid-Beta on the Proteome Of Neuronal Cells**; Maria I Indeykina[1, 2, 3]; Evgeny P Barykin[4]; Alexey S Kononikhin[2, 3,5]; Vladimir Mitkevich[4]; Igor A Popov[2, 3]; Sergey Kozin[4]; Alexander A Makarov[4]; Eugene Nikolaev[2]; *[1]Emanuel Institute of Biochemical Physics, Moscow, Russia; [2]Institute for Energy Problems of Chemical Physics, Moscow, Russia; [3]Moscow Institute of Physics and Technology, Dolgoprudny, Russian Federation; [4]Engelhardt Institute of Molecular Biology, Moscow, Russia; [5]Research Center for Obstetrics and Gynecology, Moscow, Russia*

SMALL MOLECULES: QUANTITATIVE ANALYSIS (ANIMAL, PLANT/INSECT, AND METHODOLOGY)
728 - 762

TP 728 **Quantitative Measurement of Carbidopa and Levodopa in Rat Plasma via HPLC with Tandem Mass Spectrometry**; Jingduan Chi[1]; Yonghua Ling[1]; Mofikoya Melissa[1]; Fumin Li[1]; *[1]PPD, Middleton, WI*

TP 729 **A Sensitive LC-MS-MS Method for Quantitation of Buprenorphine in Rat Brain Cerebrospinal Fluid**; Fengying Zhu[1]; Perry (Peixin) Cao[1]; Ryan Turncliff[1]; *[1]Alkermes, Inc, Waltham, MA*

TP 730 **Challenges and Solutions in the Bioanalysis of Sulprostone, a Prostaglandin E2 Analogue, in Rat and Monkey Plasma using LC-MS/MS**; Yifan Shi[1]; Shefali Patel[1]; Naidong Weng[1]; *[1]Janssen Research and Development, Spring House, PA*

TP 731 **A Novel Determination for Menthol in Rat Plasma using Salting-Out LLE and Derivatization Coupled with LC-MS/MS Detection**; Mingluan Chen[1]; Milton Furtado[1]; Anahita Keyhani[1]; *[1]Algorithme Pharma Inc., Laval, Canada*

TP 732 **Ultra Sensitive Method for Pre-clinical Quantification of Methacholine in Biological Matrices using SPE-HILIC Tandem Mass Spectrometry**; Anders Lundqvist; *AstraZeneca Gothenburg, Gothenburg, Sweden*

TP 733 **Development and Validation of a Method to Quantitate Bisphenol AF in Rodent Plasma and Amniotic Fluid by LC/MS/MS**; Bradley Collins[1]; Felicia Hubbard[2]; Kristin L. Aillon[2]; Joseph W. Algaier[2]; Suramya Waidyanatha[1]; *[1]National Institute of Environmental Health Sciences, Research Triangle Park, NC; [2]MRIGlobal, Kansas CIty, MO*

TP 734 **Simultaneous Determination of Benzocaine, N-acetyl Benzocaine, and Tetracaine in Rabbit Plasma using High Performance Liquid Chromatography-Mass Spectrometry**; Wuyi (Charlie) Zha[1]; Runlan Huo[1]; Mohamed Osman[1]; Xinping Fang[2]; Xin Zhang[2]; *[1]XenoBiotic Laboratories, Inc. WuXi AppTec Inc Plainsboro, NJ; [2]WuXi AppTec Co., Shanghai, China*

TP 735 **Validation of a Method for Quantification of DMSO in Equine Urine using Hydrophilic Interaction Liquid Chromatography Tandem Mass Spectrometry**; Matilda Salomonsson[1, 2]; Lena Ekman[3]; Mikael Hedeland[3]; Ulf Bondesson[2, 3]; *[1]The National Veterinary Institue (SVA), Uppsala, -; [2]Uppsala University, Uppsala, Sweden; [3]The National Veterinary Institute (SVA), Uppsala, Sweden*

TP 736 **A Robust LC/MS/MS Method for Quantitation of 2-morpholinoethanesulfonic acid (MES) in Dog and Rabbit Plasma**; Todd Baughman; *Covance, Durham, NC*

TP 737 **Analysis of Mycotoxins in Coix Seed using a Prototype Tandem Quadrupole Mass Spectrometer**; Kerri Smith[1]; Kelly B Doering[1]; Mark Wrona[1]; Giorgis Isaac[1]; Jimmy Yuk[1]; Sukhdev Bangar[2]; *[1]Waters Corporation, Milford, MA; [2]Waters Corporation, Beverly, MA*

TP 738 **Quantification of Biogenic Amines from Single Drosophila Cells by Direct MALDI-TOF MS**; Max Diesner[1]; Susanne Neupert[1]; *[1]Biocenter Cologne, University of Cologne 50674 Cologne, Germany*

TP 739 **CBD/THC Quantitative Analysis with Direct Analysis in Real Time-Mass Spectrometry (DART-MS)**; Bohui Lv[1]; William Hoffmann[2]; Glen P Jackson[1]; *[1]West Virginia University, Morgantown, WV; [2]Oak Ridge National Laboratory, CNMS Oak Ridge, TN*

TP 740 **A Combined MRM and SIM Method for Direct Quantitative Determination of Amino Acids in Various Samples on LC/MS/MS**; Zhe Sun[1]; Jie Xing[1]; Pei Yee Khoo[2]; Zhaoqi Zhan[1]; *[1]Customer Support Centre, Shimadzu (Asia Pacific) Pte Ltd, Singapore; [2]School of Physical & Mathematical Sciences, Nanyang Technological University Singapore, *Intern student*

TP 741 **Mass Spectrometry-Guided Refinement of Chemical Energy Buffers**; Ting-Ru Chen[1]; Pawel Lukasz Urban[2];

[1]National Chiao Tung University, Hsinchu, Taiwan; [2]Department of Applied Chemistry, National Chiao Tung University, Hsinchu, Taiwan (R.O.C.)

TP 742 **Obtain sub-ng/mL Levels for Steroids using a Simple, One-step Derivatization and a Novel, High Efficiency EI Source**; Tim Conjelko[1]; Stephan Baumann[1]; Matthew Curtis[1]; *[1]Agilent Technologies, Santa Clara, CA*

TP 743 **Novel SPE Extraction Method for Sensitive and High Throughput Quantitative Analysis of Phosphorothioate Oligonucleotides in Human Plasma Using LC-MS/MS**; Yuhuan Ji[1]; Qian Liu[1]; Qian Li[1]; Ji Chengjie[1]; Laixin Wang[2]; *[1]NovaBioAssays, LLC, Woburn, MA; [2]NovaBioAssays, LLC, Worburn, MA*

TP 744 **Quantitation of Four Chiral Drug Compounds Simultaneously Using Normal Phase LC-MS/MS Equipped With an APPI Ion Source**; Min Huang[1]; Zhongping (John) Lin[1]; *[1]Frontage Laboratories, Exton, PA*

TP 745 **The Use of Perchloric Acid as a Problem Solving Precipitating Agent to Overcome Method Development Issues**; Pierre-Yves Caron[1]; Nicolas Jean[1]; Nadine Lafontaine[1]; Louis-Charles Boisvert[1]; Sylvain Lachance[1]; Nadine Boudreau[1]; Clark Williard[1]; *[1]inVentiv Health, Québec, Canada*

TP 746 **A Novel Approach for Reducing the Isotopic Distribution Impact during Quantitation of Analyte by LCMSMS using Quadratic Regression Fit**; Nathalie Pelletier[1]; Genevieve Emond[1]; Sylvain Lachance[1]; Nadine Boudreau[1]; Clark Williard[1]; *[1]inVentiv Health, Québec, Canada*

TP 747 **Monitoring and Quantitating Genotoxic Impurities using Mass Detection and UV – Sensitive Analysis Aryl Sulfonic Acid Esters**; Mark Wrona[1]; Janet Hammond[2]; Jayne Kirk[2]; Sean Mccarthy[1]; Hillary Hewittson[1]; Margaret Maziarz[1]; *[1]Waters Corporation, Milford, MA; [2]Waters Corporation, Wilmslow, UK*

TP 748 **Development of a Low Volume Quantitative Plasma Analysis Method Using a Flexible Capillary Microsampling Technique**; Larry Mallis[1]; Wei Zhang[1]; Li Yuan[1]; Zhongping (John) Lin[1]; *[1]Frontage Laboratories, Exton, PA*

TP 749 **An Investigation on the Impact on Drug Stability in Biological Matrix when Stored in Multiple Tubes**; Nader Youssef[1]; John Chapdelaine[1]; Weixing Sun[1]; Asvinkumar Patel[1]; Zhao Heng Ge[1]; Adrien Musuku[1]; *[1]Pharmascience, Montreal, Canada*

TP 750 **Simultaneously Determination of the Enantiomers of Ketorolac in Human Plasma by Atmospheric Pressure Chemical Ionization LC/MS/MS**; Vince Windisch[1]; Feng Liang[1]; Allan Xu[1]; *[1]Keystone Bioanalytical Inc, North Wales, PA*

TP 751 **Trace Analysis of Potentially Mutagenic Impurities in Pharmaceutical Substances by Electron Ionization LC/MS (EI-LC/MS) with Supersonic Molecular Beams**; Christine Fisher[1]; Ryan Cohen[1]; Renee Dermenjian[1]; *[1]Merck & Co., Rahway, NJ*

TP 752 **Expanding Horizons in Real Time Analysis: Dual Polarity SIFT-MS**; Murray J Mcewan[1, 2]; David Hera[2]; Harry Gower[2]; Vaughan S Langford[2]; Thomas I McKellar[2]; Daniel B Milligan[2]; *[1]University of Canterbury, Christchurch, Canterbury; [2]Syft Technologies Ltd, Christchurch, New Zealand*

TP 753 **Development of LC/MS/MS Method for Screening and Quantitation of 49 Synthetic Dyes in Textiles under Restricted Substance List (RSL)**; Yin Ling Chew[1]; Jie Xing[1]; Guan Seng, Leonard Lim[2]; Zhaoqi Zhan[1]; *[1]Shimadzu (Asia Pacific) Pte Ltd, Singapore; [2]School of Physical & Mathematical Science, Nanyang Technological University, Singapore*

TP 754 **Isolation, Characterization and Color Stability of natural blue pigments**; Andrew G Newsome[1]; Luying Chen[1]; Cathy A Culver[2]; Richard B van Breemen[1]; *[1]University of Illinois at Chicago, Chicago, IL; [2]Pepsi-Cola Company, Hawthorne, NY*

TP 755 **Selective Enrichment of Flavonoids Using Pegylated Graphene Oxide and MALDI-TOF MS**; Jaesung Lee; *Konkuk University, Seoul, South Korea*

TP 756 **Development of a Sensitive Supercritical Fluid Chromatography (SFC)-MS/MS Method for the Analysis of Potential Genotoxic Impurities of Ondansetron**; Jennifer Simeone[1]; Paula Hong[1]; *[1]Waters Corporation, Milford, MA*

TP 757 **Development and Testing of a Gas Generator for Odour Transmission over Data Networks**; Stamatios Giannoukos[1]; Jeremy Smith[2]; Alan Marshall[2]; Stephen Taylor[2]; *[1]University of Liverpool, Liverpool, Please Select; [2]University of Liverpool, Liverpool, United Kingdom*

TP 758 **Novel Applications of Paired Ion Electrospray Ionization Mass Spectrometry (PIESI-MS) for Sensitive Analysis of Anionic Compounds**; Hongyue Guo[1]; Daniel W Armstrong[1]; *[1]University of Texas at Arlington, Arlington, TX*

TP 759 **Parallel Reaction Monitoring and Selected Reaction Monitoring Exhibit Comparable Analytical Performance in Quantitative Analysis of Cannabinoid**; Xiaolei Xie[1]; Thomas Carrell[1]; Marta Kozak[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

TP 760 **A Simple Systematic Strategy for Rapid Development of High-throughput and Reliable LC-MS/MS Assays for Regulated Bioanalysis**; Long Yuan; *Bristol-Myers Squibb, Princeton, NJ*

TP 761 **Commutability of LCMSMS Assays:Calibration by Internal or External Standardization?**; R. Brent Dixon; *Physician's Choice Laboratory Services, Rock Hill, SC*

TP 762 **Evaluation of an Innovative High-Throughput Online Solid Phase Extraction Tandem Mass Spectrometry System for Bioequivalence Studies**; Jinhui Zhang[1]; Patrick J. Faustino[1]; *[1]FDA, Silver Spring, MD*

TOP DOWN PROTEIN ANALYSIS (METHODOLOGY)
763 - 775

TP 763 **The National Resource for Translational and Developmental Proteomics offers novel opportunities for training and accelerated research in top-down proteomics**; Neil L Kelleher[1]; Caroline J DeHart[1]; Ryan T Fellers[1]; Richard D LeDuc[1]; Paul M Thomas[1]; *[1]Northwestern University, Evanston, IL*

TP 764 **Application of Spectral Counting for Top-down Proteomics Comparisons**; Lucia Geis-Asteggiante[1]; Nathan Edwards[2]; Suzanne Ostrand-Rosenberg[3]; Catherine Fenselau[1]; *[1]University of Maryland, College Park, MD; [2]Georgetown University Medical Center, Washington, DC; [3]University of Maryland, Baltimore County Baltimore, MD*

TP 765 **Increased Fragmentation Efficiency in Middle-down Protein Analysis using Different Collision Gases in a Modified Q-TOF Mass Spectrometer**; Christian Klein[1]; Alex Mordehai[1]; Mark Werlich[1]; William E Barry[1]; *[1]Agilent Technologies, Santa Clara, CA*

TP 766 **Protein Supercharging for Enhanced Top-Down Analysis with HCD MS/MS**; Natalia Gasilova[1]; Kristina Srzentic[2]; Yury Tsybin[3]; Hubert H Girault[4]; *[1]EPFL, Sion, Switzreland; [2]EPFL, Lausanne, Switzerland; [3]Spectroswiss Sàrl, Lausanne, Switzerland; [4]EPFL, Sion, Switzerland*

TP 767 **Difference Mass Spectra for De novo Identification of N- and C-terminal Sequences of Intact Proteins**; Harsha Gunawardena[1]; Dhanshri Bagal[1]; Daryl Bulloch[1]; Ping Cao[1]; David Chow[1]; Eddie Kast[1]; Matthew Rardin[1]; Nik Sharkov[1]; Peter Grandsard[2]; *[1]Amgen, Inc. South San Francisco, CA; [2]Amgen, Thousand Oaks, CA*

TP 768 **Top-down Targeted Proteomics Reveals Novel Molecular Mechanism in Sarcopenia**; Zachery Gregorich[1]; Ying Peng[2]; Wenxuan Cai[2]; Yutong Jin[2]; Liming Wei[3]; Albert Chen[2]; Susan McKiernan[2]; Judd Aiken[4]; Richard Moss[2]; Gary Diffee[2]; Ying Ge[2]; *[1]UW Madison, Madison,*

WI; [2]University of Wisconsin Madison, Madison, WI; [3]Fudan university, shanghai, China; [4]University of Alberta, Edmonton, Canada

TP 769 **Optimisation of intact Protein Sequencing through Testing Thousands of EThCD/ETciD MS/MS Fragmentation Conditions**; Pavel Shliaha[1]; Derek Bailey[2]; Vladimir Gorshkov[1]; Ole N. Jensen[1]; *[1]Department of Biochemistry and Molecular Biology, University of Southern Denmark Odense, Denmark; [2]Thermo Fisher Scientific, San Jose, CA*

TP 770 **Development of Mass Spectrometry-based Methods for Quality Assessment of Recombinant Proteins**; Rosa I Viner[1]; Nan Liu[2]; Seema Sharma[1]; Sergei I Snovida[3]; Krishna Vattern[3]; David M Horn[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Life Technology, South San Francisco, CA; [3]Thermo Fisher Scientific, Rockford, IL*

TP 771 **Higher-order Structure Determines the Native ETD Fragmentation Behavior of Proteins and Complexes**; Frederik Lermyte[1]; Mateusz Krzysztof Łącki[2]; Albert Konijnenberg[1]; Dirk Valkenborg[3]; Anna Gambin[2]; Frank Sobott[1]; *[1]University of Antwerp, Antwerpen, Belgium; [2]University of Warsaw, Warsaw, Poland; [3]VITO, Mol, Belgium*

TP 772 **Native Top-down Mass Spectrometry of Tau Proteins**; Piriya Wongkongkathep[1]; Michael Nshanian[1]; Michael Ehrmann[2]; Gal Bitan[1]; Joseph A Loo[1]; *[1]UCLA, Los Angeles, CA; [2]University of Duisburg-Essen, Essen, Germany*

TP 773 **Mapping p53 Proteoforms by Native and Denaturing Top-down Mass Spectrometry**; Caroline J DeHart[1]; Luca Fornelli[1]; Owen Skinner[1]; Philip D Compton[1]; Paul M Thomas[1]; Galit Lahav[2]; Jeremy Gunawardena[2]; Neil L Kelleher[1]; *[1]Northwestern University, Evanston, IL; [2]Harvard Medical School, Boston, MA*

TP 774 **High-throughput Top Down Proteomics of HeLa cell lysates using UVPD**; Timothy Cleland[1]; Ryan Parker[2]; Jennifer S Brodbelt[1]; *[1]University of Texas Austin, Pflugerville, TX; [2]University of Texas at Austin, Austin, TX*

TP 775 **Quantitative Top Down Proteomics in Translational Research: Markers for Rejection in Peripheral Blood Following Kidney Transplantation**; Timothy Toby[1]; John Savaryn[1]; Bryan P Early[1]; Paul M Thomas[1]; Ryan T Fellers[1]; Luca Fornelli[1]; Joseph B Greer[1]; Richard D Leduc[1]; Ioanna Ntai[1]; Zheng J Zhang[2]; John Friedewald[2]; Daniel Salomon[3]; Michael M Abecassis[2]; Neil L Kelleher[1]; Philip D Compton[1]; *[1]Northwestern University, Evanston, IL; [2]Northwestern Feinberg School of Medicine, Chicago, IL; [3]Scripps Center for Organ and Cell Transplantation, La Jolla, CA*

AMBIENT IONIZATION: FUNDAMENTALS AND INSTRUMENTATION (PROBES, PAPER SPRAY, DESI/ESI, TISSUE/TOOLS)
001 - 029

WP 001 **Development of a DIP-APPI-IM-qTOF-MS**; Simeon Horst[1]; Oliver Schmitz[1]; *[1]Universität Duisburg Essen, Essen, Germany*

WP 002 **Development of a DIP-ESI-MS for Drug Analysis**; Claudia Lenzen[1]; Oliver Schmitz[1]; *[1]Universität Duisburg Essen, Essen, Germany*

WP 003 **Monolith Dip-It: A Bifunctional Device for Increasing the Sensitivity of Direct Analysis in Real Time**; Li Xianjiang[1]; Yu Bai[1]; Liu Huwei[1]; *[1]Peking University, Beijing, China*

WP 004 **Inert - Atmospheric Solid Analysis Probe: A New Fast and Easy Way to Characterize Air Sensitive Compounds by Mass Spectrometry**; Mathilde Farenc[1, 2, 3]; Carlos Afonso[2, 3]; Pierre Giusti[1, 3]; *[1]TOTAL Refining and Chemicals, TRTG Gonfreville l'Orcher, France; [2]Normandie Univ, CNRS UMR 6014 COBRA Mont St Aignan, France; [3]TOTAL RC - CNRS Joint Laboratory C2MC :Complex Matrices Molecular Characterization,France,*

WP 005 **Applications and Fundamentals of Swab Touch Spray – Mass Spectrometry**; Alan K. Jarmusch[1, 2]; Valentina Pirro[1,2]; R. Graham Cooks[1, 2]; *[1]Purdue University-Department of Chemistry, West Lafayette, IN; [2]Center for Analytical Instrumentation Development, West Lafayette, IN*

WP 006 **Coupling Paper Microfluidics with Paper Spray Mass Spectrometry for Improved Versatility and Analytical Performance**; Ian Murray[1]; Glenn Walker[1]; Michael Bereman[1]; *[1]North Carolina State University, Raleigh, NC*

WP 007 ***In situ* Separation and Analysis of Lipids by Paper Spray Ionization Mass Spectrometry**; Sangwon Cha[1]; Purum Kim[1]; *[1]Hankuk Univ. Foreign Studies, Yongin, South Korea*

WP 008 **High-Throughput Copper-Catalysts Screening and Their Catalytic Activity Studies Using Paper Spray Mass Spectrometry**; Yajun Zheng[1]; Xuan Wang[1]; Teng Wang[1]; Yang Haijun[2]; Zhiping Zhang[1]; *[1]Xi'an Shiyou University, Xi'an, China; [2]Tsinghua University, Beijing, China*

WP 009 **Molecular Ionization at Low Voltage from One-Dimensional Nanostructures**; Rahul Narayanan; *Indian Institute of Technology, Chennai, Tamilnadu, India, Chennai, Tamilnadu*

WP 010 **Dehydrogenation of Tetrahydroquinolines in Corona Discharge Plasma under Ambient Conditions using Graphite-Coated Hydrophobic Paper Surface**; Kathryn Davis[1]; Abraham Badu-Tawiah[1]; *[1]The Ohio State University, Columbus, OH*

WP 011 **Mass Spectrum Real-Time Online Optimizing Paal-Knorr Spary Reaction Temperature**; XingPing Zeng[1]; Peng Zhou[1]; Huanwen Chen[2]; *[1]East China Institute of Technology, Nanchang, China; [2]East China University of Technology, Nanchang, Mainland*

WP 012 **Direct and Rapid Detection of Drugs in Urine by Extractive Electrospray Ionization Mass Spectrometry**; Peng Zhou[1]; Tenggao Zhu[1]; Yongzi Liu[2]; Huian Zhao[2]; Huanwen Chen[3]; *[1]East China Institute of Technology, Nanchang, China; [2]Jiangxi of Forensic Science Institute, Nanchang, China; [3]East China University of Technology, Nanchang, Mainland*

WP 013 **Coaxial Extractive Electrospray Ionization Mass Spectrometry**; Kenneth D Swanson[1]; Steven L Reeber[1]; Gary L Glish[1]; *[1]University of North Carolina, Chapel Hill, NC*

WP 014 **Generating Radical Cations of Aromatic Hydrocarbons through Reactive ESI Using the Single-Probe**; Rachel Vowcicefski[1]; Ning Pan[2]; Zhibo Yang[2]; *[1]University of Oklahoma, Norman, OK; [2]University of Oklahoma, Dept. of Chem & Biochem Norman, OK*

WP 015 **Pinpointing the Source of Droplet Reactivity in Contained-electrospray Ionization**; Dmytro Kulyk[1]; Abraham Badu-Tawiah[1]; *[1]Ohio State University, Columbus, OH*

WP 016 **Solvent Assisted Inlet Ionization of Airborne Nanoparticles**; Andy Horan[1]; Murray V Johnston[1]; *[1]University of Delaware, Newark, Delaware*

WP 017 **Ionization Efficiency Comparison of ESI, SAI, and vSAI Using Compounds with Different Surface Activities**; Madeline Fenner[1]; Charles N McEwen[2]; *[1]University of the Sciences, Philadelphia, PA; [2]University of the Sciences in Philadelphia, Philadelphia, PA*

WP 018 **Effects of Volatile Anions and Cations as Spray Solvent Additives on the DESI–MS Analysis of Proteins**; Andre Venter[1]; Elahe Honarvar[1]; Wisam Alisawi[1]; *[1]Western Michigan University, Kalamazoo, MI*

WP 019 **Top–down DESI-UVPD of Proteins and Lipopolysaccharides on Polyvinylidene Difluoride Membranes**; Dustin Klein[1]; Clara Feider[1]; Livia S Eberlin[1]; Jennifer S Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX*

WP 020 **DART Mass Spectrometry and Emission Spectra of Various DART Gas Sources**; William A. Harris[1]; Johnny K Ho[1]; Douglas B Henderson[1]; *[1]Northrop Grumman, Linthicum Heights, MD*

WP 021 **Ambient MS Based Analytical Platform for Rapid Identification of Brain Cancer Tumor Tissues**; Igor A Popov[1, 2]; Evgeny Zhvansky[1, 2]; Nikita Levin[1]; Vsevolod Shurkhay[3]; Denis Bormotov[1]; Maria Indeykina[2, 4]; Alexey S Kononikhin[2, 4]; Yury Kostyukevich[2, 4]; Evgeny Kukaev[1, 2]; Alexander Potapov[3]; Eugene Nikolaev[2]; *[1]Moscow Institute of Physics and Technology, Moscow, Russia; [2]Institute for Energy Problems of Chemical Physics, Moscow, Russia; [3]Burdenko Neurosurgical Institute, Moscow, Russian Federation; [4]Emanuel Institute of Biochemical Physics, Moscow, Russia*

WP 022 **Assessment of Atmospheric Pressure Surface Mass Spectrometries for Improved Characterization and Imaging of Medical Devices**; Felicia M Green[1]; Adam Taylor[2]; Rory Steven[2]; Elzbieta Gurdak[2]; Josephine Bunch[2]; *[1]National Physical Laboratory, Teddington, Middlesex; [2]National Physical Laboratory, Teddington, UK*

WP 023 **Liquid Microjunction Sampling for the Analysis of Proteins from Thin Tissue Sections**; Rian Griffiths[1]; Elizabeth C Randall[1]; Helen J Cooper[1]; *[1]The University of Birmingham, Birmingham, UK*

WP 024 **Ambient Bio-Molecular Mass Spectrometric Imaging with Subcellular Spatial Resolution**; Jae Young Kim[1]; Eunsoek Seo[1]; Hyunmin Kim[2]; Dong-Kwon Lim[3]; Dae Won Moon[1]; *[1]Department of New Biology, DGIST, Daegu, South Korea; [2]Nano and Energy Research Division, DGIST, Daegu, South Korea; [3]KU-KIST Graduate School of Converging Science and Technology, Korea University, Seoul, South Korea*

WP 025 **Spot Size, Sensitivity, and Fit for Purpose: Comparative Analysis of Extractive Analysis Techniques**; Mariam S Elnaggar; *Prosolia, Inc., Indianapolis, IN*

WP 026 **Point-of-Care Tissue Analysis with Specificity for C=C Bond Lipid Isomers**; Ran Zou[1, 2]; Xiao Wang[1, 2]; Leelyn Chong[1, 2]; Yuan Su[1, 2]; Xiaoxiao Ma[1, 2]; Jessica Page[1, 3]; Riyi Shi[1, 3]; Yu Xia[1, 4]; Zheng Ouyang[1, 2]; *[1]Purdue University, West Lafayette, IN; [2]Biomedical Engineering, Purdue University West Lafayette, IN; [3]School of Veterinary Medicine, Purdue University, West Lafayette, IN; [4]Chemistry Department, Purdue University West Lafayette, IN*

WP 027 **Robotic Surface Analysis Mass Spectrometry (RoSA-MS) for Automated Ambient Sampling of Highly-Curved Three-Dimensional Surfaces**; Martin R L Paine[1]; Rachel V Stryffler[2]; Anyin Li[1]; Jake Huckaby[3]; Alexander S Lambert[1]; Ruffin J White[1]; Henrik I Christensen[1]; Facundo M Fernández[1]; *[1]Georgia Institute of Technology, Atlanta, GA; [2]The Coca Cola Company, Atlanta, GA; [3]Energid, Boston, MA*

WP 028 **Ambient Robotic Mass Spectrometry via Cross Platform Synchonization**; Jason Wu; *Georgia Tech, Atlanta, Georgia*

WP 029 **Development of a Field-Free Ambient Pressure Desorption Thermal Ionization Probe**; Josh Swider[1]; Dale Chatfield[1]; *[1]San Diego State University, San Diego, CA*

ANTIBODIES & ANTIBODY DRUG CONJUGATES (SEQUENCING, MODIFICATIONS & HI RES)
030 - 061

WP 030 **Protease-Containing Membranes For Controlled Digestion of Antibody Cocktails and Enhancement of Monoclonal Antibody Sequencing**; Yongle Pang[1]; Merlin Bruening[1]; *[1]Department of Chemistry, Michigan State University, East Lansing, MI*

WP 031 **Validation of Originator Sequences by Antibody Domain Mass Determination and Top-Down Sequencing**; Anja Resemann[1]; Wolfgang Jabs[1]; Anja Wiechmann[1]; Elsa Wagner[2]; Colas Olivier[2]; Waltraud Evers[1]; Eckhard Belau[1]; Lars Vorwerg[1]; Catherine Evans[1]; Alain Beck[2]; Detlev Suckau[1]; *[1]Bruker Daltonic GmbH, Bremen, Germany; [2]Centre d'Immunologie Pierre-Fabre, St. Julien-en-Genevois, France*

WP 032 **Distinguishing Leucine and Isoleucine Residues in *de novo* Sequencing of mAbs using Nano LC-MSn: A Potential to Replace Edman Degradation**; Dhanashri Bagal[1]; Ping Cao[2]; Eddie Kast[2]; *[1]Amgen, South San Francisco, CA; [2]Amgen, Inc. South San Francisco, CA*

WP 033 **High Throughput Antibody *de novo* Sequencing and Its Utility in Biopharmaceutical Discovery.**; Kadir Ilker Sen[1]; Darryl Davis[1]; Wilfred Tang[2]; Marshall Bern[2]; Chris Becker[2]; *[1]Janssen Research and Development, Spring House, PA; [2]Protein Metrics Inc., San Carlos, CA*

WP 034 **Automated Antibody Sequencing Software**; Wilfred Tang[1]; Marshall Bern[1]; Chris Becker[1]; Kadir Ilker Sen[2]; *[1]Protein Metrics Inc., San Carlos, CA; [2]Janssen Research and Development, Spring House, PA*

WP 035 **Rapid Quantitation of IgG after Digestion at Elevated Temperature with a Novel Trypsin Reagent**; Michael Rosenblatt[1]; Daniel S Spellman[2]; Sergei Saveliev[1]; Kevin P Bateman[2]; Marjeta Urh[1]; *[1]Promega Corp, Madison, WI; [2]Merck & Co., Inc., West Point, PA*

WP 036 **Comparison of Various LC/MS Methods for Label-free Relative Quantitation of Site-specific Glycosylation of a Monoclonal Antibody**; Pilsoo Kang[1]; Jianmei Kochling[1]; *[1]Sanofi Genzyme, Framingham, MA*

WP 037 **Minimizing Method-induced Modifications in the Complementarity Determining Regions (CDRs) of Antibodies to Ensure Optimal Understanding of Product Quality Attributes**; Jennifer Ide[1]; Elaine Stephens[2]; Michelle A English[2]; Jason C Rouse[2]; Lisa A Marzilli[2]; *[1]Pfizer, Andover, MA; [2]Pfizer, Inc. Andover, MA*

WP 038 **A Method Comparison for Quantifying Trisulfides in Monoclonal Antibodies: Non-Reduced Peptide Mapping LC-MS vs. Hydrophilic Interaction Chromatography-Charged Aerosol Detection**; Christopher Cornell; *Genentech, South San Francisco, CA*

WP 039 **Impact of Fc N-Glycan Sialylation on IgG Structure**; Zhongqi Zhang[1, 1]; Bhavana Shah[1]; Jason Richardson[1]; *[1]Amgen, Inc., Thousand Oaks, CA*

WP 040 **Evaluation of a Rapid Method for Deamidation Profiling of Monoclonal Antibodies Suitable for Early Molecular Selection in Drug Discovery**; Heather DeGruttola[1]; Elaine Stephens[1]; Michelle English[1]; Keith A Johnson[1]; Anja Wiechmann[2]; Guillaume Tremintin[3]; Jason Wood[4]; Wolfgang Jabs[2]; Lisa A Marzilli[1]; Jason Rouse[1]; *[1]Pfizer, Inc. Andover, MA; [2]Bruker Daltonic GmbH, Bremen, Germany; [3]Bruker Daltonics, Fremont, CA; [4]Bruker Daltonics, Inc., Billerica, MA*

WP 041 **The Effect of Sialylation of IgG's N-Glycans on FcRn Binding**; Jake Pawlowski[1]; Adriana Bajardi-Taccioli[2]; Damian Houde[2]; Marina Feschenko[2]; Igor A Kaltashov[3]; Tyler Carlage[2]; *[1]UMASS Amherst, Amherst, Massachusetts; [2]Biogen Inc., Cambridge, MA; [3]University of Massachusetts, Amherst, MA*

WP 042 **Characterization of Relative N-Glycan Occupancy in Antibodies using Mass Spectrometry**; Ekaterina G. Deyanova[1]; Yun Wang[1]; Richard Huang[1]; Guodong Chen[1]; *[1]Bristol-Myers Squibb, Princeton, NJ*

WP 043 **Analysis of O-linked Glycan Released from Biopharmaceuticals by using a Chemical Reaction and ASDF-incorporated Curved Field Reflectron.**; Shuuichi Nakaya[1]; Yuzo Yamazaki[1]; *[1]Shimadzu Corporation, Kyoto, Japan*

WP 044 **Building a High Confidence, Quantitative O-glycopeptide Profile for IgA**; Amol Prakash[1]; Shadab Ahmad[1]; Scott M Peterman[2]; Julian A Saba[3]; Chu-Wei Kuo[4]; Kay-Hooi Khoo[4]; Rosa I Viner[3]; *[1]Optys Tech Corporation,*

Brighton, MA; [2]Thermo Scientific BRIMS, Cambridge, MA; [3]Thermo Fisher Scientific, San Jose, CA; [4]Academia Sinica, Taipei, Taiwan

WP 045 **A Novel Approach to Disulfide Bond Reduction in Antibodies using Electrochemistry with Online Mass Spectrometry**; Arielle Verdi[1]; Laurent Rieux[2]; Martin Eysburg[2]; Andrew Milinichik[1]; Xin Cheng[1]; Earl Albone[1]; *[1]Morphotek Inc., Exton, PA; [2]Antec LLC, Boston, MA*

WP 046 **A Novel Method for Rapid Quantitative Determination of Total Free Sulfhydryls of an Antibody Fragment**; Weitao Jia[1]; Qian Cai[1]; Jennifer Zhang[1]; *[1]Genentech Inc, South San Francisco, CA*

WP 047 **Middle-down Approach for Monitoring Monoclonal Antibody Variants and Deglycosylation**; Shanhua Lin[1]; Zoltan Szabo[1]; Yury Agroskin[1]; Terry Zhang[2]; Jonathan L Josephs[2]; Xiaodong Liu[1]; *[1]Thermo Fisher Scientific, Sunnyvale, CA; [2]Thermo Fisher Scientific, San Jose, CA*

WP 048 **Synthesis of Glycopeptides to be Used as Internal Standards for MALDI-MS Analysis of Tryptic Digestion Products from Antibodies**; Rini Roy[1]; Ronald Domalaon[1]; Frank Schweizer[1]; Helene Perreault[2]; *[1]University of Manitoba, Winnipeg, Canada; [2]University of Manitoba, Winnipeg, MB*

WP 049 **Detection and Characterization of Stress-induced Oxidation and Deamidation onVulnerableSites of Etanercept Products**; Li-Juan Huang[1]; Shu-Hui Chen[1]; *[1]Chemistry Dept. NCKU, Tainan, Taiwan (R.O.C.)*

WP 050 **Rapid Evaluation of Domain-specific PTMs in mAbs and Drug Conjugations in ADCs via a New Middle-down Proteomics Tool**; Charles Nwosu[1]; Bisola Asaolu[2]; John Piscitelli[2]; May Zhu[2]; *[1]Takeda Pharmaceuticals International Inc., Cambridge, MA; [2]Takeda Pharmaceutical International Inc., Cambridge, MA*

WP 051 **Antibody Characterization Enabled by Automated Affinity Purification, Deglycosylation, IdeS Digestion, and Reduction**; Steve Murphy[1]; Zach Van Den Heuvel[1]; Maryann Shen[2]; Jing Chen[1]; *[1]Agilent Technologies, Inc., Madison, WI; [2]Agilent Technologies, Santa Clara, CA*

WP 052 **Method Development of a Novel PK assay for Antibody-conjugated Drug Measurement of ADCs using Peptide-linker-drug Analyte**; Suk-Joon Hyung[1]; Neelima Koppada[1]; Surinder Kaur[1]; Ola M Saad[1]; *[1]Genentech Inc, South San Francisco, CA*

WP 053 **Linker-Drug Site Influences Antibody-Conjugated Drug Pharmacokinetic Assay Development for Antibody-drug Conjugates (ADCs)**; M. Violet Lee[1]; Surinder Kaur[2]; Ola Saad[2]; *[1]Genentech, South San Francisco, CA; [2]Genentech Inc, South San Francisco, CA*

WP 054 **Fast Online Characterization of Cetuximab Fd-Glycoprofile by Direct Monitoring and Control of a Mammalian Cell Cultivation Using Ultrahigh-Resolution QTOF Analysis**; Martin Hedström[1]; Constantin Issleib[1]; Fredrik Olsson[2]; Dag Erlandsson[1]; Anja Wiechmann[3]; Anja Resemann[3]; Catherine Evans[4]; Guillaume Tremintin[5]; Jason S. Wood[6]; Detlev Suckau[3]; Wolfgang Jabs[3]; *[1]CapSenze HB, Lund, Sweden; [2]Genovis AB, Lund, Sweden; [3]Bruker Daltonic GmbH, Bremen, Germany; [4]Bruker UK Ltd, Coventry, UK; [5]Bruker, Fremont, CA; [6]Bruker Daltonic, Billerica, MA*

WP 055 **Advancing Attribute Control of Antibodies Drug Conjugates (ADCs) using High Resolution Analytics**; Liuxi Chen[1]; Henry Y Shion[1]; Barbara Sullivan[2]; Ying-Qing Yu[1]; Weibin Chen[3]; *[1]Waters Corp., Milford, MA; [2]Waters Corporation, Beverly, MA; [3]Waters Corporation, Milford , MA*

WP 056 **Physicochemical Structural Characterization of Innovator and Biosimilar Eculizumab with High Resolution Mass Spectrometry Methods**; Maksim Degterev[1]; Maksim Smolov[1]; Grigoriy Poroshin[1]; Rakhim Shukurov[1]; *[1]IBC Generium, Vol'ginskiy, Vladimirskaya Oblast'*

WP 057 **Probing Monoclonal Antibody-Protein Interactions by Native Mass Spectrometry on a Quadrupole Orbitrap Mass Spectrometer**; Hongxia (Jessica) Wang[1]; Haibo Qiu[1]; Jonathan L Josephs[2]; Eugen Damoc[3]; Ning Li[1]; *[1]Regeneron Pharmaceuticals, Tarrytown, NY; [2]Thermo Fisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific, Bremen, DE*

WP 058 **Top-down Characterization of Monoclonal Antibody on an Orbitrap Fusion Lumos Tribrid Mass Spectrometer**; Seema Sharma[1]; Stephane Houel[1]; Christopher Mullen[1]; Chad Weisbrod[1]; Romain Huguet[1]; John Syka[1]; David Horn[1]; Jonathan Josephs[1]; Jae Schwartz[1]; Vlad Zabrouskov[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

WP 059 **Complete Characterization of Biotherapeutic Proteins by Automated Data Processing on High Resolution Accurate Mass Spectrometry with SWATH® Acquisition**; Milla Neffling[1]; Yang Shi[1]; Dominic Gostick[1]; Doug Simmons[2]; *[1]SCIEX, Concord ON, Canada; [2]SCIEX, Concord, ON*

WP 060 **Full Characterization of Heterogeneous Antibody Samples under Denaturing and Native/Native-Like Conditions on a Hybrid Quadrupole-Orbitrap Mass Spectrometer**; Kai Scheffler[1]; Eugen Damoc[2]; Aaron Bailey[3]; Stephane Houel[3]; Jonathan L Josephs[3]; *[1]Thermo Fisher Scientific, Dreieich, DE; [2]Thermo Fisher Scientific, Bremen, DE; [3]Thermo Fisher Scientific, San Jose, CA*

WP 061 **High Resolution Mass Spectrometry of a Bispecific Antibody for the Treatment of Pertussis**; Ellen K Wagner[1]; Andre Bui[1]; Tingting Wang[1]; Maria D Person[1]; Jennifer A Maynard[1]; *[1]University of Texas at Austin, Austin, TX*

BIOMARKERS: DISCOVERY (PART 1)
062 - 088

WP 062 **Serum Haptoglobin Glycosylation as a Potential Biomarker to Monitor Lung Cancer Development**; Ruiqing Zhang[1]; Yujie Liu[1]; Dan Zhang[1]; Zhili Li[2]; *[1]Institute of Basic Medical Sciences, CAMS & PUMC, Bejing, CN; [2]IBMS, CAMS&PUMC, Beijing*

WP 063 **Urine Peptidome Study as a Promising Approach for Preeclamsia Diagnosis**; Nataliia Starodubtseva[1, 2]; Alexey S Kononikhin[1, 2]; Anna Bugrova[1, 3]; Igor A Popov[1, 2, 3]; Victoria Shirokova[2, 4]; Maria Indeykina[3, 4]; Olga Vavina[1]; Kamila Muminova[1]; Yury Kostyukevich[2, 5]; Vitaliy Chagovets[1]; Vadim Lagutin[1]; Evgeny Kukaev[2, 3]; Vladimir E Frankevich[1]; Zulfia Khodzhaeva[1]; Gennady Sukhikh[1]; Eugene Nikolaev[4]; *[1]Research Center for Obstetrics and Gynecology, Moscow, Russia; [2]Moscow Institute of Physics and Technology, Moscow, Russia; [3]Emanuel Institute of Biochemical Physics, Moscow, Russia; [4]Institute for Energy Problems of Chemical Physics, Moscow, Russia; [5]Skolkovo Institute of Technology, Moscow, Russia*

WP 064 **Identification of Serum Protein Biomarkers Associated with Early Heterotopic Ossification Formation following Traumatic Injury**; Michael E. Hoover[1]; Claire Llamas[2]; Elizabeth C. Martin[2]; Elaine Boos[3]; Peter C. Krause[3]; Andrew G. King[3]; Harry Molligan[3]; Olivia C. Lee[3]; Vinod Dasa[3]; Thomas A. Davis[4]; Ammar Qureshi[4]; Benjamin Levi[5]; Jonathan A. Forsberg[4]; Jeffrey M. Gimble[2]; Michael A. Freitas[1]; *[1]Department of Molecular Virology, Immunology and Medical Genetics, The Ohio State University, Columbus, OH; [2]Center for Stem Cell Research and Regenerative Medicine, Tulane University, New Orleans, LA; [3]Department of Orthopedics, LSU Health Sciences Center, New Orleans, LA; [4]Department of Regenerative Medicine, Naval Medical Research Center, Silver Spring, MD; [5]Department of Surgery, University of Michigan, Ann Arbor, MI*

WP 065 **Identification of Nephropathy Prognostic Markers in Urine from Children Affected by type-1 Diabetes**; Magagnotti Cinzia[1]; Gianpaolo Zerbini[1]; Isabella Fermo[1]; Rose Mary Carletti[2, 3]; Riccardo Bonfanti[1]; Fabiana Vallone[1];

Arianna Restivo[4]; Giambattista Capasso[4]; Annapaola Andolfo[1]; *[1]OSR, Milan, Italy; [2]IEO, Milan, Italy; [3]IFOM, Milan, Italy; [4]Second University of Naples, Naples, Italy*

WP 066 **Deep Profiling of Extracellular Vesicles in µL-Scale Plasma Samples Using Miniaturized Isolation Combined with Advanced Separation and MS Data Acquisition**; Simion Kreimer[1]; Arseniy M Belov[1]; Rosa I Viner[2]; Marcia Santos[3]; Barry L Karger[1]; Alexander R. Ivanov[1]; *[1]Northeastern University, Boston, MA; [2]Thermo Fisher Scientific, San Jose, CA; [3]SCIEX, Redwood City, CA*

WP 067 **Selection of Protein Biomarkers in Dehaloccoides Mccartyistrains Enables an MRM-MS Approach for Monitoring Dechlorination Activities in Environmental Samples**; Manuel Villalobos[1, 2]; Karuna Chourey[2]; Frank Loeffler[1]; Robert Hettich[1, 2]; *[1]University of Tennessee-Knoxville, Knoxville, TN; [2]Oak Ridge National Laboratory, Oak Ridge, TN*

WP 068 **Proteome Analysis of Plasma Extracellular Vesicles and the Impact of Sampling Conditions;** Ole Østergaard[1]; Julia Tanas Tanassi[2]; Henrik Niels Helweg Heegaard[1]; *[1]Statens Serum Institut, Copenhagen, Europe; [2]Statens Serum Institut, Copenhagen, Denmark*

WP 069 **Methodological Development for Exosome Enrichment in Serum**; Yan Ren[1]; Jin Zi[1]; Liang Lin[1]; Siqi Liu[1]; *[1]BGI-Shenzhen, Shenzhen, China*

WP 070 **Serum N-glycome Analysis of Colorectal Cancer Patients Reveals Association with Survival**; Stefan W de Vroome[1]; Stephanie Holst[1]; Mar DM Rodriguez Girondo[1]; Bart JA Mertens[1]; Yuri EM van der Burgt[1]; Wilma E Mesker[1]; Manfred Wuhrer[1]; Rob AEM Tollenaar[1]; *[1]Leiden University Medical Center (LUMC), Leiden, The Netherlands*

WP 071 **Identification of Urinary Protein Biomarkers for Diagnosis of Hepatocellular Carcinoma by an Onco-proteogenomics Approach**; Thomas S.-H. Chiou[1, 2]; Chun-Hao Huang[1, 3]; Shu-Wen Chi[1]; Chao-Jen Kuo[1]; King-Teh Lee[1]; *[1]Kaohsiung Medical University, Kaohsiung, Taiwan; [2]Institute of Biological Chemistry, Academia Sinica, Taipei, Taiwan; [3]Weill Graduate School of Medicine, Cornell University, Ithaca, NY*

WP 072 **The Ascites N-glycome of Epithelial Ovarian Cancer Patients**; Karina Biskup[1, 2]; Elena I Braicu[3]; Jalid Sehouli[3]; Rudolf Tauber[1]; Véronique Blanchard[1]; *[1]Institute of Laboratory Medicine, Clinical Chemistry and Pathobiochemistry, Charité Medical University, Berlin, Germany; [2]Department of Biology, Chemistry and Pharmacy, Freie University of Berlin, Berlin, Germany; [3]Department of Gynecology, Berlin, Germany*

WP 073 **Blood Proteins with Isoelectric Point Close to 7.4 as Alzheimer Disease Biomarker**; Mohammad Pirmoradian Najafabadi[1, 2]; Thorleif Lavold[2]; Dag Aarsland[3, 4]; Roman A Zubarev[1]; *[1]Karolinska Institutet, Solna, Sweden; [2]Biomotif AB, Stockholm, Sweden; [3]Karolinska Institutet, Stockholm, Sweden; [4]King's College London, London, UK*

WP 074 **Searching for CSF Biomarkers in PGRN Associated Frontotemporal Dementia**; Diana Nijholt[1]; Lieke Meeter[1]; Christoph Stingl[1]; Lennard Dekker[1]; Jeroen van Rooij[1]; Shami Melhem[1]; Theo M. Luider[1]; John van Swieten[1]; *[1]Erasmus Medical Center, Rotterdam, The Netherlands*

WP 075 **Expanding the CSF Endopeptidome by High-pH reversed-phase Fractionation and LC-MS/MS**; Karl Hansson[1]; Elin Pernevik[1]; Silke Kern[1]; Kaj Blennow[1]; Henrik Zetterberg[1]; Johan Gobom[1]; *[1]Gothenburg University; Institute of Neuroscience and Physiology, Gothenburg, Sweden*

WP 076 **Clinical CSF Proteomics and Endopeptidomics for Biomarker Identification in Neurodegenerative Diseases**; Johan Gobom[1]; Karl Hansson[1]; Elin Pernevik[1]; Tobias Skillbäck[1]; Henrik Zetterberg[1]; Kaj Blennow[1]; *[1]University of Gothenburg, Institute of Neuroscience and Physiology, Gothenburg, Sweden*

WP 077 **Identifying Prostate Cancer Biomarkers by Profiling Glycoproteins in Human Prostate Tissue**; David Spiciarich[1]; Sophia L. Maund[2]; Sean Purcell[3]; Anthony T Iavarone[3]; Donna M. Peehl[2]; Carolyn R Bertozzi[4, 5]; *[1]University of California, Berkeley, CA; [2]Stanford University School of Medicine, Palo Alto CA, USA; [3]UC Berkeley, Berkeley, California; [4]Stanford University, Stanford, CA; [5]Howard Hughes Medical Institute, Chevy Chase, MD*

WP 078 **Mass Spectrometry-Based Proteomics of Human Breast Milk to Assess Breast Cancer Risk Using Different Protein Digestion procedures**; Roshanak Aslebagh[1]; Kathleen F Arcaro[2]; Costel C. Darie[1]; *[1]Clarkson University, Potsdam, NY; [2]University of Massachusetts Amherst, Amherst, MA*

WP 079 **Mass Spectrometric Analysis of Salivary Proteins from Medical Residents Performing Advanced Clinical Simulations Resulting in Acute Stress**; Rachel Marvin[1]; Muncharie Brooke Saepoo[1]; Paul Rega[1]; Viviane Kazan[1]; Kenneth Hensley[1]; David Giovannucci[1]; Dragan Isailovic[1]; *[1]University of Toledo, Toledo, OH*

WP 080 **High Through-Put Quantitative Proteomics for the Discovery of Circulating Biomarkers in Cancer**; Hong Wang[1]; Juan Chen[1]; Xiaoqian Liu[1]; Clemente Aguilar Bonavides[1]; Amin Momin[1]; Hiroyuki Katayama[1]; Sam Hanash[1]; *[1]MD Anderson Cancer Center, Houston, TX*

WP 081 **Proteomic Approach towards Early Diagnosis of Ventilator-Associated Pneumonia (VAP) in Critically Ill Patients**; Khyatiben Pathak[1]; Marissa Saltzman[2]; Emmanuel B Menashi[3]; Frederic Zenhausern[4]; Patrick Pirrotte[2]; *[1]Center for Proteomics, The Translational Genomics Research Institute, Phoenix, AZ; [2]Center for Proteomics, Translational Genomics Research Institute, Phoenix, AZ; [3]Laboratory for Genomics and Personalized Medicine, Honor Health Research Institute, Scottsdale, AZ; [4]Center for Applied Nanobioscience and Medicine, University of Arizona, Phoenix, AZv*

WP 082 **Intact Protein Profiling of Proteoforms Moves toward the Clinic: Intact Protein Classification of Patients with Acute Rheumatic Fever**; Giuseppe Infusini[1]; Laura Dagley[2]; Willy-John Martin[2]; Liam O'Connor[2]; Ian Wicks[2]; Andrew Webb[2]; *[1]Walter & Eliza Hall Institute, Parkville, VIC; [2]Walter & Eliza Hall Institute, Parkville, Australia*

WP 083 **A SWATH-MS Method to Monitoring Oxidative Stress and Progression to Cell Death: From Secretome to Blood Diagnosis**; Sandra Anjo[1]; Vera Mendes[1]; Mário Grãos[1, 2]; Bruno Manadas[1]; *[1]Center for Neurosciences and Cell Biology, Coimbra, Portugal; [2]Biocant - Biotechnology Innovation Center, Cantanhede, Portugal*

WP 084 **Chronic Human African Trypanosomiasis Biomarker Discovery Using Quantitative Proteomics**; Matthew Szucs[1]; Rushdy Ahmad[1]; Brett Eyford[2]; Terry Pearson[2]; Steven A Carr[1]; *[1]Broad Institute of MIT and Harvard, Cambridge, MA; [2]University of Victoria, Victoria BC, Canada*

WP 085 **Application of Adductomics for Investigating Biomarkers Associated with Ovarian Cancer**; Daniel Ladror[1]; William Funk[2]; *[1]Northwestern University, Chicago, IL; [2]Northwestern University, Evanston, IL*

WP 086 **Serialized Nanoparticle-Mediated Enrichment and Profiling of the Saliva Proteome**; Marissa Saltzman[1]; Kelsey Mitchell[2]; Kristine Tsantilas[1]; Khyati Pathak[1]; Christophe Legendre[1]; Victoria David[1]; Matthew Rosenow[1]; Shane Caswell[3]; Lance Liotta[2]; Emanuel Petricoin[2]; Patrick Pirrotte[1]; *[1]Translational Genomics Research Institute, Phoenix, AZ; [2]Center for Applied Proteomics and Molecular Medicine, Manassas, VA; [3]Sports Medicine Assessment Research and Testing (S.M.A.R.T.) Laboratory, Manassas, VA*

WP 087 **Identification of Serum Biomarker Candidates for Fatty Liver Disease through Depletion of Common High-Molecular-Weight Proteins**; Sachin Sridharan[1]; Sobanaa Jayakumar[1]; Keerthana Vinodh[1]; Adaikkalam Vellaichamy[1]; *[1]Anna University, Chennai, India*

WP 088 **Analysis of Possible Biomarkers for Complex Regional Pain Syndrome and Osteoporosis using nLC-MS**; Johan Jacksén[1]; Linus Svenberg[1]; Åsa Emmer[1]; *[1]KTH Royal Institute of Technology, Stockholm, Sweden*

BIOMARKERS: QUANTITATIVE ANALYSIS (PART 2)
089 - 116

WP 089 **Targeted Quantification of Mutant SPOP Proteins in Prostate Cancer**; Hui Wang[1]; Christopher E. Barbieri[2]; Jintang He[1]; Yuqian Gao[1]; Chaochao Wu[1]; Athena A. Schepmoes[1]; Thomas L. Fillmore[1]; Tujin Shi[1]; Sung-Suk Chae[2]; Dennis Huang[2]; Juan Miguel Mosquera[2]; Wei-Jun Qian[1]; Richard D. Smith[1]; Sudhir Srivastava[3]; Jacob Kagan[3]; David Camp[1]; Karin D Rodland[1]; Mark A. Rubin[2]; Tao Liu[1]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]Institute of Precision Medicine of Weill Cornell Medical College and New York Presbyterian Hospital, New York, NY; [3]National Cancer Institute, Bethesda, MD*

WP 090 **Quantitative Tau Isoform Differentiation**; Paul Auger[1]; Stephen Schauer[2]; W. Rodney Mathews[1]; Lee Honigberg[1]; Kristin R Wildsmith[1]; *[1]Genentech, South San Francisco, CA; [2]Genentech Inc, South San Francisco, CA*

WP 091 **Developing LC-MS Assay for Pituitary Adenylate Cyclase-Activating Polypeptide**; Ruina Li[1]; Yuzhong Deng[1]; Brian Dean[1]; Xiaorong Liang[1]; *[1]Genentech Inc, South San Francisco, CA*

WP 092 **Proteomic and Biochemical Analyses of EAM Rat**; Jong Bok Seo[1]; Soo Jeong Park[1]; Seung Min Choi[2]; *[1]Korea Basic Science Institute, Seoul, Republic of Korea; [2]Korea Basic Science Institute, Seoul, Republic of Korea*

WP 093 **Development of a Sensitive LC-MS/MS Method to Quantify Substance P Concentrations in Rat Cerebrospinal Fluid**; Hanumanth Rao Pantangi[1]; Lakshmi Prasanna Rayapati[1]; Prathyusha Chunduru[1]; Saivishal Daripelli[1]; Ganesh Ayyanki[1]; Venkatesh Kamuju[1]; Ramakrishna Nirogi[1]; *[1]Suven Life Sciences Ltd, Hyderabad, Telangana*

WP 094 **MRM-based Assay for Potential Protein Biomarker in Meningioma Patients**; Shuvolina Mukherjee[1]; Ajit Datar[2]; Rashi Kochhar[2]; Sanjeeva Srivastava[1]; Vedita Anand Singh[1]; Nikita Gahoi[1]; Saicharan Ghantasala[1]; Aliasgar Moiyadi[3]; Epari Sridhar[3]; *[1]Indian Institute of Technology Bombay, Mumbai, INDIA; [2]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, INDIA; [3]Tata Memorial Center, Mumbai, INDIA*

WP 095 **MRM Based Targeted Analysis of Serum Samples to Demonstrate Differentially Expressed Proteins in Severe Cases Of Falciparum Malaria**; Vipin Kumar[1]; Shailesh Damale[2]; Ajit Datar[2]; Sanjeeva Srivastava[1]; *[1]Indian Institute of Technology Bombay, Mumbai, India; [2]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India*

WP 096 **Development of MRM Assay for the Determination of Potential Biomarkers in Case of Severe Vivax Malaria**; Sandip Patel[1]; Shailendra Rane[2]; Ajit Datar[2]; Swati Patankar[1]; Sanjeeva Srivastava[1]; *[1]Indian Institute of Technology Bombay, Mumbai, India; [2]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India*

WP 097 **Quantitative Profiling of Hypoxia-responsive Cellular Pathways Associated with Metastasis in Osteosarcoma by Parallel Reaction Monitoring Assay**; Zifeng Song[1]; Liping Yang[1]; Luisa Zini[2]; Caleb Emmons[2]; Siva Kolluri[1]; Millan Shay[1]; Milan Milovancev[1]; Claudia S Maier[1]; *[1]Oregon State University, Corvallis, OR; [2]Proteome Software, Portland, OR*

WP 098 **Analysis of Glycosylation of Serum CD90 in Pancreatic Cancer by Mass Spectrometry**; Jun Cao[1, 2]; Jianhui Zhu[1]; Rui Yang[1]; Zhijing Tan[1]; Mingrui An[1]; David M. Lubman[1]; *[1]University of Michigan Medical Center, Ann Arbor, MI; [2]Hangzhou Normal University, Hangzhou, China*

WP 099 **Quantification of the Unique eEF2 His715-Diphthamide post-translational Modification and Its Derivatives by Parallel Reaction Monitoring Mass Spectrometry**; Axel Ducret[1]; Sabine Kux van Geijtenbeek[1]; Sebastian Stahl[2]; Ana Rita da Silva Mateus Seidl[2]; Sven Michel[2]; Gerhard Niederfellner[2]; Ruediger Rueger[2]; Ulrich Brinkmann[2]; *[1]F. Hoffmann-La Roche Ltd, Basel, Switzerland; [2]F. Hoffmann-La Roche Ltd, Penzberg, Germany*

WP 100 **Analysis of Human Dried Blood Spots for Cotinine and trans-3'-Hydroxycotinine by Reversed Phase Ultra Performance Liquid Chromatography Tandem Mass Spectrometry**; Alexandria L Anstett[1, 2]; Michael C Stagliano[2]; S. Alexandra Burt[1]; Matthew J Geiger[2]; Sara E Tomechko[2]; *[1]Michigan State University, East Lansing, MI; [2]MI Department of Health & Human Services, Lansing, MI*

WP 101 **Novel Proteomics-Based Pipeline for Identifying Predictive Biomarkers of Taxane-Induced Neuropathy**; Emily Chen[1]; Katherine D. Crew[2, 3]; Meghna Trivedi[2]; Danielle Awad[4]; Mathew Maurer[2]; Kevin Kalinsky[2, 4]; Antonius Koller[5]; Purvi Patel[5]; Jenny Kim Kim[5]; Dawn Hershman[2, 3, 4]; *[1]Columbia University Medical Center, New York, NY; [2]Department of Medicine, Columbia University Medical Center, New York, NY; [3]Department of Epidemiology, Columbia University Medical Center, New York, NY; [4]Herbert Irving Comprehensive Cancer Center, New York, NY; [5]Herbert Irving Comprehensive Cancer Center, Proteomics Shared Resource, New York, NY*

WP 102 **Quantification of Lysosomal Storage Disease Specific Urinary Oligosaccharides for Potential Treatment Monitoring**; Rongrong Huang[1]; Allison Cason[1]; Laura Pollard[1]; Tim Wood[1]; *[1]Greenwood Genetic Center, Greenwood, SC*

WP 103 **Evaluation of Stable Isotope Dimethyl Labeling and Spectra Counting for Protein Profiling in Mice with Nonalcoholic Steatohepatitis**; Zhicheng Jin[1]; Takhar Kasumov[2]; *[1]Northeast Ohio Medical University, Rootstown, OH; [2]Northeast Ohio Medical University, Rootstown, OH*

WP 104 **Rapid Detection of a Low-Abundance Biomarker from Plasma Using Combined Capture and Digestion for Improved Sensitivity**; John O'Grady[1]; Kevin Meyer[1]; Derrick Poe[1]; *[1]Perfinity Biosciences, Inc West Lafayette, IN*

WP 105 **Multiplexed Longitudinal Monitoring of Cancer Biomarkers in Dried Blood Spots using an Automated SISCAPA Workflow**; Morteza Razavi[1]; Leigh Anderson[1]; Richard Yip[1]; Matthew E. Pope[1]; Terry W Pearson[1]; *[1]SISCAPA Assay Technologies, Washington, DC*

WP 106 **Standardizing Targeted Mass Spectrometry Quantification of Dystrophin Toward Implementation in Clinical Trials**; Kristy J Brown[1]; Meng Hsuan Han[1]; Mamta Giri[1]; Shivaprasad Bhuvanendran[1]; Jyoti Jaiswal[2]; Eric P Hoffman[1]; Yetrib Hathout[1]; *[1]Children's National Healthy System, Washington DC, DC; [2]Children's National Medical Center, Washington, DC*

WP 107 **Rapid QQQ Screening and Quantification of Proteins from Complex Biological Matrices using Retention Time Predictor without Expensive Protein Standards**; Rohana Liyanage [1]; Balamurugan Packialakshmi[2]; Jeremy Post[3]; Narayan C. Rath[4]; Jackson O. Lay, Jr[2]; *[1]University of Arkansas, Fayetteville , AR; [2]University of Arkansas, Fayetteville, AR; [3]Shimadzu Scientific Instruments, Columbia, MD - Maryland; [4]PPPSRU, USDA, Agricultural Research Service, Fayetteville, AR*

WP 108 **Development of Peripheral Blood Mononuclear Cell (PBMC) Based Protein Biomarkers for Lung Cancer Diagnosis using DIA Mass Spectrometry**; Shaohua Xu[1]; Chunlin Cai[2]; Feng Yao[3]; Qian Wu[4]; Heng Zhao[3]; Wei Yan[2]; *[1]Shanghai Jiatong University, Shanghai, China; [2]Shanghai Jiao Tong University, Shanghai, China; [3]Shanghai Chest Hospital, Shanghai, China; [4]Shanghai Center for Bioinformation Technology, Shanghai, China*

WP 109 **High Sensitivity and High Specificity LC-HRMS Method to Quantify the Corticosteroid Metabolome after Exposure to Inhaled Corticosteroids**; Clementina A Mesaros[1]; Dominic Ciccimaro[1, 2]; Nathaniel W Snyder[3]; Ian A Blair[1, 2]; *[1]University of Pennsylvania, Philadelphia, PA; [2]Penn SRP Center and CEET, Philadelphia, PA; [3]AJ Drexel Autism Institute, Philadelphia, PA*

WP 110 **Quantitative Evaluation towards the Glutathione S-Transferases in Human Plasma Using Affinity Coupling with LC-MS/MS**; Feng Xian; *Beijing Institute of Genomics, CAS, Beijing, Beijing*

WP 111 **Absolute Quantitation of Biomarkers Predictive of Recovery from Acute Kidney Injury after Liver Transplantation with nano-LC - Triple-Quad Mass Spectrometry**; Jacek W Sikora[1]; Paul M Thomas[2]; Joshua Levitsky[3, 4]; Neil L Kelleher[2]; *[1]Proteomics Center of Excellence, Northwestern University, Evanston, IL; [2]Proteomics Center of Excellence, Northwestern University, Evanston, IL; [3]Comprehensive Transplant Center, Northwestern University Feinberg School of Medicine, Chicago, IL; [4]Division of Gastroenterology and Hepatology, Northwestern University Feinberg School of Medicine, Chicago, IL*

WP 112 **Towards Routine Sub 100uL Serum/Plasma Analysis of Hepcidin-25 using LC/MS/MS**; Joel Gummer[1, 2, 3]; Ben Hunter[1, 2]; Robert Trengove[2, 3, 4]; *[1]1School of Veterinary and Life Sciences, Murdoch University, Perth, Australia; [2]Separation Science and Metabolomics Laboratory, Murdoch University, Perth, Australia; [3]Metabolomics Australia, WA Node, Perth, Australia; [4]Murdoch University, Murdoch , WA*

WP 113 **Simultaneous Determination of Ceftazidime and Avibactam in Human Plasma by LC/MS**; Xiaohua Li[1]; Xu Allan[1]; *[1]Keystone Bioanalytical, Inc. North Wales, PA*

WP 114 **Integrating Glycoproteomics in the Comprehensive Multi-Omics Profiling of Obesity-mediated Progression to Type II Diabetes**; Christine Yeh; *Stanford, California*

WP 115 **An ABRF-PRG study: Identification of Low Abundance Proteins in a Highly Complex Protein Sample**; Susan Van Riper[1]; Chen Emily[2]; Allis Chien[3]; Henriette Remmer[4]; Paul M. Stemmer[5]; Wang Yan[6]; Pratik Jagtap[7]; *[1]University of Minnesota Informatics Institute, University of Minnesota, Minneapolis, MN; [2]Herbert Irving Comprehensive Cancer Center & Department of Pharmacology, Columbia University Medical Center, New York, NY; [3]Stanford University Mass Spectrometry, Stanford University, Stanford, CA; [4]Department of Biological Chemistry, University of Michigan, Ann Arbor, MI; [5]Institute of Environmental Health Science, Wayne State University, Detroit, MI; [6]Proteomics Core Facility, University of Maryland, College Park, MD; [7]Center for Mass Spectrometry and Proteomics, University of Minnesota, St. Paul, MN*

WP 116 **Particle-based N-linked Glycan Analysis of Selected Serum Proteins using Non-Glycosylated Binders as a Cancer Array Assay**; Isabella Karlsson[1]; Anna Sroka-Bartnicka[1]; Alessandro Quaranta[1]; Lorena Ndreu[1]; Matthijs Pijnappel[1]; Gunnar Thorsén[1]; *[1]Department of Environmental Science and Analytical Chemistry, Stockholm University, Stockholm, Sweden*

CARBOHYDRATES (GLYCANS)
117 - 138

WP 117 **Separation of Carbohydrate and Glycopeptide Isomers using Ion Mobility-Mass Spectrometry**; Johanna Hofmann[1, 2]; Heung Sik Hahm[3]; Weston B. Struwe[4]; Hannes Hinneburg[2, 3]; Daniel Kolarich[2, 3]; Peter H Seeberger[2, 3]; Kevin Pagel[2]; *[1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany; [2]Freie Universität Berlin, Berlin, Germany; [3]Max Planck Institute of Colloids and Interfaces, Potsdam, Germany; [4]Oxford University, Oxford, UK*

WP 118 **Non-Arbitrary Scoring Model for Structural Identification of Glycosaminoglycan Tandem MS**; Jiana Duan[1]; Jon Amster[2]; *[1]University of Georgia, Athens, GA; [2]University of Georgia, Chemistry Department Athens, GA*

WP 119 **In-depth Analysis of Non-derivatized N-linked Glycans Using Ion Chromatography- Orbitrap Mass Spectrometry**; Zoltan Szabo[1]; Junhua Wang[2]; Yury Agroskin[1]; Rosa Viner[3]; Julian Saba[3]; *[1]Thermo Fisher Scientific Japan, Yokohama, Japan; [2]Thermo Fisher Scientific Inc, San Jose, CA; [3]Thermo Fisher Scientific, San Jose, CA*

WP 120 **Hydrophilic Interaction Liquid Chromatography-Mass Spectrometric Imaging Platform for N-glycan Relative Quantitation using Stable-Isotope Labeled Hydrazide Reagents**; Zhengwei Chen[1]; Xuefei Zhong[2]; Tie Cai[3]; Yatao Shi[2]; Xinxiang Zhang[4]; Lingjun Li[2]; *[1]University of Wisconsin Madison, Madison, WI; [2]University of Wisconsin-Madison, Madison, US; [3]Peking University, Beijing, China; [4]Chinese Academy of Sciences, Shanghai, China*

WP 121 **A Comprehensive Mass Spectrometric Workflow to Investigate Glycosylation Impact on Viral Antigenic Sites**; Edward Bodnar[1]; Lisa Parsons[1]; Yanming An[1]; John F Cipollo[1]; *[1]Human and Health Services, U.S. Food and Drug Administration, Division of Bacterial, Parasitic and Allergenic Products, Laboratory of Bacterial Polysaccharides, Silver Spring, USA*

WP 122 **Mobilizing the Library: Using IMS-MS Data to Supplement GU Library Searching for Glycan Identification**; William Alley[1]; Ying-Qing Yu[1]; *[1]Waters Corp., Milford, MA*

WP 123 **Glycosaminoglycan Peak Searching: A Novel GAG-Specific Method for Automated Tandem Mass Spectra Analysis**; John D. Hogan[1]; Yu Huang[2]; Cheng Lin[2]; Joshua Klein[1]; Luis Carvalho[3]; Chengli Zong[4]; Geert-Jan Boons[4]; Joseph Zaia[2]; *[1]Program in Bioinformatics, Boston University, Boston, MA; [2]Boston University School of Medicine, Boston, MA; [3]Department of Mathematics & Statistics, Boston University, Boston, MA; [4]Complex Carbohydrate Research Center UGA, Athens, GA*

WP 124 **Speeding up the High Throughput Searches for Glycan Analysis**; Ningombam Sanjib Meitei[1]; Arun Apte[2]; Rupanjan Goswami[1]; Julian A Saba[3]; *[1]PREMIER Biosoft, Indore, India; [2]PREMIER Biosoft, Palo Alto, CA; [3]Thermo Fisher Scientific, San Jose, CA*

WP 125 **Comprehensive Assessment of Derivatization Strategies for LC-MS/MS Analysis of N-glycans**; Shiyue Zhou[1]; Xue Dong[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX*

WP 126 **Multiplex LC-MS Analysis of Isotopically Permethylated N-glycans Derived From Biological Samples**; Xue Dong[1]; Shiyue Zhou[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, Texas*

WP 127 **Capillary Electrophoresis Separation of Glycosaminoglycans Followed by Tandem Mass Spectrometry**; Morgan Stickney[1]; Patience Sanderson[1]; Robert J Linhardt[2]; Jon Amster[1]; *[1]University of Georgia, Chemistry Department Athens, GA; [2]Rensselaer Polytechnic Institute, Troy, NY*

WP 128 **Glyconote: A Software for the Automated Interpretation of Glycomics Data from Tandem Mass Spectrometry**; Mingqi Liu[1]; Guy Treves[2]; Andres Guerrero[2]; Matthew Amicucci[2]; Jasmine Davis[2]; Lauren D Wu[2]; Pengyuan Yang[1]; Carlito B Lebrilla[2]; *[1]Fudan University, Shanghai, China; [2]UC Davis Chemistry Department, Davis, CA*

WP 129 **Optimization of Dual Modifications Strategy for Simultaneous Characterization of Neutral and Sialylated N-Glycans by LC-MS/MS**; Haiying Li[1]; Patricia Cho[1]; Stephen Kostel[1]; John Froehlich[1]; Richard Lee[1]; *[1]Boston Children's Hospital, Harvard Medical School Boston, MA*

WP 130 **Semi-automated Glycan Screening and Quantitative Analysis of Longitudinal Plasma Samples**; Elizabeth S. Hecht[1]; Alison Motsinger-Reif[1]; Brendan MacLean[2]; James N Petitte[1]; Michael J MacCoss[2]; David C Muddiman[1]; *[1]North Carolina State University, Raleigh, NC; [2]University of Washington, Seattle, WA*

WP 131 **Sialyl Linkage-Specific Glycan Profiling using Solid-Phase SALSA: A Simple and Versatile Derivatization Approach**; Takashi Nishikaze[1]; Hiroki Tsumoto[2]; Yuzo Yamazaki[1]; Shinichi Iwamoto[1]; Yuri Miura[2]; Koichi Tanaka[1]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]Tokyo Metropolitan Institute of Gerontology, Tokyo, Japan*

WP 132 **MS Based Method to Quantify Rheumatoid Arthritis Serum Glycosaminoglycans Using nano UPLC-ionkey MS/MS on a Xevo G2 Q Tof**; Youjin Seo[1]; Armann Andaya[1]; Julie A Leary[1]; *[1]University of California Davis, Davis, CA*

WP 133 **Detailed Structure Elucidation of the N-linked Octasaccharide of the Archaeon *Methanosarcina mazei* by Mass Spectrometry**; Deborah R. Leon[1]; Cheng Lin[1]; Yi Pu[1]; John R Haserick[1]; Rebecca S Glaskin[1]; Rachel R Ogorzalek Loo[2]; Joseph A Loo[2]; Robert Gunsalus[2]; Catherine E Costello[1]; *[1]Boston University School of Medicine, Boston, MA; [2]UCLA, Los Angeles, CA*

WP 134 **Glyc: A New Tool for Glycan Structure Elucidation and Characterization**; Eric Joyce[1]; Jinshan Gao[1]; *[1]Montclair State University, Montcalir, NJ*

WP 135 **Developmental Profiles of Gangliosides in Prefrontal Cortex of Human Brain via Negative Ion Mode Nano-LC/MS and LC/MS/MS**; Injung Ji[1, 2]; Jae Yun Hwang[1, 2]; Su Min Kim[1, 2]; Dan Bi Park[1, 2]; David Bradley[3]; Hyun Joo An[1, 2]; *[1]Asia Glycomics Reference Site, Chungnam National University, Daejeon, Korea; [2]Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, Korea; [3]Agilent technologies Inc, Santa Clara, CA*

WP 136 **Tailoring Glycan Hydrazide Tagging Reagents for MS Functionality**; James McCord[1]; David C Muddiman[1]; *[1]North Carolina State University, Raleigh, North Carolina*

WP 137 **Acid-Induced Fucose Migration**; Yi Pu[1]; Yang Tang[1]; John Haserick[2]; Catherine E Costello[2]; Cheng Lin[2]; *[1]Boston University, Boston, MA; [2]Boston University School of Medicine, Boston, MA*

WP 138 **Automated N-Glycan Sample Preparation with an Instant Glycan Labeling Dye for Mass Spectrometry**; Ted Haxo[1]; Aled Jones; Michael J Kimzey[1]; Emily Dale[1]; Sergey vlasenko[1]; Steve mast[1]; *[1]ProZyme, Hayward, CA*

DISEASE BIOMARKERS
139 -153

WP 139 **Identification of Novel Biomarker Candidates for Diagnosis of Follicular Carcinoma**; Xianyin Lai; *Indiana University School of Medicine, Indianapolis, IN*

WP 140 **Identification of a CNS-specific Proteome Biomarker for Clinical Relapses and Progression of Multiple Sclerosis using a Systems-Biology Approach**; Itay Raphael[1]; Carol A Huizar[1]; Yanyan Qu[2]; Wendell P Griffith[2]; Thomas G Forsthuber[1]; *[1]Department of Biology, University of Texas at San Antonio, San Antonio, TX; [2]Department of Chemistry, University of Texas at San Antonio, San Antonio, TX*

WP 141 **Biomarkers of Early Chronic Obstructive Pulmonary Disease (COPD) in Smokers and Former Smokers - A Comparison of Two Methods**; Karin Barbara Sahlin[1]; Johan Malm[2]; Mikael Truedsson[2, 3]; May Bugge[3]; Elisabet Wieslander[2]; Maria Yokaleva[2]; Magnus Dahlbäck[2]; Roger Appelqvist[2]; Thomas Fehniger[2]; György Marko-Varga[2]; *[1]Lund University, Lund , Sweden; [2]Lund University, Lund, Sweden; [3]Örestadskliniken, Malmö, Swden*

WP 142 **Large-Scale Analysis of Protein Conformational Changes for Biomarker Discovery**; Fang Liu[1]; Michael C Fitzgerald[1]; *[1]Duke University, Durham, NC*

WP 143 **Study of Traumatic Brain Injury Biomarkers by Mass Spectrometry-Based Proteomics**; Manasi Mangaonkar[1]; Richard A Yost[1]; Kari Green[1]; Kevin Wang[1]; *[1]University of Florida, Gainesville, FL*

WP 144 **Lipidomics Approach in Biliary Atresia for a Potential Diagnostic Method Based on Mass Spectrometry**; Cibele Esteves[1]; Diogo Noin de Oliveira[1]; Carlos Fernando Odir Rodrigues Melo[1]; Luciana Di Paolo[1]; Gabriel Hessel[1]; Rodrigo Ramos Catharino[1]; *[1]University of Campinas, Campinas, Brazil*

WP 145 **Neonatal Neurodegeneration in 5XFAD Alzheimer's Disease Transgenic Mouse Model**; Aise Rumeysa Mazi[1, 2]; Aysegul Sumeyye Arzuman[1, 2]; Mehmet Ozansoy[1, 3]; Ahmet Tarik Baykal[4]; *[1]Regenerative and Restorative Medicine Research Center, REMER, Istanbul, Turkey; [2]Institute of Health Science, Istanbul Medipol University, Istanbul, Turkey; [3]Department of Physiology, International School of Medicine, İstanbul Medipol University, Istanbul, Turkey; [4]Acibadem University, Ataşehir-Istanbul*

WP 146 **A Proteomic Investigation of the Role of Neurotoxins Linked to Amyotrophic Lateral Sclerosis Disease Pathogenesis**; Joshua Beri[1]; Michael S Bereman[1]; *[1]NC State University, Raleigh, NC*

WP 147 **Prediction of Response to Sorafenib in Hepatocellular Carcinoma: A Multimarker Panel of Potential Biomarkers by Multiple Reaction Monitoring-Mass Spectrometry**; Hyunsoo Kim[1]; Injoon Yeo[1]; Su Jong Yu[2]; Taesung Park[3]; Jung-Hwan Yoon[2]; Youngsoo Kim[1]; *[1]Department of Biomedical Engineering, Seoul National University College of Medicine, Seoul, Korea; [2]Department of Internal Medicine and Liver Research Institute, Seoul National University College of Medicine, Seoul National University Hospital, Seoul, Korea; [3]Department of Statistics, Seoul National University, Seoul, Korea*

WP 148 **Simultaneous Quantification of Tryptophan-Relatedmetabolitesas Biomarkers for Prediabetes**; Norihide Yokoi[1]; Ritsuko Hoshikawa[1]; Toshiya Matsubara[2]; Susumu Seino[1]; *[1]Kobe University Graduate School of Medicine, Kobe, JPN; [2]SHIMADZU Corporation, Kyoto, JPN*

WP 149 **Comparison of Plasma Protein Profiles of Selected Cardiovascular Diseases by iTRAQ Quantification**; Helena Rehulkova[1]; Alena Myslivcova Fucikova[1]; Pavel Rehulka[1]; Radek Pudil[2]; Jiri Stulik[1]; *[1]Faculty of Military Health Sciences, University of Defence, Hradec Kralove, Czech Republic; [2]1st Department of Internal Medicine – Cardioangiology, Faculty Hospital, Hradec Kralove, Czech Republic*

WP 150 **Proteomics Analysis of Aged Healthy Human White Blood Cells**; Ceereena Ubaida-Mohien[1]; Alexey Lyashkov[1]; Arsun Bektas[1]; Robert Wersto[1]; Nan Ping Weng[1]; Ranjan Sen[1, 2]; Luigi Ferrucci[1]; *[1]Intramural Research Program, National Institute on Aging, National Institutes of Health, Baltimore, MD - Maryland; [2]Laboratory of Molecular Biology and Immunology, National Institute on Aging, Baltimore, MD*

WP 151 **Cardiovascular Disease - Metabolic Syndrome Induced Protein/PTM Changes**; Mark E. McComb[1]; Stephen A. A Whelan[1]; Chunxiang Yao[1]; Jessica B. Behring[1]; Jean L. Spencer[1]; Christian F. Heckendorf[1]; Nancy M. Leymarie[1];

Deborah A. Siwik[1]; Wilson S. Colucci[1]; Richard A. Cohen[1]; Markus M. Bachschmid[1]; Catherine E. Costello[1]; *[1]Boston University School of Medicine, Boston, MA*

WP 152 **An Adductomics Pipeline for Untargeted Analysis of Post Translational Modifications**; Hasmik Grigoryan[1]; William Edmands[2]; Sixin S Lu[2]; Yukiko Yano[2]; Anthony Iavarone[2]; Evan R Williams[2]; Stephen M Rappaport[2]; *[1]University Of California, Berkeley, CA; [2]University of California, Berkeley, CA*

WP 153 **Localized Quantitative Proteomics on Amyloid Plaques Microdissected from Postmortem Tissue to Characterize Difference between Rapidly Progressive and Typical Alzheimer's Disease**; Shruti Nayak[1]; Eleanor Drummond[1]; Manor Askenazi[2]; Arline Faustin[1]; Geoffrey Pires[1]; Richard Hickman[1]; Jiri Safar[3]; Thomas Wisniewski[1]; Beatrix M Ueberheide[1]; *[1]NYULMC, New York, NY; [2]Biomedical Hosting LLC, Arlington, MA; [3]Case Western Reserve University, Cleveland, OH*

DRUG DISCOVERY/DMPK/ADME (GENERAL)
154 - 177

WP 154 **High Throughput Screening of Competitive Binders for Target Proteins using Rapid LC-MS Analysis**; Kasun Imaduwage[1]; Eden P Go[2]; Heather Desaire[1]; *[1]University Of Kansas, Lawrence, KS; [2]University of Kansas, Lawrence, KS*

WP 155 **Implementation of Mass Spectrometry into High Throughput Screening Workflows to Improve Hit Quality**; Gregory Adam[1]; Juncai Meng[2]; Adam Amoss[2]; Amita Patel[2]; Daniel Riley[2]; Victor Uebele[2]; Jeffrey Hermes[2]; *[1]Merck & Co., Inc., North Wales, PA; [2]Merck & Co., North Wales, PA*

WP 156 **Application of High-Throughput Micro-Flow LC/MS/MS to a Metabolic Stability Screening Workflow**; Brendon Kapinos[1]; John S Janiszewski[1]; Mary Piotrowski[1]; Wayne Lootsma[2]; Steven Ainley[2]; William Schramm[2]; Hui Zhang[1]; *[1]Pfizer, Groton, CT; [2]Sound Analytics, Niantic, CT*

WP 157 **Ultra High Throughput Drug Discovery Screening by MALDI-TOF Mass Spectrometry– Exceeding One Million Samples per Week**; Peter S. Marshall[1]; Michelle Pemberton[1]; Carl Haslam[1]; Gabriella Clarke[1]; Jessica Chandler[1]; Adrian Dunn[1]; Neil Hardy[1]; Melanie Leveridge[1]; *[1]GlaxoSmithKline, Stevenage, UK*

WP 158 **High Throughput Screening- ADME; Transitioning from Triple Quadrupole to High Resolution Accurate Mass Spectrometry**; Jason Causon[1]; Graeme Clark[2]; *[1]SCIEX, Warrington, UK; [2]Cyprotex, Macclesfield, UK*

WP 159 **Utilizing High Resolution Accurate Mass Spectrometry for Quantification, MRMHR and SWATH® Acquisition Workflows**; Jason Causon[1]; Lee Mendil[2]; Donna-Michelle Smith[2]; Neil Devenport[1]; Thomas Knapman[1]; Milla Neffling[1]; *[1]SCIEX, Warrington, UK; [2]CRUK Cambridge Institute - University Of Cambridge, Cambridge, UK*

WP 160 **Simultaneous Analysis of Supernatant Components of Cell Culture using Triple Quadrupole LC/MS/MS**; Qiaoxia Liu[1]; Hongyuan Hao[1]; Yuling Song[1]; Qiang Li[1]; Zhao Liu[1]; Taohong Huang[1]; Yuki Hashi[1]; *[1]Shimadzu, Shanghai, CHINA*

WP 161 **Assay Development of *in vitro* Blood-Brain Barrier Models for Drug Permeability Screening**; Lie Min[1]; Jennifer L. Mantle[1]; Kelvin H. Lee[1]; *[1]Department of Chemical and Biomolecular Engineering and Delaware Biotechnology Institute, University of Delaware, Newark, DE*

WP 162 **Labeled Compound Detection Using Compound Discoverer Pattern Scoring From High Resolution Mass Spectrometry**; Caroline Ding[1]; Tim J Stratton[1]; Martin Strohalm[2]; Ji Ma[3]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Bremen, DE; [3]Amgen, Inc. South San Francisco, CA*

WP 163 **Evaluation of Ion Mobility Enabled Collisional Cross Section Measurements for the Differentiation of Acyl and Phenolic Glucuronide Metabolites**; Catherine Holdsworth[1]; Richard Clayton[1]; Daniel Weston[2]; Nick Tomczyk[2]; Martin Palmer[2]; Darren Hewitt[2]; *[1]Covance, Harrogate, UK; [2]Waters, Wilmslow, UK*

WP 164 **Resolution and Characterisation of Co-eluting Isomeric Metabolites by Collision Cross Section Measurements using a Novel Geometry Travelling-Wave IMS-QTof Mass Spectrometer**; Richard Clayton[1]; Catherine Holdsworth[1]; Daniel Weston[2]; Nick Tomczyk[2]; Martin Palmer[2]; Darren Hewitt[2]; *[1]Covance, Harrogate, UK; [2]Waters, Wilmslow, UK*

WP 165 **Automatic Calculation and Layout of MS/MS Fragmentation Pathways**; Ismael Zamora[1]; Blanca Serra[2]; Morettoni Luca[3]; *[1]Lead Molecular Design, S.L., Sant Cugat del Valles, Barcelona; [2]Molecular Discovery, Ltd London, UK; [3]Molecular Discovery, London, UK*

WP 166 **Drug Stability Study using Q Exactive Bench-Top Mass Spectrometer**; Jie Ding[1]; Thomas Leitzinger[1]; Kate Comstock[2]; *[1]PPD Inc, Middleton, WI; [2]Thermo Fisher Scientific, San Jose , CA*

WP 167 **Novel Drug Target Identification via Label Free Differential Mass Spectrometry and Thermal Stability Profiling**; Harris Bell-Temin[1]; Steven J Mullett[1]; David Zaidins[2]; Andrey Bondarenko[3]; Mark E Schurdak[2]; Andrew Michael Stern[2]; D. Lansing Taylor[2]; Nathan A Yates[1]; *[1]School of Medicine, University of Pittsburgh, Pittsburgh, PA; [2]Drug Discovery Institute, University of PIttsburgh, Pittsburgh, PA; [3]Infoclinika, Seattle, WA*

WP 168 **Quantitative Kinome Analysis as a Tool for Discovering Molecular Targets for Cancer Therapy**; Weili Miao[1]; Yongsheng Xiao[1]; Yinsheng Wang[2]; *[1]University of California - Riverside, Riverside, CA; [2]University of California, Riverside, CA*

WP 169 **Rapid Rank Ordering of Compounds in Mixtures by Orthogonal Affinity Selection – Mass Spectrometry**; Christine L. Andrews[1]; Matthew P Richards[1]; Jacqueline Hicks[1]; John Caldwell[1]; Jared Cumming[1]; Andrew Stamford[1]; Corey Strickland[1]; Peter Dandliker[1]; *[1]Merck & Co, Kenilworth, NJ*

WP 170 **Platform Agnostic Data Processing Routine for Targeted and Untargeted Metabolite Identification in Drug Discovery**; Richard Lee[1]; Vitaly Lashin[2]; Alexandr Sakarov[2]; *[1]ACD/Labs, Toronto, Canada; [2]ACD/Labs, Moscow, Russia*

WP 171 **A MS Approach to Understand the Most Metabolically Labile Amide Bonds in Peptides**; Ismael Zamora[1]; Tatiana Radchenko[1]; Elisabeth Ortega[1]; *[1]Lead Molecular Design S.L., Sant Cugat de Valles, Spain*

WP 172 **Identification of Active Herbal Ingredients by Affinity Selection Mass Spectrometry Coupled with Ultrafiltration**; Yan Jin[1]; Fangzhou Xie[1]; Lei Fu[1]; *[1]Shanghai Jiao Tong University, Shanghai, China*

WP 173 **Glue Medicines Analysis by UHPLC Tandem Quadrupole-Time of Flight Mass Spectrometry**; Hu Nan[1]; Zuo Shuai[1]; Du Wei[1]; Bo Tao[1]; *[1]Agilent Technologies (China) Limited, Beijing, China*

WP 174 **Rapid Determination of Protein Binding Affinity Using Solid Phase Micro Extraction**; Emily Barrey[1]; Craig Aurand[1]; David Bell[1]; Sara Smith[1]; *[1]Sigma Aldrich, Bellefonte, PA*

WP 175 **Biochemical Assay Development Using Novel MALDI High-Throughput Screening System**; Sergei Dikler[1]; Paul J Kowalski[2]; *[1]Bruker Daltonics, Billerica, MA; [2]Bruker Daltonics, Inc., Billerica, MA*

WP 176 **Assessment of Chemical Probes for Identification of Cellular Targets of Small Molecules**; Jeffrey Martin[1]; Mercedes Beyna[1]; Ceren Korkut[1]; Rajesh Prakash[1]; Jeffery Vessels[1]; Kevin Guckian[1]; Erik Hett[1]; Peter Juhasz[1]; *[1]Biogen, Cambridge, MA*

ENERGY: BIOFUELS AND ALGAE
178 - 189

WP 177 **Evaluating the Impact of Freezing Biologic Fluids on Drug Distribution and Its Impact on Frozen Aliquotting for Quantitative Drug Analysis**; Glenn Smith[1]; Joseph Fraone[1]; Graham Long[1]; Tanya Shih[1]; *[1]Cryoxtract Instruments, Woburn, MA*

WP 178 **Detection of Creatine from Single Algae Cells using Mass Spectrometry**; Mei Sun[1]; Ning Pan[1]; Boris Wawrik[1]; Zhibo Yang[1]; *[1]The University of Oklahoma, Norman, OK*

WP 179 **Quadrupole–Time-of-Flight Tandem Mass Spectrometry Identifies and Quantifies Eugenol in Extraction from Bio-oils Into Diesel**; Kelsey Boes[1]; Nelson R Vinueza[1]; Yufei F Chen[1]; Hoyong Kim[1]; Park Sunkyu[1]; *[1]North Carolina State University, Raleigh, NC*

WP 180 **Application of Molecular Dynamic Simulation to Improve the CCS Calculation Accuracy of Aromatic Compounds with Long Alkyl Chains**; Arif Ahmed[1]; Dongwan Lim[1]; Hugh I. Kim[2]; Sunghwan Kim[1, 3]; *[1]Kyungpook National University, Daegu, Republic of Korea; [2]Korea University, Seoul, Republic of Korea; [3]Green-Nano Materials Research Center, Daegu, Republic of Korea*

WP 181 **Characterization of a β-O-4 Trimeric Lignin Model Compound and Post Fenton Chemistry Products using HRAM Mass Spectrometry**; Fan Huang[1]; Bert C Lynn[1]; *[1]University of Kentucky, Lexington, KY*

WP 182 **Investigating the Mechanism of Lipid Body Obesity in *C. reinhardtii* under Nitrogen Starvation Conditions using High Resolution Mass Spectrometry**; Carter Lantz[1]; Ryan Rho[1]; Jeremy Sieker[1]; Matthew Brantley[1]; Alireza Abdolvahabi[1]; James Chang[1]; Sung-Joon Kim[1]; Touradj Solouki[1]; *[1]Baylor University, Waco, TX*

WP 183 **Effect of Alkali Metals on Pyrolysis Kinetics of Carbohydrates Using dAPCI-TOF MS**; Kristen O'Connor[1]; Carolyn Hutchinson[1]; Young Jin Lee[1]; *[1]Iowa State University, Ames, IA*

WP 184 **Characterization of Fast Pyrolysis Oil from Pine Feedstock**; Ashley Wittrig[1]; Ross Mabon[1]; Boris Sheludko[1]; *[1]ExxonMobil, Annandale, NJ*

WP 185 **Exploring the Mechanisms of Fast Pyrolysis of Hemicellulose via Tandem Mass Spectrometry and Quantum Chemical Calculations: A Model Compound Study**; Priya Murria[1]; John Degenstein[1]; Mckay Easton[1]; Hanyu Zhu[1]; John Nash[1]; Rakesh Agrawal[1]; Nicholas Delgass[1]; Fabio Ribeiro[1]; Kenttämaa Hilkka[1]; *[1]Purdue University, West Lafayette, IN*

WP 186 **Chemical Reactions Causing Instability in Wood-Derived Bio-Oils: Enhanced Detection of Aldehydes using Peracetylation with Pyridine or DMAP**; Elizabeth A. Stemmler[1]; Paige E. Speight[2]; Mason A. Bosse[2]; Matthew J. Rasmussen[2]; *[1]Bowdoin College, Brunswick , ME; [2]Bowdoin College, Brunswick, ME*

WP 187 **Integrated Omics Reveals the Details of Metabolic Adaptation of Clostridium thermocellumATCC-27405 Grown on Switchgrass**; Suresh Poudel[1, 2]; Richard J Giannone[1]; Miguel Rodriguez[1]; Babu Raman[3]; Madhavi Z Martin[1]; Nancy L Engle[1]; Nookaew Intawat[1]; Steven D Brown[1]; Timothy J Tschaplinski[1]; David Ussery[1]; Hettich L Robert[1]; *[1]Oak Ridge National Laboratory, Oak Ridge, TN; [2]University of Tennesse, Knoxville, TN; [3]Dow AgroSciences, Indianapolis, IN*

WP 188 **Large scale Identification of Polymorphic Peptides via Cross-Species Spectral Networks in Microbial Proteomics**; Seungjin Na[1]; Sam Payne[2]; Nuno Bandeira[1]; *[1]University of California San Diego, La Jolla, CA; [2]Pacific Northwest National Lab, Richland, WA*

WP 189 **Development of GeLC-MRM Approach to Study Carbon Concentrating Mechanism during Nitrogen Starvation in Chlorella sp IITG FC2**; Vineeta Rai[1]; Deepti Bhandarkar[2]; Ajit Datar[2]; Sanjeeva Srivastava[1]; *[1]Indian Institute of Technology Bombay, Mumbai, India; [2]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India*

ENVIRONMENTAL ANALYSIS: WATER QUALITY
190 - 206

WP 190 **Development of Method for Quantification of Iodoacetic Acids in Drinking Water Using GC/EI-MS/MS**; Hannah Liberatore[1]; Amy A. Cuthbertson[1]; Susan D Richardson[1]; *[1]University of South Carolina, Columbia, SC*

WP 191 **Water Quality Growth and Change, Advanced Technology Method Change to Prescribe a Desirable Future to US EPA Method 521, (2004)**; Andrew Eaton[1]; Konjit Tadigo[1]; Charles Grady[1]; Ron Honnold[2]; *[1]Eurofins Eaton Analytical Inc, Monrovia, CA; [2]Agilent Technologies, Prescott, AZ*

WP 192 **A New Approach for Identification of Unknown Disinfection Byproducts in Drinking Water using Multiplex Solid Phase Extraction /HPLC-tandem Mass Spectrometry**; Xing-Fang Li[1]; Yanan Tang[2]; Guang Huang[2]; Lindsay Jmaiff[2]; Ian Vander Meulen[2]; *[1]University of Alberta, Edmonton, AB; [2]University of Alberta, Edmonton, Canada*

WP 193 **Direct Analysis of PFAAs in Water using Differential Mobility Spectrometry-Mass Spectrometry**; Matthew Noestheden[1]; KC Hyland[2]; Simon Roberts[2]; Chris Higgins[3]; *[1]SCIEX, Concord, ON; [2]SCIEX, Redwood City, CA; [3]Colorado School of Mines, Golden, CO*

WP 194 **Significantly Improved Detection in Volatile Organic Analysis (VOA) of Water using Static Headspace and GCMS with a High Efficiency Source;** Harry Prest[1]; Melissa Churley [2]; Peter Gautschi[3]; *[1]Agilent Technologies, Santa Clara, CA; [2]Agilent Technologies, Santa Clara , CA; [3]Agilent Technologies Sales & Services GmbH, Waldbronn, Deutschland*

WP 195 **Increased Capabilities for the Analysis of Hormones in Drinking and Waste Water using SPE and LC/MS/MS**; Xianrong (Jenny) Wei[1]; Sean Orlowicz[2]; *[1]Phenomenex, Torrance, ca; [2]Phenomenex, Torrance, CA*

WP 196 **Analysis and "Fingerprinting" of Non-Ionic Surfactants in Hydraulic Fracturing Waters by Ion Mobility Mass Spectrometry**; E. Michael Thurman[1]; Imma Ferrer[2]; Jerry Zweigenbaum[3]; Aaron Boice[4]; John Fjeldsted[4]; *[1]University of Colorado, Boulder, CO; [2]University of Colorado, Boulder, Colorado; [3]Agilent Technologies, Little Falls, DE; [4]Agilent Technologies, Santa Clara, CA*

WP 197 **Cloud-based Analysis of Complex Sample Systems for Outlier and Trend Analysis in the Context of Water Monitoring**; Ralf Tautenhahn[1]; Tim J Stratton[1]; Dipankar Ghosh[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

WP 198 **Two Birds with One Stone: Simultaneous GC/MS Analysis of Volatile and Semivolatile Water Pollutants**; Olga V Polyakova[1]; Dmitry Mazur[1]; Viatcheslav Artaev[2]; Albert T. Lebedev[3]; *[1]Moscow State University, Moscow, Russia; [2]LECO Corporation, St Joseph, MI; [3]Moscow State University, Moscow, Moscow*

WP 199 **Unknown Profiling of Drinking Water Using High Resolution LC-MS/MS and New Software**; Caroline DING[1]; Anastasia Kalli[1]; Charles Yang[1]; Tim J Stratton[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

WP 200 **Environmental Screening of Water Samples utilizing Ion Mobility Enable High Resolution Mass Spectrometry**; Lauren Mullin[1]; Douglas Stevens[1]; Gareth Cleland[1]; Adam Ladak[1]; *[1]Waters, Milford, MA*

WP 201 **Using Mass Spectrometry to Detect Silanol Compounds in Water from the International Space Station**; Jeffrey A. Rutz[1]; C.K. Mike Kuo[1]; James T. Alverson[1]; William T. Wallace[1]; Daniel B. Gazda[2]; *[1]Wyle Science, Technology, and Engineering Group, Houston, TX; [2]NASA Johnson Space Center, Houston, TX*

WP 202 **Quantitative Analysis of Nonylphenol Ethoxylates in Surface Water with UHPLC and HRAM Mass Spectrometry**; Cindy Lai[1]; Claudia Martins[1]; Keith Waddell[1]; Mark Tracy[2]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Sunnyvale, CA*

WP 203 **MALDI-TOF MS for Identification of Organic-Degrading Bacteria in Contaminated Groundwater near Unconventional Natural Gas Extraction Sites**; Inês C. Santos[1]; Doug D. Carlton Jr.[1]; Zacariah L. Hildenbrand[2,3]; Kevin A Schug[1,3]; *[1]Department of Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, TX; [2]Inform Environmental, LLC, Dallas, TX; [3]Affiliate of the Collaborative Laboratories for Environmental Analysis and Remediation, The University of Texas at Arlington, Arlington, TX*

WP 204 **Screening for Pollutants in Water using a GC/MSD Extractor Source with MassHunter Deconvolution Software and Customized Reporting**; Chris Sandy[1]; Angela Henry[2]; Bruce Quimby[2]; Lei Tao[1]; Sue Zhang[1]; Vadim Kalmeyer[1]; Sun Li[1]; *[1]Agilent Technologies, Santa Clara, CA; [2]Agilent Technologies, Little Falls, DE*

WP 205 **Identification of Halobenzoquinones, an Emerging Class of Disinfection By-Products in Drinking Water, using High Resolution Mass Spectrometry**; Wei Wang; *University of Alberta, Edmonton, AB*

WP 206 **Medical Imaging Compounds as a Source for New Iodo-Disinfection Byproducts in Drinking Water**; Christina M Joseph[1]; Cristina Postigo[2]; Michael J Plewa[3]; Thomas A Ternes[4]; Friedrich Wendel[4]; Christian Luetke-Eversloh[4]; Stephen E Duirk[5]; Susan D Richardson[1]; *[1]University of South Carolina, Columbia, SC; [2]Institute of Environmental Assessment and Water Research (IDAEA-CSIC) Water and Soil Quality Research Group, Department of Environmental Chemistry, Barcelona, Spain; [3]University of Illinois at Urbana-Champaign, Urbana-Champaign, IL; [4]Federal Institute of Hydrology (BfG), Koblenz, Germany; [5]University of Akron, Akron, OH*

FOOD SAFETY: OTHER CONTAMINANTS (PART 1)
207 - 235

WP 207 **Characterization of the Volatile Degradation Products of Soybean Oil after Frying Process by HS-SPME-GC-MS**; Ya-Ting Tsai[1]; Maw-Rong Lee[2]; *[1]Department of Chemistry, National Chung-Hsing University, Taichung, Taiwan; [2]National Chung-Hsing University, Taichung, Taichung*

WP 208 **Non-targeted Analysis Approach for Distinguishing of Various Vegetable Oils and Adulterated Oils using HS-SPME-GC-MS**; Yu-Hao Chen[1]; Maw-Rong Lee[2]; *[1]Department of Chemistry, National Chung-Hsing University, Taichung, Taiwan; [2]National Chung-Hsing University, Taichung, Taichung*

WP 209 **Significant Robustness Improvements of PAHs Analysis in Palm Oil using the Self-Cleaning Ion Source (SCIS) in a GC/MS/MS System;** Michel Lesieur[1]; Elizabeth Almasi[2]; Terry Sheehan[2]; *[1]Agilent Technologies, Les Ulis, France; [2]Agilent Technologies, Santa Clara, CA*

WP 210 **Analysis of Fish Oil for Contaminants by LC Time-of-Flight Mass Spectrometry with All Ions Confirmation**; Sue Dantonio[1]; Joan Stevens[2]; *[1]Agilent Technologies, Flatonia, TX; [2]Agilent Technologies, Wilmington, DE*

WP 211 **Quality Control of Cooking Oils by Metabolic Profiling and Spectral Fingerprinting**; Chi Yuen Cheung; *HKUST, Hong Kong*

WP 212 **Direct Analysis of Brominated Vegetable Oil in Commercial Soft Drinks by LC-MS**; Priyanka Chitranshi[1]; Goncalo Gamboa Da Costa[1]; *[1]US FDA NCTR, Jefferson, AR*

WP 213 **Determination of Phthalates in Vegetables by GPC–GCMS**; Zhang Xi; *SHIMADZU (CHINA) CO., LTD., Beijing Branch, Beijing, China*

WP 214 **Representative, Two-Gram Incurred Food Samples using mini-QuEChERS, Cryomilling and GC/MS/MS Analysis with a High Efficiency Ion Source**; Joan Stevens[1]; Melissa Churley[2]; *[1]Agilent Technologies, Wilmington, DE; [2]Agilent Technologies, Santa Clara, CA*

WP 215 **Identification of Contaminants in Powdered Beverages by Direct Extraction Thermal Desorption GC/MS**; Ronald Shomo[1]; Christopher W Baker[1]; John Manura[1]; *[1]Scientific Instrument Services, Ringoes, NJ*

WP 216 **Simultaneous Separation and Determination of Fifteen Organic UV Filters in Sunscreen Cosmetics by HPLC-ESI-MS/MS**; Qiang Ma[1]; Xianshuang Meng[1]; Guangcheng Xi[1]; *[1]Chinese Academy of Inspection and Quarantine, Beijing, China*

WP 217 **Determination of Chlorinated Compounds Arising from the Thermal Degradation of Sucralose**; Diogo Noin de Oliveira[1]; Maico Menezes[1]; Rodrigo Ramos Catharino[1]; *[1]Innovare Biomarkers Laboratory - UNICAMP, Campinas, Brazil*

WP 218 **A High Throughput, Low Cost and Green Approach to Automated Extraction, Clean Up, and Concentration for Same Day POPs Analysis**; Tom Hall[1]; Ruud Addink[1]; *[1]Fluid Management Systems, Watertown, MA*

WP 219 **Total Residue Analysis of Glyphosate and Three Metabolites in Soy and Milk-Based Nutritional Ingredients by Liquid Chromatography – Mass Spectrometry**; Stefan Ehling[1]; Todime Reddy[1]; *[1]Abbott Nutrition, Columbus, OH*

WP 220 **Infant Formula and Milk: Chlorinated Dioxins and Furans Analysis Using Automated Extraction and Column Chromatography**; Aleks Sharapov[1]; Rudolf Addink[1]; *[1]Toxic Report, Watertown, MA*

WP 221 **Simultaneous Determination of Total vitamins B1, B2, B3, B5, and B6 and Total Folate in Infant Formula and Related Nutritionals**; Nicholas Cellar[1]; Todime Reddy[1]; *[1]Abbott Nutrition, Columbus, OH*

WP 222 **Simultaneous Determination of Choline, Carnitine, and Myo-inositol by LC-MS/MS**; Jonathan Draher[1]; Nicholas A Cellar[2]; Todime Reddy[2]; *[1]Abbott Nutrition, Columbus, OH; [2]Abbott Nutrition, Columbus, OH*

WP 223 **Multi-residue Antibiotic Analysis of Dairy Products using UHPLC-MS/MS with a Heated Laminar Flow Interface and a Modified QuEChERS Method**; Avinash Dalmia[1]; Sharanya Reddy[1]; Thomas P White[1]; Tong Chen[1]; Wilhad Reuter[1]; David Welkie[1]; Lisa Cousins[2]; Joshua Ye[2]; Reza Javahery[2]; *[1]PerkinElmer Health Sciences, Inc., Shelton, CT; [2]IONICS Mass Spectrometry, Bolton, Canada*

WP 224 **Rapid Determination of Lactulose in Heat Treated Milk using Ultraperformance Convergence Chromatography Coupled with Mass Spectrometry**; Fang Wen[1]; Yao Tian[1,2]; Yongwei Xu[3]; Nan Zheng[1,2]; Qinglong Sun[3]; Songli Li[1,2]; Jiaqi Wang[1,2]; *[1]Ministry of Agriculture Laboratory of Quality & Safety Risk Assessment for Dairy Products (Beijing), Institute of Animal Science, Chinese Academy of Agricultural Sciences, Beijing, China; [2]Ministry of Agriculture - Milk and Dairy Product Inspection Center (Beijing), Beijing, China; [3]Waters Corporation, Shanghai, China*

WP 225 **Mass Barcode-Based Signal Amplification for Highly Sensitive Multiplex Diagnosis of Allergy**; Xiaoqin Zhong[1]; Liang Qiao[1,2]; Natalia Gasilova[1]; Baohong Liu[2]; Hubert H Girault[1]; *[1]Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland; [2]Fudan university, Shanghai, China*

WP 226 **Multi-Allergen Quantitation in Thermally Processed Foods by Liquid Chromatography Tandem Mass Spectrometry**; Chelsea M. Coffey[1]; Christine H. Parker[1]; Timothy R Croley[1]; *[1]U.S. Food and Drug Administration, College Park, MD*

WP 227 **Ultra-Fast Analysis of Allergens using Capillary Electrophoresis Coupled to Mass Spectrometry and Ultraviolet Photodissociation**; Chien-Hsun Chen[1];

Andreas Krupke[1]; Monica Carrera[2]; Chad R Weisbrod[1]; Romain Huguet[1]; Shiaw-Min Chen[3]; Achim Karger[3]; Steve Williams[3]; Michael Wenz[3]; Andreas Huhmer[1]; Aran Paulus[1]; Daniel Lopez Ferrer[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Marine Research Institute, Vigo, Spain; [3]Thermo Fisher Scientific (South San Francisco), South San Francisco, CA - California*

WP 228 **Chlorinated Dioxins, Furans and Biphenyls Analysis in Beverages Using Automated Extraction and Reduced Solvent Volume Column Chromatography**; Matt Falkenstein[1]; Rudolf Addink[1]; *[1]Toxic Report, Watertown, MA*

WP 229 **Rapid Analysis of Key Aflatoxins in Rice by Microwave Plasma Torch Mass Spectrometry**; Tao Jiang[1]; Runzhi Zhou[1]; Zhiqiang Zhu[1]; Huanwen Chen[2]; *[1]East China Institute of Technology, Nanchang, China; [2]East China University of Technology, Nanchang, Mainland*

WP 230 **A High Sensitivity LC/MS/MS Method with QuEChERS Sample Pre-treatment for Determination of Aflatoxins in Milk Powders**; Yin Ling Chew[1]; Jie Xing[2]; Guan Seng Leonard Lim[3]; Zhaoqi Zhan[1]; *[1]Shimadzu (Asia Pacific) Pte Ltd, Singapore; [2]Shimadzu (Asia Pacific) Pte Ltd, Singapore, Singapore; [3]School of Physical & Mathematical Science, Nanyang Technological University SPMS-CBC-02-01 Singapore, Singapore*

WP 231 **Development of Automated Screening and Quantitation Method on a Novel On-line SFE-SFC-MS/MS Platform – (II) For Aflatoxins in Powdered Food**; Jie Xing[1]; Yin Ling Chew[1]; Jun Xiang Lee[1]; Liw Wan Tung[1]; Zhaoqi Zhan[1]; *[1]Shimadzu (Asia Pacific) Pte Ltd, Singapore*

WP 232 **Simultaneous Analysis of 23 Mycotoxins using Ultra-High Speed LC-MS/MS with a Pentafluorophenyl Column**; Matsumoto Keiko[1]; Jun Watanabe[2]; Mochizuki Naoki[3]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]Shimadzu Corporation, Kyoto; [3]Asahi Group Holdings, Limited Moriya, Japan*

WP 233 **LC-MS Analysis of Graviola and Other Neurotoxic Fruits**; Kevin Tran[1]; Pushkar Shejwalkar[2]; Kenji Hara[2]; Ingrid de Moraes[3]; *[1]US FDA, Lenexa, KS; [2]Tokyo University of Technology, Tokyo, JP; [3]State University of Campinas, Campinas, Brazil*

WP 234 **Rapid Development of Quantitative Method for Determination of Plant Growth Regulators and Streptomycin in Fruits using LC/MS/MS**; Anant Lohar[1]; Shailendra Rane[1]; Ashutosh Shelar[1]; Purushottam Sutar[1]; Shailesh Damale[1]; Deepti Bhandarkar[1]; Rashi Kochhar[1]; Ajit Datar[1]; Jitendra Kelkar[1]; Pratap Rasam[1]; *[1]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India*

WP 235 **A Streamlined Processing Method for High Resolution Mass Spectrometric Data to Compare Food-Grade-Glycerin with Crude-Glycerins to Screen for Jatropha Toxins**; Kithsiri B Herath[1]; Lauren Girard[1]; Renate Reimschuessel[1]; Hiranthi Jayasuriya[1]; *[1]Center for Veterinary Medicine/FDA, Laurel, MD*

FOOD"OMICS" MS CHARACTERIZATION OF FOOD AND NUTRITIONAL SUPPLEMENTS (PART 2)
236 - 252

WP 236 **Determination of Relative Amounts of iso- and n-Alpha Acids in Beer without Prior Separation via Chemometric Analysis of MS/MS Data**; Kevin D. Clark[1]; Joshua Driver[1]; Jon Amster[1]; *[1]Univ of Georgia, Athens, GA*

WP 237 **SPME and Liquid-Liquid Extraction, Complimentary Methods for Analysis of Coffee Flavor Components by GCMS?**; Emily P Erdman[1]; Stephanie I Allred[1]; Steven B Foster[1]; Ronald L Halterman[1]; *[1]University of Oklahoma, Dept. of Chem & Biochem Norman, OK*

WP 238 **New Analytical and Statistical Tools to Study the Flavor-formation during the Roasting Process of Coffee Beans, Cacao Beans and Nuts**; Sven Ehlert[1]; Hendryk Czech[1]; Jessalin Howell[2]; Romy Hertz-Schuenemann[1]; Chahan Yeretzian[3]; Thorsten Streibel[1]; Ralf Zimmermann[4,5]; *[1]University of Rostock, Rostock, Germany; [2]JM Smucker Inc., Orrville, Ohio; [3]ZAHW, Zuerich, Switzerland; [4]University of Rostock, Rostock; [5]Helmholtz Zentrum Muenchen, Oberschleissheim, Germany*

WP 239 **Understanding the Role of Origin, Roasting & Storage on Flavor Components in Coffee Employing Gas Chromatography Mass Spectrometry**; Steven B Foster[1]; Emily P Erdman[1]; Melissa M Henniger[1]; Jessica R McConahey[1]; Gabrielle C Thng[1]; Ronald L Halterman[1]; *[1]University of Oklahoma, Dept. of Chem & Biochem Norman, OK*

WP 240 **New Approach Analyzing Food Functionality using MALDI-MS-based Metabolic Profiling Technique: Evaluation of Green Tea Extracts**; Chihiro Kawano[1]; Yoshinori Fujimura[1]; Ayaka Maeda-Murayama[1]; Eisuke Hayakawa[1]; Takanori Ishii[1]; Hiroyuki Wariishi[1,2]; Daisuke Miura[1]; *[1]ICMRN, Kyushu University, Fukuoka, Japan; [2]Faculty of Arts and Science, Kyushu University, Fukuoka, Japan*

WP 241 **Non-targeted Modification-Specific Metabolomics Investigation of Glycosylated Metabolites in Tea (Camellia sinensis L.) by Liquid Chromatography−High Resolution Mass Spectrometry**; Weidong Dai[1,2]; Meiling Lu[2]; Zhi Lin[1]; Shan Zhou[2]; Junfeng Tan[1]; *[1]Tea Research Institute of Chinese Academy of Agricultural Sciences, Hangzhou, China; [2]Agilent Technologies (China) Limited, Beijing, China*

WP 242 **Study of the Aroma Variation in Oolong Tea Processing by Solid-Phase Micro-Extraction and Gas Chromatography-Mass Spectrometry**; Chengying Ma[1]; Shan Zhou[2]; Aiqing Miao[1]; Wenwen Wang[2]; Junxi Cao[1]; *[1]Tea Research Institute, Guangdong Academy of Agricultural Sciences, GuangZhou, China; [2]Agilent Technologies Company. Ltd, Beijing, China*

WP 243 **Analysis of Catechins in Brewed Tea by LC-TOF Mass Spectrometry**; Robert J. Seward[1]; Jason Weisenseel[1]; Craig Young[1]; Wilhad M. Reuter[1]; *[1]PerkinElmer, Waltham, MA*

WP 244 **Determination of Catechins in Tea by using *in-situ* Derivatization with a Direct Analysis in Real Time Source Equipped Mass Spectrometer**; Robert Goguen[1]; Brian D. Musselman [2]; *[1]IonSense, Inc. Saugus, MA; [2]IonSense, Inc., Saugus , MA*

WP 245 **Foodomic Profiling of Vinegars in China with Metabolomics Workflow by Agilent 6545 UHPLC-ESI/QTOF**; Shaozhen Wang[1]; Shan-An Chan[2]; *[1]Agilent Technology, Inc., Shanghai, China; [2]Agilent Technology, Inc., Shanghai, China*

WP 246 **High Sensitive LC-MS Analysis of Stevia Sweeteners Using a Polymer-Based Amino Column**; Junji Sasuga[1]; Tomokazu Umezawa[1]; Leah Block[2]; *[1]Showa Denko K.K., Kawasaki, Japan; [2]Shodex, Showa Denko America, Inc., New York, NY*

WP 247 **Differences in the Composition of Milk during Lactation using High-Resolution Mass Spectrometry**; Tatiane Melina Guerreiro[1]; Rodrigo Ramos Catharino[1]; *[1]Innovare Biomarkers Laboratory - UNICAMP, Campinas, Brazil*

WP 248 **Analysis of Water Soluble Vitamins in Infant Formula using UHPLC with Tandem Mass Spectrometry and a Heated Laminar Flow Interface;** Wilhad Reuter[1]; Sharanya Reddy[1]; Avinash Dalmia[1]; Tong Chen[1]; Thomas White[1]; Lisa Cousins[2]; Joshua Ye[2]; *[1]PerkinElmer, Shelton, CT; [2]IONICS Mass Spectrometry, Bolton, Canada*

WP 249 **Preliminary Investigation of Canadian Wheat Varieties Low Molecular Weight Glutenin Subunits Relative to Functional Gluten Strength**; Dave Hatcher[1]; Bin Xiao Fu[1]; Ray Bacala[1]; *[1]Grain Research Laboratory, Canadian Grain Commission, Winnipeg, Canada*

WP 250 **Direct Separation and Quantitation of Amino Acids in Commercial Supplements and Nutraceuticals using LC-MS and HILIC Chromatography**; Kimberly Dunn-Meynell[1]; Patricia Atkins[1]; *[1]Spex Certiprep, Metuchen, NJ*

WP 251 **Reductive Amination Assistance to Quantitate Garlic Components in Isotope Dilution Analysis**; Shih-Shin Liang; *Kaohsiung*

WP 252 **A Metabolomics Approach to Characterize Raw, Pasteurized and Ultra-High Temperature Milk using UPLC-QTOF-MS and Multivariate Data Analysis**; Yangdong Zhang; *Chinese Academy of Agricultural Sciences, Beijing, China*

FORENSICS (PART 2)
253 - 278

WP 253 **Mass Spectrometry by Paper Spray Ionization (PS-MS) – A Swiss Army Knifein Forensic Chemistry**; Eloilson Domingos[1]; Heloa Santos[1]; Lilian V Tose[1]; Radigya M Correia[1]; Flávia Tosato[1]; Thays C. Carvalho[2]; Christopher Thompson[3]; Paulo R Filgueiras[1]; Boniek G Vaz[2]; Wanderson Romão[4]; *[1]UFES, Vitória, Brazil; [2]UFG, Goiania, Goias; [3]Bruker Daltonic, Billerica, MA; [4]IFES/UFES, Vila Velha, ES*

WP 254 **Quantification of Cocaine and Its Adulterants by Paper Chromatography reveled byDragendorff Reagent and Paper Spray Ionization Mass Spectrometry**; Heloa Santos[1]; Flavia Tosato[1]; Aryanne Souza Lima[2]; Eloilson Domingos[1]; Boniek G Vaz[3]; Wanderson Romão[1]; *[1]UFES, Vitória, Brazil; [2]IFES, Vila Velha, Brazil; [3]UFG, Goiânia, Brazil*

WP 255 **Detection of NBOMe Designer Drugs on Blotter Paper using Ambient Ionization High Resolution Time-of-Flight Mass Spectrometry: A Forensic Case Study**; Jamie Foss[1]; David Barajas[2]; Sabra Botch-Jones[2]; Frank Kero[3]; Craig Young[3]; Jason Weisenseel[3]; *[1]Maine Health & Environmental Testing Lab, Augusta, ME; [2]Boston University School of Medicine, Boston, MA; [3]PerkinElmer, Shelton, CT*

WP 256 **Evaluating an All Ions Method for the Identification of NBOMEs on Seized Blotter Papers using Q-TOF LC/MS**; Andrey Giovanni Gomes de Oliveira[1]; Luciano Chaves Arantes[1]; *[1]Criminalistics Institute, Brazilian Federal District Civil Police (PCDF), Brasilia, Brazil*

WP 257 **Forensic Applications of Probe Electrospray Ionization Mass Spectrometry (PESI-MS) using a Needle Coated with Polypyrrole**; Carla S. de Freitas[1]; Ricardo Alves Bernardo[1]; Gessica Adriana Vasconcelos[1]; Veronica Vale Cavalho[1]; Thays Colletes Carvalho[1]; Wanderson Romão[2]; Andrea Chaves[1]; Boniek G Vaz[1]; *[1]Federal University of Goias, Goiania, GO; [2]Federal University of Espirito Santo, Vitoria, Brazil*

WP 258 **Rapid Detection of Drugs-of-abuse in Body Fluid by Mass Spectrometry**; Tsz-Tsun Ng[1]; Pui-Kin So[1]; Bin Hu[1]; Zhong-Ping Yao[1]; *[1]Department of Applied Biology and Chemical Technology, The Hong Kong Polytechnic University, Hong Kong SAR, China*

WP 259 **Classification of Synthetic Cathinones Using Neutral Mass Losses by Direct Analysis in Real Time Mass Spectrometry (DART-MS)**; Kristen Fowble[1]; Jason Shepard[1]; Rabi A. Musah[1]; *[1]University at Albany-SUNY, Albany, NY*

WP 260 **Solid-phase Microextraction Combined with a Laminar Flow LC-MS/MS for High-Throughput and High Sensitive Analysis of Drugs in Oral Fluids**; Vincent Bessonneau[1]; Janusz Pawliszyn[2]; *[1]University of Waterloo, Waterloo, Canada; [2]University of Waterloo, Waterloo ON, Canada*

WP 261 **Magnetic Graphene Framework as Adsorbent for the Enrichment of Flunitrazepam from Beverage Samples Prior to Its Determination by Mass Spectrometry**; Qiuhua Wu[1]; Si Cheng[2]; Zhi Li[1]; Hao Chen[1]; *[1]Ohio University, Athens, OH; [2]Ohio, Athens, OH*

WP 262 **LC-MS/MS Analysis of Drugs of Abuse Using Biocompatible Solid Phase Micro Extraction**; Sara Smith[1]; Emily Barrey[1]; Craig Aurand[1]; David Bell[1]; Candace Price[1]; *[1]MilliporeSigma, Bellefonte, PA*

WP 263 **Evaluation of Solid Phase Micro Extraction Sample Preparation for LC-MS Analysis of Drugs in Urine and Plasma for Forensics**; Marta Kozak[1]; Nathaly Reyes Garces[2]; German Augusto Gomez-Rios[3]; Cornelia Boeser[4]; Sarracino David[4]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]University of Waterloo, Waterloo, Ontario (ON); [3]University of Waterloo, Waterloo ON, Canada; [4]ThermoFisher Scientific, San Jose, CA*

WP 264 **The Development of a Two-Dimensional Liquid Chromatography-Tandem Mass Spectrometry Method for the Analysis of Designer Drugs in Urine**; Holly Castellano; *Duquesne University, Pittsburgh, PA*

WP 265 **Drugs of Abuse Extraction from Whole Blood using Supported Liquid Extraction (SLE) Prior to GC/MS Analysis**; Katie-Jo Teehan[1]; Rhys Jones[1]; Lee Williams[2]; Paul Roberts[1]; Helen Lodder[1]; Adam Senior[1]; Alan Edgington[1]; Geoff Davies[1]; Steve Jordan[1]; Claire Desbrow[1]; Victor Vandell[3]; Dan Menasco[3]; *[1]Biotage GB Limited, Cardiff, UK; [2]Biotage GB Limited, Cardiff; [3]Biotage LLC, Charlotte, NC*

WP 266 **Illegal Drugs Analysis by Thermal Desorption and Pyrolysis Combined with Direct Analysis in Real Time- Mass Spectrometry (TDP/DART-MS)**; Hiroko Abe[1]; Chikako Takei[2]; Yasuo Shida[3]; Motoshi Sakakura[4]; Teruhisa Shiota[4]; Kayako Suga[5]; Daisuke Yajima[1]; Hirotaro Iwase[6]; *[1]University of Chiba, Chiba, Japan; [2]BioChromato, Inc. Fujisawa, Japan; [3]University of Yamanashi, Kofu, Japan; [4]AMR Inc., Meguro-Ku, Japan; [5]AB SCIEX, Tokyo, Japan; [6]University of Tokyo, Tokyo, Japan*

WP 267 **Developement of an LC-MS/MS Screening Method for 101 Targeted Compounds in Whole Blood, Using Library Searching on a QTRAP MS**; Heather Singletary[1]; Amanda Sweet[1]; *[1]Metro Nashville PD-Crime Lab, Madison, TN*

WP 268 **Fast and Reliable Quantitation of Z-drug Hypnotics and Benzodiazepines in Serum using UHPLC-QTOF Mass Spectrometry**; Sebastian Goetz[1]; Karin Wendt[1]; Tony Drury[2]; Matt Willetts[3]; Carsten Baessmann[1]; *[1]Bruker Daltonik GmbH, Bremen, Germany; [2]Bruker Daltonics, Coventry, UK; [3]Bruker Daltonic, Billerica, MA*

WP 269 **Urine and Serum Ultra-Rapid Analysis of Flakka (alpha-PVP) in 9 Seconds per Sample by Laser Diode Thermal Desorption Mass Spectrometry** ; Jonathan Rochon[1]; Annie-Claude Bolduc[1]; Réal Paquin[1]; Alex Birsan[2]; Serge Auger[2]; Jean Lacoursiere[2]; Pierre Picard[2]; *[1]Université Laval, Québec, Canada; [2]Phytronix Technologies, Inc. Quebec, Canada*

WP 270 **SWATH Data Used for Data Mining: What kind of Adulterants, Diluents and Other Toxic Compounds are Consumed Together with Cocaine?**; Stefan König[1]; Thomas Wüthrich[2]; Marie Martin[2]; Werner Bernhard[2]; Wolfgang Weinmann[2]; Susanne Nussbaumer[2]; *[1]Institut für Rechtsmedizin, Universität Bern, Bern, Switzerland; [2]Institut für Rechtsmedizin, Bern, Switzerland*

WP 271 **Quantitative Multi Target Screening (MTS) using Liquid Chromatography-Tandem Mass Spectrometry with MS/MS Library Based Identification for Forensic Toxicology**; Alan Barnes[1]; Tiphaine Robin[2]; Simon Ashton[1]; Neil Loftus[1]; Pierre Marquet[2]; Sylvain Dulaurent[2]; Franck Saint-Marcoux[2]; *[1]Shimadzu, Manchester, UK; [2]CHU Limoges, Limoges, France*

WP 272 **Comprehensive and Sensitive Quantitation of More Than 100 Synthetic Cannabinoids in Serum by LC-MS/MS**; Laura M. Huppertz[1]; Rafaela Martin[2]; Markus Meyer[2]; Ronja Peter[3]; Juergen Kempf[3]; *[1]Institute of Forensic Medicine Freiburg, Freiburg, Germany; [2]Bruker Daltonik*

GmbH, Bremen, Germany; [3]Institute for Forensic Medicine Freiburg, Freiburg, Germany

WP 273 **Rapid Update of Screening Methods for the Detection of Synthetic Cannabinoid Use in Human Urine by Software Assisted Metabolite Identification**; Bjoern Moosmann[1]; Laura M. Huppertz[1]; Florian Franz[1]; Sebastian Götz[2]; Volker Auwärter[1]; *[1]Institute of Forensic Medicine Freiburg, Freiburg, Germany; [2]Bruker Daltonic GmbH, Bremen, Germany*

WP 274 **Strategies for Classification and Annotation of Novel Synthetic Designer Drugs**; Fanny Chu[1, 2]; A. Daniel Jones[2, 3]; Ruth Waddell Smith[1]; *[1]Forensic Science Program, School of Criminal Justice, Michigan State University, East Lansing, MI; [2]Department of Chemistry, Michigan State University, East Lansing, MI; [3]Department of Biochemistry and Molecular Biology, Michigan State University, East Lansing, MI*

WP 275 **Comprehensive Detection and Identification of Prescription Analgesics and Illicit Opioids in Post-Mortem Specimens using Ion Trap LC-MSn;** Elisa N. Shoff[1]; George W. Hime[1]; Carsten Baessmann[2]; Diane M. Boland[1]; *[1]Miami Dade Medical Examiner Dept., Miami, FL; [2]Bruker Daltonik GmbH, Bremen, Germany*

WP 276 **CE-MS Analysis of Controlled Substances with Optical Isomer Resolution in about a Minute**; Mehdi Moini[1]; Christopher Rollman[1]; *[1]George Washington University, Washington, DC*

WP 277 **Screening Procedure to Detect Peptide Hormones Prohibited in Sports. CESI-MS vs LC-ESI-MS**; Monica Mazzarino[1]; Xavier de la Torre[2]; Francesco Botrè[2]; *[1]Antidoping laboratory of Rome, Rome, Italy; [2]Antidoping laboratory of Rome, FMSI Rome, Italy*

WP 278 **Hydrophilic Interaction Liquid Chromatography Tandem Mass Spectrometry (HILIC-MS/MS) Method for the Quantitation of gamma-Aminobutyric Acid (GABA) in Equine Plasma**; Rong Yi[1]; Sarah Zhao[1]; Noel Kong[1]; Julia Zhang[1]; Devan Loganathan[1]; Sandrine Merette[1]; Barbara Morrissey[1]; *[1]MAXXAM, Burnaby, Canada*

GCMS: INSTRUMENTATION AND APPLICATIONS (INSTRUMENTATION-NEW DEVELOPMENTS)
279 - 293

WP 279 **Development of a Multi-Turn TOF Mass Spectrometer with a Cold Trap "infiTOF-CT" for Trace Gas Analysis**; Hirofumi Nagao[1]; Shinichi Miki[1]; Ikunori Kannoh[1]; Michisato Toyoda[2]; *[1]MSI.TOKYO Inc, Chofu, Tokyo, Japan; [2]Osaka University, Toyonaka, Osaka, Japan*

WP 280 **GC-MS with Cold EI and Its Unexpected Benefits**; Aviv Amirav[1]; Alexander B. Fialkov[2]; Tal Alon[2]; Uri Keshet[2]; Svetlana Tsizin[2]; *[1]Tel-Aviv University, Tel-Aviv; [2]Tel Aviv University, Tel Aviv, Israel*

WP 281 **Evaluation of Organometallic Compounds using GC/Q-TOF with a Novel High Efficiency Source**; David Kaz[1]; Jennifer Sanderson[1]; Sofia Nieto[1]; *[1]Agilent Technologies, Santa Clara, CA*

WP 282 **On-Line Coupling of Microscale Distillation with GC-MS for Analysis of Complex Samples**; Ya-Ru Tang[1]; Pawel Lukasz Urban[2]; *[1]National Chiao Tung University, Hsinchu, Taiwan; [2]Department of Applied Chemistry, National Chiao Tung University, Hsinchu, Taiwan (R.O.C.)*

WP 283 **Fast Analysis Workflow with No Sample Preparation for Forensic Applications using Open Probe FastGC/MS: Unit and High Resolution Mass Spectrometers**; Luis Cuadra-Rodriguez[1]; Jennifer Sanderson[1]; Bjorn Flatt[1]; Bill Russ[1]; *[1]Agilent Technologies, Santa Clara, CA*

WP 284 **Vacuum Ultraviolet (VUV) Spectroscopy – an Alternative to Mass Spectrometry for Gas Chromatography Detection**; Changling Qiu[1]; Allegra Leghissa[1]; Jonathan Smuts[2]; Kevin A Schug[1]; *[1]University of Texas at Arlington, Arlington, TX; [2]VUV Analytics, Inc., Cedar Park, TX*

WP 285 **Gas Chromatography Electrospray Ionization Mass Spectrometry Analysis of Trimethylsilyl Derivatives**; Ren-Yu Hsu[1]; Jhan-Hong Liao[1]; Hsin Wen Tien[1]; Guor-Rong Her[1]; *[1]National Taiwan University, Taipei, Taiwan*

WP 286 **Characterization of lignans of *Schisandra sphenanthera* Fruit by Flash Evaporation-Gas Chromatography/Mass Spectrometry**; Huijun Liu[1]; Yilei Huang[1]; Zhongping Huang[1]; Yutian Chen[1]; Lili Wang[1]; *[1]Zhejiang University of Technology, Hangzhou, China*

WP 287 **Interfacing Gas and Liquid Chromatography with High Temperature Plasma Mass Spectrometry**; Sychyi Cheng[1]; Jentaie Shiea [1]; *[1]National Sun Yat- Sen University, Kaohsiung, Taiwan*

WP 288 **EPA Method 325B, Novel Thermal Desorption Instrument Modification to Improve Sensitivity**; Ronald Shomo[1]; John Manura[1]; Christopher W Baker[1]; *[1]Scientific Instrument Services, Ringoes, NJ*

WP 289 **Trace Elemental Quantification of Carbon via the Production of Cyanide Anions in Plasma Assisted Reaction Chemical Ionization Mass Spectrometry (PARCI-MS)**; Peter Haferl[1]; Haopeng Wang[1]; Kaveh Jorabchi[1]; *[1]Georgetown University, Washington, DC*

WP 290 **How We Can Improve Number of Compounds Found by Deconvolution in One Essential Oil Sample with GCMS?**; Celso Blatt[1]; Romao Beserra[1]; *[1]Agilent Technologies Brasil Ltda, São Paulo, Sao Paulo*

WP 291 **Raising the Identification Confidence in Non-Target Analysis of House Dust by Combining Classic and Soft Electron Ionization GC-HRMS**; Peter Haglund[1]; Sofia Nieto[2]; Vadim Kalmeyer[2]; Nathan Eno[2]; Jennifer Sanderson[2]; *[1]Umea University, Umea; [2]Agilent Technologies, Santa Clara, CA*

WP 292 **GCxGC with Simultaneous Mass Spectrometry/Flame Ionization Detection for Routine Petrochemical Analyses**; Laura McGregor[1]; Nick P Bukowski[1]; Matthew Edwards[1]; Pete Grosshans[2]; Chris Hall[2]; Massimo Santoro[1]; *[1]Markes International, Cardiff, UK; [2]Markes International Inc, Cincinnati, OH*

WP 293 **A High Efficiency Ion Source for GC/MS**; Jeffrey Kernan; *Agilent Technologies, Santa Clara, CA*

GLYCOPROTEINS (TANDEM MS, SEPARATIONS, AND AUTOMATION/SOFTWARE)
294 - 313

WP 294 **Extending the Energy-resolved Collision-Induced Dissociation Method for Structural Characterization of Sialylated N-Glycopeptides**; Venkata Kolli[1]; Katherine N Schumacher[1]; Eric D Dodds[1]; *[1]University of Nebraska - Lincoln, Lincoln, NE*

WP 295 **Detailed Characterization of Glycans and Glycopeptides by Collisional and Electron Activated Dissociation**; Kshitij Khatri[1]; Yi Pu[1]; Joshua Klein[1]; Cheng Lin[1]; Joseph Zaia[1]; *[1]Boston University, Boston, MA*

WP 296 **Glycopeptide Analysis Using Parallel Data-Dependent Acquisition at Varied Normalized Collision Energies**; Crystal Daniels[1]; Joseph Otto[1]; Jana Rocker[1]; Lindsay Schambeau[1]; *[1]Mitchell Cancer Institute, Mobile, AL*

WP 297 **Sequential Chemical Charge Enhancement with Electron-Transfer Dissociation for the Site-Specific Characterization of Doubly Glycosylated Peptides**; Yanyan Qu[1]; William R Alley[1]; Stephan Bach[1]; Wendell P Griffith[1]; *[1]Department of Chemistry, University of Texas at San Antonio, San Antonio, TX*

WP 298 **Comparing Effectiveness and Specificity of Glycopeptide Enrichment Strategies for Qualitative LC-MS/MS Analysis of Depleted Human Plasma**; Sarah Michelle Totten[1]; Majlinda Kullolli[2]; Christa Feasley[3]; Sharon J Pitteri[2]; *[1]Stanford University School of Medicine, Palo Alto,*

CA; [2]Stanford University School of Medicine, Palo Alto CA; [3]Thermo Fisher Scientific, West Palm Beach, FL

WP 299 **Online Cotton HILIC: An Easily Accessible and Affordable Enrichment of Glycopeptides**; Jingfu Zhao[1]; Ehwang Song[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, Texas*

WP 300 **Affinity-capture Based Methods for N-glycan Analysis of Specific Serum Proteins**; Gunnar Thorsén[1]; Alessandro Quaranta[2]; Isabella Karlsson[2]; Anna Sroka-Bartnicka[2]; Matthijs Pijnappel[2]; Lorena Ndreu[2]; *[1]Stockholm University, Stockholm, Stockholm; [2]Department of Environmental Science and Analytical Chemistry, Stockholm University, Stockholm, SE*

WP 301 **Separation and Detection of PSA-derived Sialic Acid Attachment Isomers Using a Heated PGC Column and LC-MS/MS**; Yifan Huang[1]; Shiyue Zhou[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX*

WP 302 **N-glycosylation Analysis of Specific Serum Proteins using an Automated Microfluidic Platform and MALDI-MS**; Alessandro Quaranta[1]; Anna Sroka-Bartnicka[1]; Isabella Karlsson[1]; Lorena Ndreu[1]; Matthijs Pijnappel[1]; Thorsén Gunnar[1]; *[1]Stockholm University, Stockholm*

WP 303 **Identification and Separation of N-glycans by HILIC/MS**; Zsuzsanna Lakos[1]; Elena Dremina[1]; Robert Carney[1]; John L. Snyder[1]; *[1]Eurofins Lancaster Laboratories, Lancaster, PA*

WP 304 **Silk-Based Glyco-Enrichment Tip for Purification and Enrichment of Glycans and Glycopeptides**; Haci Mehmet Kayili[1, 2]; Mehmet Atakay[1]; Bekir Salih[1]; *[1]Hacettepe University, Department of Chemistry, Ankara, Turkey; [2]Çankırı Karatekin University, Department of Chemistry, Çankırı, Turkey*

WP 305 **N-linked Glycosylation Analysis of Seasonal Influenza Vaccine Hemagglutinins**; Yanming An[1]; Lisa Parsons[1]; John Cipollo[1]; *[1]FDA/CBER, Silver Spring, MD*

WP 306 **Assisting the Identification of Isomeric Glycoforms with a Hydrophilic Interaction Liquid Chromatography Retention Time Model for Procainamide Tagged N-linked Glycans**; Emily Betchy[1]; Barry Boyes[2]; Ron Orlando[1]; *[1]CCRC, University of Georgia Athens, GA; [2]Advanced Materials Technology, Wilmington, DE*

WP 307 **Glycopeptidomics with Ion Mobility Spectrometry for Elucidating Glycan Structures**; Miklos Guttman[1]; Kelly Lee[1]; *[1]University of Washington, Seattle, WA*

WP 308 **Automated Processing of LC-MSMS Data for Quantitative Analysis of the Human-like N-glycosylation of Glycoproteins Produced by a Glyco-optimization Cell Platform**; Robert Wilmanowski[1]; Catherine Evans[2]; Anja Resemann[3]; Peter Hufnagel[3]; Rainer Paape[3]; Detlev Suckau[3]; Wolfgang Jabs[3]; Sven Bahrke[1]; Keven Lothert[1]; Andrea Hahne[1]; *[1]Glycotope GmbH, Berlin, Germany; [2]Bruker Ltd, Coventry, UK; [3]Bruker Daltonic GmbH, Bremen, Germany*

WP 309 **N-glycan Analysis using GIG-automation on Sialylglycotransferase Knock-in CHO Cell Line**; Shuang Yang[1]; Qiong Wang[2]; Lijun Chen[3]; Bojiao Yin[2]; Li Shuwei[4]; Michael Betenbaugh[2]; Hui Zhang[3]; *[1]John Hopinks Dept. of Pathology, Baltimore, MD; [2]Johns Hopkins University, Baltimore, MD; [3]Johns Hopkins School of Medicine, Baltimore, MD; [4]University of Maryland, College Park, MD*

WP 310 **GPQuest: A Free Software for Identification of Glycans and Intact Glycopeptides**; Yingwei Hu[1]; Shadi Toghi Eshghi[2]; Weiming Yang[1]; Punit Shah[1]; Shisheng Sun[1]; Shuang Yang[1]; Lingquan Deng[1]; Xingde Li[2]; Hui Zhang[1]; *[1]Department of Pathology, School of Medicine, Johns Hopkins University, Baltimore, MD; [2]Department of Biomedical Engineering, School of Medicine, Johns Hopkins University, Baltimore, MD*

WP 311 **Scalable Computational Tool for Identifying Intact Glycopeptides in Complex Samples Using Mass Spectrometry**; Lei Wang[1]; Chuan-Yih Yu[1]; Anoop M Mayampurath[2]; Rui Zhu[3]; Ehwang Song[3]; Yehia Mechref[3]; Haixu Tang[1]; *[1]Indiana University, Bloomington, IN; [2]University of Chicago, Chicago, IL; [3]Texas Tech University, Lubbock, Texas*

WP 312 **GLYMPS: A Tool to Automatically Assign Glycopeptides from MSEdata**; Lisa Parsons[1]; Yanming An[1]; John F Cipollo[1]; *[1]FDA/CBER, Silver Spring, MD*

WP 313 **Confident, Automated N-glycoproteomics Profiling in Unenriched and Glycopeptide-Enriched Cancer Cell Samples**; Shadab Ahmad[1]; Amol Prakash[1]; Sergei I Snovida[2]; Scott M Peterman[3]; Chu-Wei Kuo[4]; Kay-Hooi Khoo[4]; Gauri Muradia[5]; Jeremy P Kunkel[5]; Jessie R Lavoie[5]; Nina Soltero[2]; Julian A Saba[2]; *[1]Optys Tech Corporation, Brighton, MA; [2]Thermo Fisher Scientific, San Jose, CA; [3]Thermo Scientific BRIMS, Cambridge, MA; [4]Academia Sinica, Taipei, Taiwan; [5]Health Canada, Ottawa, Canada*

H/D EXCHANGE: HARDWARE, SOFTWARE AND METHODOLOGY
314 - 327

WP 314 **The Development of a Fully Customized HDX-MS Platform with Exceptional Performance on Back-Exchange, Robustness and Reproducibility**; Chengjie Ji[1]; Jeff Zhu[1]; Qian Li[1]; Yankun Li[1]; *[1]Novabioassays LLC, Woburn, MA*

WP 315 **MALDI Compatible Protease Chips - A Novel Platform For Protein H/D Exchange**; Michal Rosulek[1, 2]; Petra Darebna[1, 2]; Daniel Kavan[1, 2]; Petr Man[1, 2]; Michael Volny[3]; Petr Pompach[1, 2]; Petr Novak[1, 2]; *[1]Institute of Microbiology CAS, Prague, Czech Republic; [2]Faculty of Science, Charles University in Prague, Prague, Czech Republic; [3]AffiPro, s.r.o, Mratin, Czech Republic*

WP 316 **Protease Type XVIII Columns for Enhanced Digestion Efficiency and Sequence Resolution for Protein HDX Monitored by Q Exactive MS**; Chengjie Ji[1]; Qian Li[1]; Yankun Li[1]; *[1]Novabioassays LLC, Woburn, MA*

WP 317 **Improvements to HDX Workbench Software for Analysis and Interpretation of HDX MS Data**; Bruce D. Pascal[1]; Venkatasubramanian Dharmarajan[1]; Scott Novick[1]; Jie Zheng[1]; Vinh Lam[1]; *[1]The Scripps Research Institute, Jupiter, Florida*

WP 318 **In-source Column Cooling for nanoHX-MS on Complex Druggable Protein Scaffolds**; Joey Sheff[1]; David Schriemer[1]; *[1]University of Calgary, Calgary, Canada*

WP 319 **Post-column Hydrogen-deuterium Exchange Method for the Identification of Organic Compounds**; Emmanuel Eysseric[1]; Xavier Bellerose[1]; Jean-Michel Lavoie[1]; Pedro A Segura[1]; *[1]Université de Sherbrooke, Sherbrooke, QC*

WP 320 **How Precise are HDX-MS Measurements? Results from the NIST HDX-MS Interlaboratory Comparison Project**; Jeffrey W. Hudgens[1, 2]; Elyssia S Gallagher[1, 2]; Ioannis Karageorgos[1, 2]; *[1]National Institute of Standards and Technology, Rockville, MD; [2]Institute for Bioscience and Biotechnology Research, Rockville, MD*

WP 321 **Phosphoform-Specific Characterization of Protein Conformational Changes Induced by Multisite Phosphorylation**; Jingxi Pan[1]; Albert Chou[1]; Suping Zhang[2]; Christoph H. Borchers[1, 3]; *[1]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [2]MRM Proteomics Inc, Victoria, BC, Canada; [3]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada*

WP 322 **Top-Down Analysis of 'On-the-Fly' HDX of NativeProtein Ions**; Ken Chanthamontri[1]; Nawaporn Sanguantrakun[2, 3]; Michael L Gross[3]; *[1]Washington University in St Louis, St Louis, MO; [2]Saint Louis College of Pharmacy, St. Louis, MO; [3]Washington University in St. Louis, Saint Louis, MO*

WP 323 **HDXMS Studies of Membrane Proteins (GPCR) Expressed in Virus like Particles (VLP)**; Deepa Balasubramaniam[1]; Carrie A Shipley[1]; Beata A Zamlynny[1]; Margarita Garcia-Calvo[1]; Payal Sheth[1]; Michael Kavana[1]; David G McLaren[1]; *[1]Merck Research Labs, Kenilworth, NJ*

WP 324 **HX-MS Reveals a Loss of Helical Structure in an Intrinsically Disordered Protein under Highly Crowded Conditions**; Farai Rusinga; *University of Kansas, Lawrence, KS*

WP 325 **Observation of H/D Exchange at Non-labile C-H Sites Capable by an Increase in Desolvation Temperature in ESI-source**; Alexander Zherebker[1, 2]; Yury Kostyukevich[2,3,4]; Alexey S Kononikhin[2, 4]; Vitaliy Roznyatovsky[1]; Igor A Popov[4, 5]; Yuri K. Grishin[1]; Irina V Perminova[1]; Eugene Nikolaev[2]; *[1]Lomonosov Moscow State University, Moscow, Russia; [2]Institute for Energy Problems of Chemical Physics, Moscow, Russia; [3]Skolkovo Institute of Technology, Moscow, Russia; [4]Moscow Institute of Physics and Technology, Moscow, Russia; [5]Emanuel Institute of Biochemical Physics, Moscow, Russia*

WP 326 **Towards a High Throughput Binding-Site Specific Drug Screening by HDX MS**; ROMAN ZUBAREV [1]; Juan Astorga-Wells[2, 3, 4]; Thorleif Lavold[3]; *[1]Karolinska Institutet, Stockholm, Sweden; [2]Karolinska Institutet, Solna, Sweden; [3]Biomotif AB, Stockholm, Sweden; [4]HDXperts AB, Stockholm, Sweden*

WP 327 **Negative Ion Electron Capture Dissociation (niECD) of Deuterated Peptides**; Qingyi Wang[1]; Kristina Håkansson[1]; *[1]University of Michigan Department of Chemistry, Ann Arbor, MI*

H/D EXCHANGE: PROTEIN STRUCTURE/FUNCTION (PART 1) 328 - 336

WP 328 **Utilizing Hydrogen Exchange Mass Spectrometry to Interrogate KRas Binding to SOS1 at Two Distinct Sites**; Rane A Harrison[1]; Andreas Zoephel[2]; Klaus Rumpel[3]; John R Engen[1]; *[1]Department of Chemistry and Chemical Biology, Northeastern University, Boston, MA; [2]Department of Medicinal Chemistry, Boehringer Ingelheim RCV GmbH & Co KG, Vienna, Austria; [3]Department of New Therapeutic Concept Discovery, Boehringer Ingelheim RCV GmbH & Co KG, Vienna, Austria*

WP 329 **Local Dynamics in Lipid-Associated Apolipoprotein A-I and Effects of Disease-Causing Mutations Probed by Hydrogen-Deuterium Exchange MS**; Christopher Jay Wilson[1]; Madhurima Das[2]; Xiaohu Mei[2]; John R Engen[1]; Olga Gursky[2]; *[1]Department of Chemistry and Chemical Biology, Northeastern University, Boston, MA; [2]Department of Physiology and Biophysics, Boston University School of Medicine, Boston, MA*

WP 330 **Integrating XL-MS and HX-MS2 Data to Develop a Model of DNA Binding to DNAPKcs**; Morgan Hepburn[1]; Daniel Saltzberg[2]; Yapping Yu[1]; Susan Lees-Miller[1]; Andrej Sali[2]; David Schriemer[1]; *[1]University of Calgary, Calgary, Canada; [2]University of California, San Francisco, CA*

WP 331 **Identification of a Structural Conduit for Thermal Energy Transfer from Solvent to Enzyme Active Site using Hydrogen/Deuterium Exchange Mass Spectrometry**; Anthony T Iavarone[1]; Adam R Offenbacher[1]; Judith P Klinman[1]; *[1]UC Berkeley, Berkeley, CA*

WP 332 **Examining the Importance of Conformational Dynamics for the Function of Pyruvate Kinase: Insights from HDX-MS**; Courtney S Fast[1]; Siavash Vahidi[1]; Stanley D Dunn[1]; Lars Konermann[1]; *[1]Western University, London, Canada*

WP 333 **Analysis of HIV Nef Dimerization and Binding Partner Interactions by Hydrogen Exchange Mass Spectrometry**; Jamie Moroco[1]; John Jeff Alvarado[2]; Thomas E Smithgall[2]; John R Engen[1]; *[1]Northeastern University, Boston, MA; [2]University of Pittsburgh School of Medicine, Pittsburgh, PA*

WP 334 **Pre-Amyloid Oligomer Dissociation Kinetics Studied by Hydrogen/Deuterium Exchange Mass Spectrometry**; Zhe Zhang[1]; Richard W Vachet[1]; *[1]University of Massachusetts Amherst, Amherst, MA*

WP 335 **Gas-Phase H/D Exchange Monitored by MS Reveals a Dense Network of Side-Chain Interactions Stabilizing Oligomers of Alzheimer's Disease Aβ Peptide**; Kaja Przygonska[1]; Kinga Fituch[1]; Ewa Sitkiewicz[1]; Kasper D Rand[2]; Michal Dadlez[1]; *[1]Institute of Biochemistry and Biophysics, Polish Academy of Science, Warsaw, Poland; [2]Department of Pharmacy, University of Copenhagen Copenhagen, Denmark*

WP 336 **Effect of Protein Structure on Antibody Deamidation Rates: A Combination of Peptide Mapping, 3D Modeling, and Hydrogen/Deuterium Exchange Mass Spectrometry**; Paul Mawson; *Ridgefield, CT*

ICP AND ISOTOPE RATIO MS: ELEMENTAL 337 - 341

WP 337 **Measurement of the Molar Mass of 28Si-enriched Silicon Crystal with High Resolution Inductively Coupled Plasma Mass Spectrometer**; Tongxiang Ren[1]; Jun Wang[2]; Tao Zhou[2]; Hai Lu[2]; *[1]National Institute of Metrology, Beijing, Chaoyang; [2]National Institute of Metrology, Beijing, China*

WP 338 **Selenium Accumulation and Speciation in Supplemented Aquaponic Systems Using Reverse Phase HPLC and ICP-QQQ**; Skyler Smith[1]; Julio A. Landero-Figueroa[1]; Megan Schmale[1]; *[1]University of Cincinnati, Cincinnati, OH*

WP 339 **Environmental Source Determination Using Stable Lead Isotope Ratios in American Woodcock (Scolopax minor) Feathers and Bone**; Amanda D. French[1]; Warren C Conway[1]; Daniel S Sullins[2]; David Klein[3]; *[1]Texas Tech University, Lubbock, Texas; [2]Kansas State University, Manhattan, KS; [3]Texas Tech University, Lubbock, TX*

WP 340 **Rapid Determination of Calcium in Water by Spray Microwave Plasma Torch Mass Spectrometry**; Meiling Yang[1]; Xinchen Wang[1]; Tao Zhong[1]; Huanwen Chen[2]; *[1]East China Institute of Technology, Nanchang, China; [2]East China University of Technology, Nanchang, Mainland*

WP 341 **Determination of Absolute Isotopic Composition of Mo by MC-ICP-MS using Synthetic Isotope Mixtures and Uncertainty Evaluation**; Panshu Song[1]; Jun Wang[1]; *[1]National Institute of Metrology, Beijing, China*

IMAGING MS: METHOD DEVELOPMENT (DESI/SIMS/MISC) 342 - 364

WP 342 **A Novel Quantitative Imaging Strategy of Elements in Biological Tissue by Isotope Dilution Laser Ablation ICP-MS**; Liuxing Feng; *National Metrology Institute, China, Beijing, Beijing*

WP 343 **Differential Protein Profiling using Virtual 2D Gel-Mass Spectrometry**; Neil R Quebbemann[1]; Joseph A Loo[1]; Rachel R. Ogorzalek Loo[1]; *[1]University of California, Los Angeles, Los Angeles, CA*

WP 344 **Targeted DESI Mass Spectrometry Imaging in Ovarian Cancer**; Luisa Doria[1]; James McKenzie[1]; Anna Mroz[1]; Abigail Speller[1]; Francesca Rosini[1]; David Phelps[1]; Emrys A Jones[2]; Renata Soares[1]; Kirill Veselkov[1]; Sadaf Ghaem-Maghami[1]; Zoltan Takats[1]; *[1]Imperial College, London, UK; [2]Waters, Manchester, UK*

WP 345 **Tissue Imaging with Specificity for Unsaturated Lipid Isomers Using Mass Spectrometry with Photochemical Reactions**; Chengan Guo[1]; Xiaoxiao Ma[2]; Yuan Su[2]; Ran Tian[2]; Ruyi Shi[2]; Fei Tang[1]; Yu Xia[2]; Zheng Ouyang[2]; *[1]Tsinghua University, Beijing, China; [2]Purdue University, West Lafayette, IN*

WP 346 **Methodology for Drug Delivery Quantitation in Single Cells using TOF-SIMS**; Anthony Castellanos[1]; Quentin Vanbellingen[1]; Francisco Fernandez-Lima[1, 2]; *[1]Florida International University, Miami, FL; [2]Biomolecular Science Institute, Miami, FL*

WP 347 **Single Cell Analysis using nano-DESI Mass Spectrometry**; Hilde-Marléne Bergman[1]; Ingela Lanekoff[1]; *[1]Uppsala University, Uppsala, Sweden*

WP 348 **Region- and Enzyme-Specific Bioconversion of Dynorphin Neuropeptide Detected by *in situ* Histochemistry and MALDI Imaging Mass Spectrometry.**; Erik Bivehed[1]; Stromvall Robert[1]; Malin Andersson[1]; *[1]Uppsala University, Uppsala, Sweden*

WP 349 **Combining SRS Microscopy and MS Imaging**; Elizabeth C. Randall[1, 2]; Alasdair Rae[2]; Alan M. Race[2]; Helen J. Cooper[1]; Josephine Bunch[2]; *[1]University of Birmingham, Birmingham, UK; [2]National Physical Laboratory, Teddington, UK*

WP 350 **Tissue Classification using Mass Spectrometry and Membrane Microarrays**; Jone Garate[1]; Roberto Fernandez[1]; Tarson Tolentino-Cortez[2]; Sergio Lage[1]; Gabriel Barreda-Gómez[2]; Egoitz Astigarraga[2]; Jose A Fernandez[1]; *[1]University of Basque Country, UPV/EHU Leioa Basque Country, Spain; [2]IMG Pharma Biotech, Zamudio, Spain*

WP 351 **Ambient Ionization Mass Spectrometry for Preoperative Diagnosis of Indeterminate Thyroid Nodules**; Jialing Zhang[1]; Wendong Yu[2]; Clara L Feider[3]; Jerry Buentello[2]; Robert Tibshirani[4]; James W Suliburk[2]; Livia S Eberlin[3]; *[1]UT Austin, Austin, TX; [2]Baylor College of Medicine, Houston, TX; [3]University of Texas at Austin, Austin, TX; [4]Stanford University, Stanford, CA*

WP 352 **Mass Spectrometry Imaging of the Human Pancreas Lipidome**; Grant Barry[1]; Daniel Cavazos[1]; Igor Veryovkin[1]; Manami Hara[2]; Graeme Bell[2]; Luke Hanley[1]; *[1]University of Illinois at Chicago, Chicago, IL; [2]University of Chicago, Chicago, IL*

WP 353 **Simultaneous Detection and Imaging of Drugs and Delivery Vehicles using LDI-MS**; Bo Zhao[1]; Mine Canakci[1]; Sankaran Thayumanavan[1]; Richard W Vachet[1]; *[1]University of Massachusetts Amherst, Amherst, MA*

WP 354 **Polarity Switching and Quantitative Mass Spectrometry Imaging of Healthy and Cancerous Hen Ovarian Tissue Sections using IR-MALDESI**; Milad Nazari[1]; Mark T Bokhart[1]; Kenneth P Garrard[1]; David C Muddiman[1]; *[1]North Carolina State University, Raleigh, NC*

WP 355 **Rapid Detection and Imaging of Fire-Retardant-Cyclodextrin-Inclusion Complexes on fibers and films by using IR-MALDESI Mass Spectrometry**; Yufei Chen[1]; Nanshan Zhang[1]; Milad Nazari[1]; Mark Bokhart[1]; Maans Ekeloef[1]; David C Muddiman[1]; Nelson R Vinueza[1]; *[1]North Carolina State University, Raleigh, NC*

WP 356 **Metabolomic Imaging of Biofilm and Other Biological Materials for Studying Metabolomic Heterogeneity**; Tomasz Ruman[1]; Joanna Nizioł[1]; Vincent Bonifay[1]; Jon Brauer[1]; Christine Gaylarde[1]; Iwona B Beech[1]; Jan A Sunner[1]; *[1]University of Oklahoma, Norman, OK*

WP 357 **Matrix-free Analysis of Resveratrol in Intact Rat Retina Tissue Using REDIchip**; Amanda Martinez[1]; Andrea Kelley[1]; Madeline Colley[1]; Stephan Bach[1]; *[1]University of Texas at San Antonio, San Antonio, TX*

WP 358 **Lanthanide Labeled Antibody Detection by SIMS nano-TOF II of Human Intestinal Injury Markers**; Keely Pierzchalski; *Maastricht, Limburg*

WP 359 **Mass Spectrometric and FT-IR Spectroscopic Imaging to Probe Organic Ligands and Their Binding Schemes on Nanocrystals**; Tae Lee[1]; Jin Gyeong Son[2]; Jeong Hee Moon[3]; Sang Woo Han[2]; *[1]KRISS, Daejeon; [2]KAIST, Daejeon, Republic of Korea; [3]KRIBB, Daejeon, Republic of Korea*

WP 360 **Analysis of Medical Devices in 2D and 3D by Secondary Ion Mass Spectrometry**; Adam Taylor[1]; Felicia Green[1]; Bonnie Tyler[1]; Josephine Bunch[1]; *[1]National Physical Laboratory, Teddington, UK*

WP 361 **Multiplex Proteins and Lipids SIMS Imaging of Mouse Hippocampus Tissues**; Eunseok Seo[1]; Sun young Lee[1]; Young-ho Park[1]; EunSook Choi[1]; Eunjoo Kim[1]; Dong Kwon Lim[2]; Su-Il In[1]; DaeWon Moon[1]; *[1]DGIST, Daegu, Korea; [2]Korea University, Seoul, Korea*

WP 362 **Imaging Mass Spectrometry as a Novel Approach to Measure Synaptic Zinc;** Masoumeh Dowlatshahi Pour[1, 2]; Lin Ren[1]; Andrew G Ewing[1, 2]; Per Malmberg[1, 2]; *[1]Chalmers University of Technology, Gothenburg, Sweden; [2]National Center for Imaging Mass Spectrometry, Gothenberg, Sweden*

WP 363 **Precursor Ion Selector Scan for Discovery of Analyte Specific Fragments in MALDI-TOF/TOF-MS/MS**; Stanislav Rubakhin[1]; Jonathan V Sweedler[2]; *[1]Beckman Institute, UIUC, Urbana, IL; [2]University of Illinois at Urbana-Champaign, Urbana, IL*

WP 364 **MS Imaging to Analyse the Transition from Early Goal-Directed Phase to Late Habituation Phase of Spatial Learning in Mice**; Geert Baggerman[1, 2]; Jeroen Aerts[3]; Laurens Minerva[3]; Dirk Valkenborg[1, 2, 4]; Annelies Laeremans[3]; D'hooge Rudi[3]; Kurt Boonen[3]; Lutgarde Arckens[3]; *[1]Flemish Institute for Technological Research (VITO), Mol, Belgium; [2]University of Antwerp, Antwerp, Belgium; [3]KU Leuven, Leuven, Belgium; [4]Hasselt University, Diepenbeek, Belgium*

INFORMATICS: ALGORITHMS AND STATISTICAL ADVANCES
365 - 389

WP 365 **A Processing Pipeline for Dramatically Increased Statistical Power in Label-Free Quantitative Proteomics**; Michael J Sweredoski[1]; Annie Moradian[1]; Tanya R Porras-Yakushi[1]; Sonja Hess[1]; *[1]Caltech, Pasadena, CA*

WP 366 **Missing Value Prediction in Metabolite-Intensity Matrix of a Quantitative Metabolomic Dataset Generated by Chemical Isotope Labeling Liquid Chromatography Mass Spectrometry**; Yunong Li[1]; Tao Huan[1]; Liang Li[1]; *[1]University of Alberta, Edmonton, Canada*

WP 367 **Improved Qualitative and Quantitative Analysis of the Human Mitochondrial Proteome by Hybrid Acquisition**; Maurizio Ronci[1]; Enrico Cilio[1]; Steven Ciavarini[2]; Curt Devlin[2]; Brad Williams[2]; Scott Geromanos[2]; Chris Hughes[3]; Johannes Vissers[4]; Andrea Urbani[1]; *[1]University of Rome Tor Vergata, Rome, Italy; [2]Waters, Milford, MA; [3]Waters, Wilmslow, UK; [4]Waters Corporation, Wilmslow, Greater Manchester*

WP 368 **Development of MSn Spectral Database and the Search Algorithm using Multiple MSn Spectra**; Yohei Yamada[1]; Akemi Suzuki[2]; Umemura Yoshikatsu[1]; Hiroyuki Yasuda[1]; Yutaro Yamamura[1]; Hideshi Fujiwake[1]; Kageyama Tetsuya[1]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]Tohoku Pharmaceutical University, Miyagi, Japan*

WP 369 **Analysis of Polarity-Switched DESI Images of Colorectal Tissue Samples**; James Stuart McKenzie[1]; Anna K Mróz[1]; Renata Filipe-Soares[1]; Zoltan Takats[1]; *[1]Imperial College, London, UK*

WP 370 **Mass Graph-Based Proteoform Identification by Top-Down Mass Spectrometry**; Qiang Kou[1]; Si Wu[2]; Nikola Tolic[3]; Ljiljana Pasa-Tolic[3]; Xiaowen Liu[4, 5]; *[1]Indiana University-Purdue University, Indianapolis, IN; [2]University of Oklahoma, Dept. of Chem & Biochem Norman, OK; [3]Pacific Northwest National Laboratory, Richland, WA; [4]Indiana University-Purdue University Indianapolis, Indianapolis, IN; [5]Indiana University School of Medicine, Indianapolis, IN*

WP 371 **A Very Fast Bayesian Engine for Truly unified MS1- and MS2-based Protein Inference**; Julianus Pfeuffer[1]; Xiao Liang[2]; Knut Reinert[2]; Oliver Kohlbacher[1]; Oliver Serang[3]; *[1]Eberhard Karls Universität Tübingen, Tübingen, BW, Deutschland; [2]Freie Universität Berlin, Berlin, Germany; [3]Freie Universität Berlin, Berlin*

WP 372 **An Adjusted-Median Approach to Missing Values in Label Free Quantitation**; Seth Just[1]; Luisa Zini[1]; Nick Vincent-Maloney[1]; Brian C Searle[1, 2]; *[1]Proteome Software, Portland, OR; [2]University of Washington, Seattle, WA*

WP 373 **Machine Learning Algorithms for Advanced Identification of Tumor Tissue and Tumor Borders**; Evgeny Zhvansky[1, 2]; Igor A Popov[1, 2]; Anatoly Sorokin[1]; Nikita Levin[1]; Vsevolod Shurkhay[3]; Denis Bormotov[1]; Maria Indeykina[2, 4]; Alexey S Kononikhin[2, 4]; Yury Kostyukevich[2, 4]; Evgeny Kukaev[1, 2]; Alexander Potapov[3]; Eugene Nikolaev[2]; *[1]Moscow Institute of Physics and Technology, Moscow, Russia; [2]Institute for Energy Problems of Chemical Physics, Moscow, Russia; [3]Burdenko Neurosurgical Institute, Moscow, Russian Federation; [4]Emanuel Institute of Biochemical Physics, Moscow, Russia*

WP 374 **Making the Most of Multi-Modality Imaging: Exploring Fusion of Mass Spectrometry Imaging with Stimulated Raman Spectroscopy**; Alan Race[1]; Alasdair Rae[2]; Jean-Luc Vorng[2]; Rory Steven[2]; Josephine Bunch[2]; Ian Gilmore[2]; *[1]National Physical Laboratory, Teddington, Middlesex; [2]National Physical Laboratory, Teddington, UK*

WP 375 **Automated Tumor Typing of Tissue Sections Based on Characteristic Spectral Patterns Extracted from MALDI Mass Spectrometry Imaging Data**; Tobias Boskamp[1, 2]; Delf Lachmund[1]; Nicolas Jathe[1]; Christian Etmann[1]; Janina Oetjen[1]; Rita Casadonte[3]; Jan Hendrik Kobarg[2]; Dennis Trede[2]; Jörg Kriegsmann[3, 4]; Peter Maass[1, 2]; *[1]University of Bremen, Bremen, Germany; [2]SCiLS GmbH, Bremen, Germany; [3]Proteopath GmbH, Trier, Germany; [4]Center for Histology, Cytology and Molecular Diagnostic, Trier, Germany*

WP 376 **Virtual Lock Masses: An Algorithmic Method to Enable Mass Spectra Comparison in Untargeted Studies**; Francis Brochu[1]; Pier-Luc Plante[1, 2]; Alexandre Drouin[1]; Louis-Émile Robitaille[1]; François Laviolette[1]; Mario Marchand[1]; Jacques Corbeil[1, 2]; *[1]Université Laval, Québec, Canada; [2]Centre de Recherche du CHU de Québec, Québec, Canada*

WP 377 **Isotopic Tree: Fast Calculation of Fine and Coarse Isotopic Envelopes up to a Predefined Margin of Error**; Dmitry Avtonomov[1]; Alexey I Nesvizhskii[1]; *[1]University of Michigan, Ann Arbor, MI*

WP 378 **DISCO - Data Independent Signal Correlator**; David Shteynberg[1]; Samuel L Bader[1]; Andrew Keller[1]; Michael Hoopmann[1]; Luis Mendoza[1]; Eric Deutsch[1]; Robert L Moritz[1]; *[1]Institute for Systems Biology, Seattle, WA*

WP 379 **A Parameterized Averagine Model Improves Feature Detection of Oligonucleotides and Increases Wider Applicability of Feature Finding Algorithm**; Samuel Wein[1]; Benjamin A Garcia[2]; *[1]University of Pennsylvania, Philadelphia, Pa; [2]University of Pennsylvania, Philadelphia, PA*

WP 380 **MassTodon - Electron Transfer driven Fragmentation Analyzer and Automatic Spectrum Calibrator**; Mateusz Krzysztof Łącki[1, 2]; Frederik Lermyte[3, 4]; Michał Startek[2]; Dirk Valkenborg[4, 5, 6]; Frank Sobott[3, 4]; Anna Gambin[2]; *[1]University of Warsaw, Warszawa, Mazowieckie; [2]Faculty of Mathematics, Informatics, and Mechanics, University of Warsaw, Warsaw, Poland; [3]Biomolecular & Analytical Mass Spectrometry group, University of Antwerp, Antwerpen, Belgium; [4]UA-VITO Center for Proteomics, University of Antwerp, Antwerpen, Belgium; [5]Interuniversity Institute for Biostatistics and Statistical Bioinformatics, Hasselt University, Hasselt, Belgium; [6]VITO, Mol, Belgium*

WP 381 **IsoSpec - a Hyperfast Generator of Fine Isotopic Structure Peaks with Preset Total Probability**; Mateusz Krzysztof Łącki[1]; Michał Startek[1]; Dirk Valkenborg[2, 3, 4]; Anna Gambin[1]; *[1]Faculty of Mathematics, Informatics, and Mechanics, University of Warsaw, Warsaw, Poland; [2]UA-VITO Center for Proteomics, University of Antwerp, Antwerpen, Belgium; [3]Interuniversity Institute for Biostatistics and Statistical Bioinformatics, Hasselt University, Hasselt, Belgium; [4]VITO, Mol, Belgium*

WP 382 **Robust Algorithms for Denoising, Eliminating Dispersion Similar to Phasing in 1D_FT-MS Spectra and Reconstructing Non Uniformly Sampled 2D_FT-ICR Data**; Lionel Chiron[1]; Fabrice Bray[2]; Christian Rolando[3]; Marc-André Delsuc[4]; *[1]CASC4DE, Strasbourg, France; [2]Université de Lille, Villeneuve d'Ascq, France; [3]Univ. de Lille 1, Sciences et Technologies, Villeneuve d'Ascq; [4]Université de Strasbourg, Strasbourg, France*

WP 383 **Finding the Peaks: Performance Enhancement of Portable MS using a Bayesian Approach**; Simon Maher[1]; Simon Maskell[1]; Sarfaraz Syed[2]; Fred Jjunju[1]; Stephen Taylor[1]; *[1]Department of Electrical Engineering and Electronics University Of Liverpool, Liverpool, UK; [2]Maastricht University, Maastricht, NL*

WP 384 **Integrated GlycoProteome Analyzer (I-GPA) for Automatic Identification and Quantitation of Site-Specific N-Glycosylation**; Gun Wook Park[1, 2]; Jin Young Kim[2]; Heeyoun Hwang[2]; Ju Yeon Lee[2]; Young Hee Ahn[3]; Hyun Kyoung Lee[2]; Eun Sun Ji[2]; Hoi Keun Jeong[2]; Ki Na Yun[2]; Yong-Sam Kim[4]; Jeong-Heon Ko[4]; Hyun Joo An[5]; Jae Han Kim[5]; Young-Ki Paik[6]; Jong Shin Yoo[2]; *[1]Chungnam National University, Cheongju, Chungbuk; [2]Korea Basic Science Institute, Cheongju-Si, Republic of Korea; [3]Cheongju University, Cheongju-Si, Republic of Korea; [4]Korea Research Institute of Bioscience and Biotechnology, Daejeon, Republic of Korea; [5]Chungnam National University, Daejeon, Republic of Korea; [6]Yonsei University, Seoul, South Korea*

WP 385 **Identification of N-glycopeptides using Open Spectral Library Search**; Zhiwu An[1]; Qingbo Shu[1]; Hao Lv[1]; Jianjun Yu[1]; Fuquan Yang[1]; Yan Fu[1]; *[1]Chinese Academy of Sciences, Beijing, Beijing*

WP 386 **Extending MS Interpreter: A Freely-Available Tool for Structure/Spectrum Self-Consistency of High Resolution Tandem Mass Spectra**; Alexey V. Mayorov[1, 2]; Yuri Mirokhin[3]; Dmitrii Tchekhovskoi[3]; Stephen Stein[3]; *[1]NIST, Gaithersburg; [2]N.M. Emanuel Institute of Biochemical Physics RAS (IBCP RAS), Moscow, Russian Federation; [3]NIST, Gaithersburg MD*

WP 387 **Machine Learning-Driven Validation Platform for Mass Spectrometry Imaging using Tandem Mass Spectra and Chemical Structure Databases**; Ivan Laponogov[1]; Emilie J L Cauet[2]; James McKenzie[2]; Robert C Glen[2]; Zoltan Takats[2]; Kirill Veselkov[2]; *[1]Imperial College London, London, London; [2]Imperial College, London, UK*

WP 388 **Improving LC-MS Coverage through New Charge State and Monoisotopic m/z Assignment Algorithms**; Graeme McAlister[1]; Derek Bailey[1]; Romain Huguet[1]; Michael Senko[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

WP 389 **SAINTq: Robust Scoring of Protein-Protein Interactions in Quantitative AP-SWATH Experiments**; Guoci Teo[1]; Hiromi WL Koh[1]; Damian Fermin[2]; Jean-Philippe Lambert[3]; James Knight[3]; Anne-Claude Gingras[3]; Hyungwon Choi[4]; *[1]National University of Singapore, Singapore, Singapore; [2]Yale University, New Haven, CT; [3]Lunenfeld Tanenbaum Research Institute, Toronto, Canada; [4]National University of Singapore, Singapore*

INFORMATICS: WORKFLOW AND DATA MANAGEMENT
390 - 405

WP 390 **Galaxy-P: Recent Developments and Emerging Applications**; Pratik Jagtap[1, 2]; James Johnson[3]; Thomas McGowan[3]; Innocent Onsongo[3]; Benjamin Lynch[3]; Candace Guerrero[1]; Kevin Murray[1]; Lloyd M Smith[4]; Michael R Shortreed[4]; Anthony J Cesnik[4]; Lennart Martens[5, 6]; Adrian Hegeman[1]; Timothy Griffin[1, 2]; *[1]University of Minnesota, Minneapolis, MN; [2]Center for Mass Spectrometry and Proteomics, UMN St.Paul, MN; [3]University of Minnesota Supercomputing Institute, Minneapolis, MN; [4]University of Wisconsin Madison, Madison, Wisconsin; [5]Ghent University, Ghent, Belgium; [6]VIB, Ghent, Belgium*

WP 391 **Optide-Hunter: Informatics Solutions for Optimized Peptide Drug Development through the Integration of Heterogeneous Data and Adaptation of Various LC-MS Technologies**; Mi-Youn Brusniak[1]; Emily Girard[1]; Bernard Lee[2]; Chris Mehlin[1]; Yuko Ogata[1]; Philip Gafken[1]; Hector Ramos[1]; Jim Olson[1]; *[1]Fred Hutchinson Cancer Research Center, Seattle, WA; [2]LabKey Software, Seattle, WA*

WP 392 **APOSTL: An interactive Galaxy Pipeline For Reproducible Analysis of Affinity Proteomics Data**; Brent Kuenzi[1]; Adam Borne[1]; Jiannong Li[1]; Uwe Rix[1]; Paul Stewart[1]; Eric Haura[1]; *[1]H. Lee Moffitt Cancer Center & Research Institute, Tampa, FL*

WP 393 **Enabling Collaborative Discovery in Big Data Visual Analytics**; Joon-Yong Lee[1]; Ryan Wilson[1]; Grant M Fujimoto[1]; Gary R Kiebel[1]; Richard D Smith[1]; Nick Cramer[1]; Samuel H Payne[1]; *[1]Pacific Northwest National Lab, Richland, WA*

WP 394 **Scientific Workflows for Data Analysis and Visualization in Quantitative Proteomics**; Arzu Tugce Guler[1]; Dmitrii Travin[2]; Yassene Mohammed[1]; Magnus Palmblad[1]; *[1]Leiden University Medical Center, Center for Proteomics and Metabolomics, Leiden, Netherlands; [2]Faculty of Bioengineering and Bioinformatics, Lomonosov Moscow State University, Moscow, Russia*

WP 395 **Integration of Peptide-Centric Searching of Data Independent Acquisition Data without an MS/MS Spectrum Library with Data in the Chorus Project**; Michael J. MacCoss[1]; Brian C Searle[1]; Sonia Ying Ting[1]; Jarrett Egertson[1]; Christine C Wu[2]; Andrii Laboda[3]; Oleksii Tymchenko[3]; Andrey Bondarenko[3]; *[1]Univ of Washington, Seattle, WA; [2]Stratus Biosciences, Seattle, WA; [3]Infoclinika, LLC, Seattle, WA*

WP 396 **High Performance Computing at the National Resource for Translational and Developmental Proteomics**; Ryan T Fellers[1]; Richard D LeDuc[1]; Bryan P Early[1]; Joseph B Greer[1]; Alexandra J Van Nispen[1]; Paul M Thomas[1]; Neil L Kelleher[1]; *[1]Northwestern University, Evanston, IL*

WP 397 **The MassIVE Repository for Interactive Annotation of Proteomics Big Data**; Jeremy Carver[1]; Mingxun Wang[1]; Nuno Bandeira[1]; *[1]UCSD, La Jolla, CA*

WP 398 **The Potential of Functional Annotation of Mass Spectrometry Tools**; Magnus Palmblad[1]; Arzu Tugce Guler[1]; Kristian Davidsen[2]; Jon Ison[2]; Veit Schwämmle[3]; *[1]Leiden University Medical Center, Leiden, the Netherlands; [2]Technical University of Denmark, Copenhagen, Denmark; [3]University of Southern Denmark, Odense, Denmark*

WP 399 **Recent Developments in ProteomicsDB: From FDR Estimates to Proteomic Assays and More**; Mathias Wilhelm[1]; Daniel Paul Zolg[1]; Hans-Christian Ehrlich[2]; Stephan Aiche[2]; Mohammed AbuJarour[2]; David Weese[2]; Judith Schlegl[3]; Tobias Schmidt[1]; Wilhelm Becker[2]; Lars Rückert[2]; Jan Huenges[2]; Susan Klaeger[1, 4, 5]; Stephanie Heinzlmeir[1, 4, 5]; Hannes Hahne[1, 6]; Bernhard Kuster[1, 4, 5]; *[1]Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; [2]Innovation Center Potsdam, SAP SE, Potsdam, Germany; [3]SAP SE, Walldorf, Germany; [4]German Cancer Consortium (DKTK), Muenchen, Germany; [5]German Cancer Research Center, Heidelberg, Germany; [6]OmicScouts GmbH, Freising, Germany*

WP 400 **Dredging the Mass Spectrometry Data Lake for Hidden Information with Teradata Database and Business Intelligence Software**; Alan Dickson[1]; Tony Ly[1]; Vackar Afzal[1]; Dalila Bensaddek[1]; Jens Hukelmann[1]; Angus Lamond[1]; *[1]Centre for Gene Regulation and Expression, Dundee, UK*

WP 401 **Comparison of Data Processing Strategies for Optimal Detection of Protein-Protein Interactions**; Gerhard Duernberger[1, 2]; Florian Stanek[3]; Johannes Doblmann[3]; Zuzana Demianova[3]; Karl Mechtler[3]; *[1]GMI - Gregor Mendel Institute of Molecular Plant Biology, Vienna, Austria; [2]IMP - Research Institute of Molecular Pathology, Vienna, Vienna; [3]IMP - Research Institute of Molecular Pathology, Vienna, Austria*

WP 402 **Proteomics in Perl: A Streamlined Approach**; Jeremy D Volkening[1]; Michael R Sussman[1]; *[1]University of Wisconsin-Madison, Madison, WI*

WP 403 **RAId GUI: A Graphical User Interface for RAId Tandem Mass-Spectrometry Database Search Tool**; Danny Lee[1]; Aleksey Ogurtsov[1]; Gelio Alves[1]; Yi-Kuo Yu[1]; *[1]National Center for Biotechnology Information, NLM, NIH, Bethesda, MD*

WP 404 **Xcalibur Workbench: A Lua Based Data Browser**; Michael W. Senko[1]; Graeme C McAlister[1]; Derek Bailey[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

WP 405 **CHORUS is Innovative and User Friendly Platform for Third Party Mass Spectrometry Software Integration**; Andrey Bondarenko[1]; Andrii Loboda[1, 2]; Oleksii Tymchenko[1, 2]; Vladimir Moiseiev[1, 2]; Nathan Yates[3]; Mai Sun[3]; Michael J MacCoss[4]; Brendan Maclean[4]; Christine Wu[4]; Brian C Searle[4]; Sonia Ying Ting[4]; Jimmy K Eng[4]; Nick Shulman[4]; Juergen H Cox[5]; Chris Becker[6]; *[1]InfoClinika, Bellevue, WA; [2]TeamDev, Kharkiv, Ukraine; [3]University of Pittsburgh, Pittsburgh, PA; [4]University of Washington, Seattle, WA; [5]Max Planck Institute for Biochemistry, Martinsried, Germany; [6]Protein Metrics Inc., San Carlos, CA*

INSTRUMENTATION: MINI/PORTABLE/FIELDABLE MS
406 - 425

WP 406 **Fingerprinting of Falsified Artemisinin Combination Therapies (ACTs) via DART Ionization Coupled to a Compact Single Quadrupole Mass Spectrometer**; Matthew Bernier[1]; Frederick Li[2]; Joseph LaPointe[2]; Brian D Musselman[2]; Paul Newton[3, 4]; Facundo M Fernandez[1]; *[1]Georgia Institute of Technology, Atlanta, GA; [2]IonSense, Inc. Saugus, MA; [3]Lao-Oxford-Mahosot Hospital Wellcome Trust Research Unit (LOMWRU), Vientiane, Laos; [4]Centre for Tropical Medicine and Global Health, University of Oxford, Oxford, UK*

WP 407 **Explosive Detection Using a Portable Benchtop Cylindrical Ion Trap-Mass Spectrometer**; Stephen Davila[1]; Corey Stedwell[1]; Daniel DeBord[1]; *[1]1st Detect Corporation, Webster, TX*

WP 408 **Establishing a Baseline for a Portable Stable Carbon Isotope Detection System**; Brian Thomas[1]; Steve Taylor[1]; Tim Clarey[2]; Dave McIntosh[1]; *[1]University of Liverpool, Liverpool, UK; [2]The King's University, Southlake, TX*

WP 409 **Micro Mass Spectrometer Approach for Cometary Exploration**; Ashish Chaudhary[1]; Friso van Amerom[1]; Tim Short[1]; Emily Barrentine[2]; Yun Zheng[2]; Daniel Glavin[2]; William Brinckerhoff[2]; Paul Mahaffy[2]; *[1]SRI International, St. Petersburg, FL; [2]NASA GSFC, Greenbelt, MD*

WP 410 **Development of Compact Laser Desorption/Ionization Time-of-Flight Mass Spectrometer for Planetary Missions**; Xiang Li[1]; Stephanie Getty[2]; Andrej Grubisic[3]; Kyle Uckert[4]; William Brinckerhoff[2]; Timothy J Cornish[5];

Scott Ecelberger[5]; *[1]University of Maryland, Baltimore County, Greenbelt, MD; [2]NASA Goddard Space Flight Center, Greenbelt, MD; [3]University of Maryland, College Park, College Park, MD; [4]New Mexico State University, Las Cruces, NM; [5]C&E Research, Inc, Columbia, MD*

WP 411 **Mars Organic Molecule Analyzer (MOMA) Mass Spectrometer: Performance Testing in GC-MS and LD-MS Modes of Operation**; Veronica Pinnick [1]; Ryan Danell[2]; Friso van Amerom[3]; Samuel Larson[3]; Arnaud Buch[4]; Cyril Szopa[5]; Xiang Li[1]; Andrej Grubisic[6]; Ricardo Arevalo[3]; Stephanie Getty[3]; William Brinckerhoff[3]; Paul Mahaffy[3]; Francois Raulin[7]; Fred Goesmann[8]; *[1]University of Maryland, Baltimore County Greenbelt, MD; [2]Danell Consulting, Inc. Winterville, NC; [3]NASA GSFC, Greenbelt, MD; [4]Ecole Centrale, Paris, France; [5]Laboratoire Atmosphères, Paris, France; [6]University of Maryland, College Park, MD; [7]5Laboratoire Interuniversitaire des Systèms Atmosphériques, Paris, France; [8]Max Planck Institut für Sonnensystemforschung, Göttingen, Germany*

WP 412 **Characterization of the Mars Organic Molecule Analyzer Mass Spectrometer Intrinsic Dynamic Range**; Friso H.W. Van Amerom[1]; Xiang li[2]; Ryan Danell[3]; Veronica T Pinnick[2]; Stephanie Getty[4]; Ricardo Arevalo[4]; Andrej Grubisic[5]; Lars Hovmand[6]; William Brinckerhoff[4]; Paul Mahaffy[4]; Fred Goesmann[7]; *[1]Mini-Mass Consulting, Inc, Hyattsville, MD; [2]University of Maryland, Baltimore County Greenbelt, MD; [3]Danell Consulting, Winterville, NC; [4]NASA GSFC, Greenbelt, MD; [5]University of Maryland, College Park, MD; [6]Linear Labs, Washington DC; [7]Max Planck Institut für Sonnensystemforschung, Goettingen, Germany*

WP 413 **The Europa Mass Spectrometer for Planetary Exploration (MASPEX). A High-Resolution Multi-Pass Time-of-Flight Mass Spectrometer**; Gregory P. Miller[1]; Jack Hunter Waite, Jr.[2]; Tim Brockwell[2]; John Roberts[2]; Keith S Pickens[2]; Ryan C. Blase[2]; Paul Wilson V[2]; *[1]Southwest Research Institute, San Antonio , TX; [2]Southwest Research Institute, San Antonio, TX*

WP 414 **Silence is Golden: Detector Radiation Shielding at Europa for MAss Spectrometer for Planetary EXploration (MASPEX)**; Ryan C. Blase[1]; Roland R. Benke[2]; Keith S. Pickens[1]; Gregory P. Miller[1]; Tim Brockwell[1]; John Roberts[1]; Paul Wilson IV[1]; J.H. Waite, Jr.[1]; *[1]Southwest Research Institute, San Antonio, TX; [2]Atom Consulting LLC / Consultant to SwRI, Austin, TX*

WP 415 **Development of an Integrated LC-MS Prototype for an *in situ* Mission to an Icy Body in the Solar System**; Adrian Southard[1]; Stephanie Getty[2]; Jerome P Ferrance[3]; Brian N Stamos[4]; Jamie E Elsila[2]; Manuel A Balvin[2]; Daniel P Glavin[2]; Daniel S Stewart[2]; Brandon J Colon-Curiel[5]; *[1]Universities Space Research Association, Columbia, MD; [2]NASA GSFC, Greenbelt, MD; [3]J2f engineering, Charlottesville, VA; [4]University of Texas at Arlington, Arlington, TX; [5]University of Puerto Rico Mayaguez, Mayaguez, PR*

WP 416 **Towards Remote Chemical Sensing Using an Aerodynamic Assisted Portable Mass Spectrometer**; Yanbing Zhai[1]; Ting Jiang[1]; Wei Xu[1]; *[1]Beijing Institute of Technology, Beijing, China*

WP 417 **Portable Multiple Ionization Sources Biological Mass Spectrometer**; Jung-Lee Lin[1]; Ming-Lee Chu[1]; Chung-Hsuan Chen[1]; *[1]Academia Sinica, Taipei, Taiwan*

WP 418 **Low Temperature Co-fired Ceramic (LTCC)-Packaged MEMS Micro-ion Source for Miniature Mass Spectrometry Applications**; Charles B Parker[1]; Erich J Radauscher[1]; Kristin H Gilchrist[2]; Shane DiDona[1]; Zachary E Russell[1]; Stephen D Hall[2]; James B Carlson[2]; Sonia Grego[2]; Steven J Edwards[3]; Roger P Sperline[3]; M. Bonner Denton[3]; Brian R Stoner[1, 2]; Jeffrey T Glass[1]; Jason J Amsden[1]; *[1]Department of Electrical and Computer Engineering, Duke University, Durham, NC; [2]Engineering and Applied Physics Division, RTI International, Research Triangle Park, NC; [3]Department of Chemistry and Biochemistry, University of Arizona, Tucson, AZ*

WP 419 **Handheld and Portable DAPCI Source for Point and Shoot Applications: Towards Onsite *in-situ* Explosives Analysis**; Fred Paul Mark Jjunju[1]; Simon Maher[2]; Stephen Taylor[2, 3]; Graham R Cooks[4]; *[1]Department of Electrical Engineering and Electronics University of Liverpool, Liverpool, UK; [2]University of Liverpool, Liverpool, UK; [3]Q-Technologies Ltd, Liverpool, UK; [4]Department of Chemistry Purdue University, West Lafayatte, IN*

WP 420 **Development of HPLC Methods for Use with Mobile Ambient Ionization Mass Spectrometry**; Leonard Rorrer,III[1]; Mitch Wells[1]; *[1]FLIR Systems, Inc., West Lafayette, IN*

WP 421 **Improving the Selectivity of a High Pressure Mass Spectrometry**; Andrew Hampton; *UNC - Chapel Hill, Chapel Hill, NC*

WP 422 **Falling Through the Cracks: High Resolution Quadrupole Mass Spectrometry**; Dave McIntosh[1]; Mariya Antony-Joseph[1]; Simon Maher[1]; John Ray Gibson[1]; Stephen Taylor[1]; *[1]University of Liverpool, Liverpool, UK*

WP 423 **Utilizing Silicon on Insulator Materials to Fabricate Miniature Ion Traps for High Pressure Mass Spectrometry**; Zachary Dyer[1]; Craig Cavanaugh[2]; Kenion Blakeman[2]; Tina Stacy[1]; Michael J Ramsey[1]; *[1]UNC Ramsey Group, Chapel Hill, NC; [2]University of North Carolina at Chapel Hill, Chapel Hill, NC*

WP 424 **Miniaturized Toroidal Ion Trap using Cylindrical Electrodes**; Daniel Austin[1]; Jessica Higgs[1]; Kit White[1]; Yuan Tian[1]; *[1]Brigham Young University, Provo, UT*

WP 425 **Overcoming the Tradeoff between Resolution and Sensitivity in Miniature Mass Spectrometry using Spatially Coded Apertures**; Zachary E Russell[1, 2]; Evan X Chen[1]; Shane T DiDona[1]; Jason J Amsden[1]; Charles B Parker[1]; Scott D Wolter[3]; Ryan M Danell[4]; Brian R Stoner[5]; Gottfried Kibelka[6]; Michael E Gehm[1]; David W Brady[1]; Jeffrey T Glass[1]; *[1]Duke University, Durham, NC; [2]Stanford University, Stanford, CA; [3]Elon Univesity, Elon, NC; [4]Danell Consulting, Inc. Winterville, NC; [5]RTI International, Raleigh, NC; [6]Xylem/OI Analytical, College Station, TX*

INSTRUMENTATION: NEW DEVELOPMENTS IN IONIZATION AND SAMPLING (SAMPLING)
426 - 438

WP 426 **Coupling Thin-Layer Chromatography with Matrix Assisted Inlet Ionization for Small Molecule Analysis**; Khoa Hoang[1]; Charles N McEwen[2, 3]; *[1]MStm, philadelphia, pa; [2]University of the Sciences in Philadelphia, Philadelphia, PA; [3]MSTM, LLC. Hockessin, DE*

WP 427 **Interfacing UPLC to Mass Spectrometry via a Liquid-junction, Secondary Ultrasonic API Source**; Steve Bajic[1]; David S Douce[1]; Gordon A Jones[1]; *[1]Waters Corporation, Manchester, England*

WP 428 **Development and Optimization of an Inlet System for Desorption Atmospheric Pressure Photoionization – Mass Spectrometry (DAPPI-MS)**; Kai Kroll[1]; Christine Polaczek[1]; Tiina Kauppila[2]; Anu Vaikkinen[2]; Hendrik Kersten[1]; Thorsten Benter[1]; *[1]University of Wuppertal, Wuppertal, Germany; [2]University of Helsinki, Helsinki, Finland*

WP 429 **Glove Box MS Interface for the Measurement of Reaction Kinetics of Airsensitive Compounds**; Alan T. Taylor[1]; Ruth Dooley[2]; Mark Baumert[3]; Clive Aldcroft[3]; Mark Allen[3]; C. Logan Mackay[2]; Guy Lloyd-Jones[2]; *[1]University of Edinburgh, Edinburgh, Lothian; [2]School of Chemistry, The University of Edinburgh Edinburgh, UK; [3]Advion UK Ltd, Essex, UK*

WP 430 **Volatile Terpene Analysis in Cannabis, Spices and Fresh Produce by Tandem Mass Spectrometry Fitted with a Modified Plasma Source**; Frank Kero[1]; Craig Young[1]; Heather Gamble[2]; Joshua Ye[2]; Lisa Cousins[2]; Chuck Joliffe[2]; Chai Yuan-Cheng[3]; Lin Jing-Chao[3]; *[1]PerkinElmer, Downers Grove, IL; [2]Ionics, Bolton, Canada; [3]PerkinElmer, Shanghai, China*

WP 431 **A New Interface Design for Coupling a Liquid Stream to an Electron Ionization Source**; Alexander Lekkas[1]; Dimitris Papanastasiou[1]; Emmanuel Raptakis[1]; Francesca Rigano[2]; Danilo Sciarrone[3]; Luigi Mondello[2,3]; *[1]Fasmatech, Athens, Greece; [2]Chromaleont s.r.l., Messina, Italy; [3]Dipartimento di Scienze Chimiche, Biologiche, Farmaceutiche ed Ambientali", University of Messina, Messina, Italy*

WP 432 **LC-MS with Cold EI – The New System and Recent Applications**; Svetlana Tsizin[1]; Aviv Amirav[2]; Alexander B Fialkov[1]; Tal Alon[1]; *[1]Tel Aviv University, Tel Aviv, Israel; [2]Tel-Aviv University, Tel-Aviv*

WP 433 **Study of Vaporization Surfaces in Liquid Chromatography – Electron Ionization Mass-Spectrometry**; Federica Bianchi[1]; Laura Magrini[2]; Nicolò Riboni[1]; Maria Careri[1]; Achille Cappiello[2]; *[1]University of Parma, Parma, Italy; [2]University of Urbino, Urbino, Italy*

WP 434 **DEI vs. LEI: A Novel, Advanced System for Interfacing Liquid Chromatography and Electron Ionization Mass Spectrometry**; Achille Cappiello[1]; Maurizio Piergiovanni[1]; Giorgio Famiglini[1]; Veronica Termopoli[1]; Pierangela Palma[1]; *[1]University of Urbino, Urbino, Italy*

WP 435 **Evaluation of an Induction-Based Fluidics System for Delivery of Low Volume (nL) Samples;** Kelly Hanssen Smith[1]; Susan M Schulz[1]; Bryce F Doxzon[1]; Ernest H Braue[1]; Irwin Koplovitz[1]; Kathleen Housman[1]; Lee I Roberts[1]; Jonathan Oyler[1]; *[1]USAMRICD, Aberdeen Proving Ground, MD*

WP 436 **AP-to-vacuum Inlet with New Features - Optimization of Desolvation Conditions in Liquid AP-MALDI MS**; Jeff Brown[1, 2]; Pavel Ryumin[1]; Michael Morris[2]; Rainer Cramer[1]; *[1]University of Reading, Reading, UK; [2]Waters, Wilmslow, UK*

WP 437 **Gas Chromatography Plasma-Assisted Reaction Chemical Ionization Time of Flight Mass Spectrometry (GC-TOF-MS) for Identification and Quantification of Halogenated Compounds**; Kunyu Zheng[1]; Hamid Badiei[2]; Kaveh Jorabchi[1]; *[1]Georgetown University, Washington, DC; [2]PerkinElmer, Woodbridge, ON*

WP 438 **A Novel Method for Online Analysis of Electronic Cigarette Aerosol**; Christian Lindinger[1]; Alfons Jordan[1]; Philipp Sulzer[1]; Kostiantyn Breiev[1]; Kerstin M.M. Burseg[2]; Grant O'Connell[2]; Eugen Hartungen[1]; Stefan S. Biel[2]; Xavier Cahours[3]; Stephane Colard[3]; Tilmann D. Märk[1, 4]; *[1]IONICON Analytik GmbH., Innsbruck, AUSTRIA; [2]Fontem Ventures B.V., Amsterdam, The Netherlands; [3]SEITA - Imperial Tobacco Group, Fleury-les-Aubrais, France; [4]Institut für Ionenphysik und Angewandte Physik, Leopold-Franzens Universität Innsbruck, Innsbruck, Austria*

ION MOBILITY: FUNDAMENTALS
439 - 463

WP 439 **Collision Cross Section (CCS) Measurements for Small Molecular Mixture by Fourier Transform Ion Cyclotron Resonance Mass Spectrometry**; Hu Miao[1]; Zhang Linzhou[1]; Xu Chunming[1]; Quan Shi[2]; *[1]China University of Petroleum, Beijing, China; [2]State Key Laboratory of Heavy Oil Processing, Changping, Beijing*

WP 440 **Assessment of using Projection Superposition Approximation (PSA) with Molecular Modeling to Compute Collision Cross Sections For Ion Mobility Spectrometry**; Glenn Spangler; *Technispan LLC, Lutherville, MD*

WP 441 **Predicting Theoretical Collision-cross Sections for Peptides and Peptide Fragments**; Bela Paizs[1]; Oscar Hernandez[1]; Daniel Chaplin[1]; Ash Buck[1]; Keith Richardson[2]; Jeff Brown[2]; Kevin Giles[2]; Zoltan Takats[3]; *[1]Bangor University, Bangor, UK; [2]Waters, Wilmslow, UK; [3]Imperial College, London, UK*

WP 442 **Evaluation of Collision Cross Section Measurements Obtained by Uniform Field Drift Tube IM-MS: Insight into Instrument Settings and Theoretical Calculations**; Sarah Stow[1]; Jody C May[1]; James N Dodds[1]; Andrzej Balinski[1]; Emma E Rennie[2]; Ruwan T Kurulugama[2]; John Fjeldsted[2]; John A McLean[1]; *[1]Vanderbilt University, Nashville, TN; [2]Agilent Technologies, Santa Clara, CA*

WP 443 **Hide-and -Seek: The effect of Localisation of Partial Charges on Ions on Their Calculated CCS Values**; Lukasz Grzegorz Migas[1]; Eleanor Sinclair[1]; Christopher Gray[1]; Sabine Flitsch[1]; Perdita Barran[1]; *[1]University of Manchester, Manchester, UK*

WP 444 **On the Structural Denaturation of Biological Analytes in Trapped Ion Mobility Spectrometry - Mass Spectrometry**; Fanny Caroline Liu[1]; Samuel R. Kirk[1]; Christian Bleiholder[1]; *[1]Florida State University, Tallahassee, FL*

WP 445 **Collision Cross Section Accuracy of Common MS Calibrants Across a Large Number of Measurements in Positive and Negative Ion Modes**; Jody C. May[1]; Ruwan T Kurulugama[2]; George C Stafford[2]; John C Fjeldsted[2]; John A McLean[1]; *[1]Vanderbilt University, Nashville, TN; [2]Agilent Technologies, Santa Clara, CA*

WP 446 **Elucidating the Structural Heterogeneity of Biomolecules in the Gas Phase using Traveling Wave Ion Mobility Arrival Time Distributions**; Sugyan Dixit[1]; Brandon T Ruotolo[1]; *[1]University of Michigan, Ann Arbor, MI*

WP 447 **Towards using Trapped IMS in Structural Biology Applications**; Christian Bleiholder[1]; Fanny C Liu[2]; Samuel R Kirk[2]; Meggie Young[2]; Mengqi Chai[2]; *[1]Florida State University, Tallahassee, FL; [2]Florida State University, Tallahassee, FL*

WP 448 **Characterizing Instrumental Parameters in Trapped Ion Mobility Spectrometry (TIMS) for Transmission and Preservation of Native Analyte Structures and Their Complexes**; Samuel Kirk[1]; Christian Bleiholder[1]; *[1]Florida State University, Tallahassee, FL*

WP 449 **Fundamentals of Trapped Ion Mobility Spectrometry: Fluid Dynamics**; Melvin A. Park[1]; Karsten Michelmann[2]; Mark E Ridgeway[1]; Joshua Silveira[1]; *[1]Bruker Daltonics, Inc., Billerica, MA; [2]Bruker Daltonik GmbH, Bremen, Germany*

WP 450 **Decomposition Pathways during Explosive Analysis Using TIMS-MS and Molecular Dynamics**; Alan McKenzie[1]; Mark E Ridgeway[2]; Melvin Park[2]; Francisco Alberto Fernandez Lima[3]; *[1]Florida Int'l University, Miami, FL; [2]Bruker Daltonic, Billerica, MA; [3]Florida International University, Miami, FL*

WP 451 **Improving Ion Mobility – Mass Scan for the High Performance Ion Mobility Spectrometry – Mass Spectrometry**; Jianglin Wu[1]; Adam M Graichen[1]; Mark Osgood[1]; Ching Wu[1]; *[1]Excellims Corporation, Acton, MA*

WP 452 **Structures for Lossless Ion Manipulations (SLIM) using Multilevel Traveling Wave Ion Escalators for Obtaining Ultrahigh Resolution Ion Mobility Separations**; Ahmed M Hamid[1]; Yehia M Ibrahim[1]; Sandilya V. B Garimella[1]; Ian K Webb[1]; Liulin Deng[1]; Gordon A Anderson[1]; Spencer A Prost[1]; Jeremy A Sandoval[1]; Randolph V Norheim[1]; Erin S Baker[1]; Richard D Smith[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

WP 453 **Development and Evaluation of Long Serpentine Path Traveling Wave SLIM Modules for High Resolution Ion Mobility Separations**; Liulin Deng[1]; Yehia M Ibrahim[2]; Ahmed M Hamid[2]; Sandilya Garimella[2]; Ian Webb[2]; Xing Zhang[2]; Tsung-Chi Chen[2]; Xueyun Zheng[2]; Erin Baker[2];

Richard D Smith[2]; [1]*Pacific NW National Laboratory, Richland, WA;* [2]*Pacific Northwest National Lab, Richland, WA*

WP 454 **Comparing Ion Multiplexing Techniques: Tangible Enhancement for Ion Mobility-Mass Spectrometry**; Brian H. Clowers[1]; Austen L. Davis[1]; Kelsey A Morrison[1]; [1]*Washington State University, Pullman, WA*

WP 455 **A Comparative Study of nanoESI and ESI on an Atmospheric Pressure High Performance Ion Mobility Spectrometer**; Mark Osgood[1]; Adam M Graichen[1]; Ching Wu[1]; [1]*Excellims Corporation, Acton, MA*

WP 456 **Modeling Space Charge Effects on the Performance of Transversal Modulation Ion Mobility Spectrometry: A Numerical Approach**; Cesar Barrios[1]; Guillermo Vidal-de-Miguel[2]; [1]*SEADM, Boecillo, Spain;* [2]*Fossil Ion Technology S.L., Madrid, Spain*

WP 457 **Coupling of High-Resolution Atmospheric Pressure Drift Tube Ion Mobility Spectrometry with High-Resolution Accurate Mass Orbitrap Mass Spectrometry**; Joel D Keelor[1]; Anyin Li[1]; Brian H Clowers[2]; Facundo M Fernandez[1]; [1]*Georgia Institute of Technology, Atlanta, GA;* [2]*Washington State University, Pullman, WA*

WP 458 **Peak Width Analysis for Automated Detection of Unresolved Isomers in Ion Mobility**; Matthew Brantley[1]; Michael Pettit[1]; Brett Harper[1]; Brooke Brown[1]; Touradj Solouki[1]; [1]*Baylor University, Waco, TX*

WP 459 **Altering the Mobility-Time Continuum: Methods for Targeted, Yet Lossless, High Resolution Trapped Ion Mobility-Mass Spectrometry**; Joshua Adam Silveira[1]; William Danielson[2]; Jacob Meier[1]; Mark E Ridgeway[1]; Melvin Park[1]; [1]*Bruker Daltonics, Billerica, MA;* [2]*Danielson Software Consulting, Richland, WA*

WP 460 **Comprehensive Electric Field Analysis of Resistive Glass Drift Tubes, Reflectrons, and Other Electro-Optical elements**; Robert Jackson[1]; Matthew Breuer[2]; Paula Holmes[2]; Jeffrey DeFazio[3]; [1]*Instrumental Design Physics, LLC, Littleton, MA;* [2]*Photonis USA, Sturbridge, MA;* [3]*PHOTONIS USA, Lancaster, PA*

WP 461 **Ion Mobility Coupled to Extended Mass Range Orbitrap for Structural Analysis of Large Proteins and Protein Complexes**; Michael Poltash[1]; Kyle Fort[2]; David H Russell[3]; [1]*Texas A&M University, College Station, Texas;* [2]*Utrecht University, Utrecht, The Netherlands;* [3]*Texas A&M University, College Station, TX*

WP 462 **Multistage Transversal Modulation IMS Coupled with IonMax Electrospray and Ion Trap MS to Provide a Modular ESI-IMS-MS Solution**; Guillermo Vidal-de-Miguel[1]; Miriam Macia[1]; Gonzalo Arranz[2]; Alberto Tejero[2]; [1]*Fossil Ion Technology S.L., Madrid, Spain;* [2]*SEADM, Boecillo, Spain*

WP 463 **Development of a Drift Tube Mass Spectrometer Associated with Plasma Microjets**; Joel Lemaire[1]; Bessem Brahim[1]; Michel Heninger[1]; Essyllt Louarn[1]; Helene Mestdagh[1]; Gérard Bauville[2]; Nicole Blin Simiand[2]; Et-Touhami Es-Sebbar[2]; Michel Fleury[2]; Stephane Pasquier[2]; Joao Santos Sousa[2]; Elsa Bauchard[3]; Julien Leprovost[3]; [1]*LCP, UMR8000, CNRS-Université Paris Sud, Université Paris Saclay, Orsay, France;* [2]*LPGP, UMR8578, CNRS-Université Paris Sud, Université Paris Saclay, Orsay, France;* [3]*AlyXan, Juvisy sur Orge, France*

ION STRUCTURE/ENERGETICS
464 - 482

WP 464 **Gas Phase Conformation of the Complex of Cyclodextrins with Amino Acids Revealed by Ion Mobility-Mass Spectrometry and Molecular Dynamics Calculation**; Yinjuan Chen[1]; ZhiCheng Zuo[1]; Xinhua Dai[2]; Wenning Wang[1]; Chuanfan Ding[3]; [1]*Fudan University, Shanghai, China;* [2]*National Institute of Metrology, Beijing, China;* [3]*Fudan University, Shanghai, CN*

WP 465 **Fragmentation of Nickel Nitrate Anions**; Daniel Goebbert; *The University of Alabama, Tuscaloosa, AL*

WP 466 **Effects of Solvent Systems and Source Conditions on Protonation Site: The Case of p-Aminobenzoic Acid**; Amanda L Patrick[1]; Nicolas C Polfer[1]; [1]*University of Florida, Gainesville, FL*

WP 467 **How Does Zinc Do It? Transformations of Alcohols by Gas-Phase Zinc Cation Complexes**; Evan Perez[1]; Cassandra Hanley[1]; Theodore A Corcovilos[1]; John K Gibson[2]; Jonathan Martens[3]; Jos Oomens[3, 4]; Michael J. Van Stipdonk[1]; [1]*Duquesne University, Pittsburgh, PA;* [2]*Lawrence Berkeley National Lab, Berkeley, CA;* [3]*Radboud University Nijmegen, Nijmegen, Netherlands;* [4]*University of Amsterdam, Amsterdam, The Netherlands*

WP 468 **Synthesis and Study of Metal Oxide Cores through Sequential Fragmentation of Co(NO3)3−**; Thomas Hester[1]; Daniel J. Goebbert[1]; [1]*The University of Alabama, Tuscaloosa, AL*

WP 469 **Effects of D-amino Acids on the Gas Phase Acidity of Oligopeptides**; Zachary Buen[1]; Jianhua Ren[1]; [1]*University of the Pacific, Stockton, CA*

WP 470 **Fragmentation Mechanisms of Metal-yersiniabactin Complexes by Low-Energy Collision-Induced Dissociation Tandem Mass Spectrometry: An Empirical and Theoretical Study**; Daryl Giblin[1]; Eun-Ik Koh[2]; Jan R Crowley[2]; Michael L Gross[2]; Jeffrey P Henderson[2]; [1]*Washington University in St. Louis, St. Louis, MO;* [2]*Washington University in St. Louis, Saint Louis, MO*

WP 471 **A Study of Diaryl Iodonium Complexes with Crown Ethers in the Gas Phase**; Dmitri Zagorevski[1]; Michael F Aldersley[1]; [1]*Rensselaer Polytechnic Institute, Troy, NY*

WP 472 **Underwater: A Computational Examination of the Gas-phase Basicity Scale Weaker than 700 kJ/mol**; John Bartmess; *University of Tennessee, Knoxville, TN*

WP 473 **Potential Energy Surface of the Gd+ Reaction with O2 Mapped with GIBMS and Theory** ; Maria Demireva[1]; Peter B Armentrout[1]; [1]*Department of Chemistry, University of Utah, Salt Lake City, UT*

WP 474 **The Spider versus the Fly: Cationized Carbohyrdate Gas-phase Fragmentation Chemistry informs Saccharide Sequence Elucidation**; Maha T Abutokaikah[1]; Ashley R. Wagoner[1]; Benjamin J. Bythell[1]; [1]*University of Missouri-St.Louis, St. Louis, MO*

WP 475 **Structure, Thermochemistry, and Reactivity Studies of Gas-Phase Alkali Metal Ion-Coordinated ProLeu and LeuPro**; Yasaman Jami Alahmadi[1]; Travis D Fridgen[2]; [1]*Memorial Univ of NL-Canada, St. John's, NL;* [2]*Memorial University of NL, St. John's, Canada*

WP 476 **Studies of Dihalogen Radical Anion Formation from Maleic Acid-Acene Compounds by Negative Chemical Ionization (NCI) and Time-of-Flight Mass Spectrometry (TOFMS)**; Daryl Giblin[1]; Jonathan P Hopwood[2]; Brittni A Qualizza[2]; Jacob W. Ciszek[2]; M. Paul Chiarelli[2]; Michael L Gross[1]; [1]*Washington University, St Louis, MO;* [2]*Loyola University, Chicago, IL*

WP 477 **Solution pH Can Affect Electrosprayed Metal-Ion Binding Patterns: IRMPD Structures of Metal-Ion/Tripeptide Complexes**; Robert C. Dunbar[1]; Jonathan Martens[2]; Giel Berden[2]; Jos Oomens[3]; [1]*Case Western Reserve Univ, Cleveland, OH;* [2]*Radboud University Nijmegen, Nijmegen, Netherlands;* [3]*Radboud University, Nijmegen, Netherlands*

WP 478 **Prediction of CID/HCD Spectra by First-Principle Molecular Dynamics for Aimed Routine Compound ID**; Michal Raab[1]; Robert Mistrik[2]; [1]*HighChem, Bratislava, Slovakia;* [2]*HighChem, Bratislava, SK*

WP 479 **Unimolecular Dissociation and Structures of Gaseous Self-Assembled [Ca(Uracil)4,5,6]2+ Complexes**; Ruodi Cheng[1]; Travis Fridgen[2]; [1]*Memorial university of NL, St. John's, Canada;* [2]*Memorial University of NL, St. John's, NL*

WP 480 **Ligand Binding Energies and Structural Isomerism Accompanying Phosphine Exchange on the Cationic Gold Clusters**; Marshall Ligare[1]; Jose Ulises Reveles[2]; Grant E Johnson[1]; Erin Baker[1]; Julia Laskin[1]; *[1]Pacific Northwest National Lab, Richland, WA; [2]Virginia Commonwealth University, Richmond, VA*

WP 481 **Metal Ion Adducts of Cysteine and Cysteine-Containing Peptide Radicals: Structure and Reactivity**; Victor Ryzhov[1]; Michael Lesslie[1]; John Lawler[1]; Kai-Chi Justin Lau[2]; Alan C Hopkinson[2]; *[1]Northern Illinois University, DeKalb, IL; [2]York University, Toronto, Canada*

WP 482 **Mass Spectrometric and Computational Investigation of the Protonated Carnosine−Carboplatin Complex Fragmentation**; Ida Ritacco[1]; Emilia Sicilia[1]; Tamer Shoeib[2, 3]; Mohamed Korany[2]; Nino Russo[1]; *[1]Dipartimento di Chimica e Tecnologie Chmiche, Università della Calabria, Calabria, Italy; [2]Department of Chemistry, The American University in Cairo, New Cairo, Egypt; [3]Centre for Analytical Science, Department of Chemistry, Loughborough University, Loughborough, UK*

LC-MS: SAMPLE PREPARATION (PART 1)
483 - 504

WP 483 **Improved Recovery, Reproducibility and Matrix Effects with an Advanced Technology in Solid Phase Extraction (SPE) –Oasis PRiME HLB**; Xin Zhang[1]; Jonathan Danaceau[1]; Erin Chambers[1]; *[1]Waters, Milford, MA*

WP 484 **Comprehensive Analysis of Protein Glycosylation using NGAG Method**; Shisheng Sun[1]; Punit Shah[1]; Shadi Toghi Eshghi[1]; Hui Zhang[1]; *[1]Johns Hopkins University, Baltimore, MD*

WP 485 **Methylmalonic Acid: Evaluation of Sample Preparation and Simplicity of Method Implementation using Automated Sample Preparation Prior to LC-MS/MS Analysis**; Rhys Jones[1]; Helen Lodder[1]; Lee Williams[2]; Geoff Davies[1]; Alan Edgington[1]; Adam Senior[1]; Steve Jordan[1]; Claire Desbrow[1]; Paul Roberts[1]; Victor Vandell[3]; Dan Menasco[3]; *[1]Biotage GB Limited, Cardiff, UK; [2]Biotage GB Limited, Cardiff; [3]Biotage LLC, Charlotte, NC*

WP 486 **Integration of Steroids Analysis in Serum using LC-MS/MS with Full-Automated Sample Preparation**; Toshikazu Minohata[1]; Kawakami Daisuke[1]; *[1]Shimadzu Corporation, Kyoto, Japan*

WP 487 **Determination of Pharmaceuticals in Wastewater using Online SPE Coupled to Liquid Chromatography Mass Spectrometry**; Andreas Bruchmann[1]; Claudia vom Eyser[2]; Thorsten Teutenberg[2]; Jochen Tuerk[2]; *[1]Axel Semrau GmbH & Co.KG, Sprockhoevel; [2]IUTA, Duisburg, Germany*

WP 488 **Applying a Tangential Flow Filtration Approach for Low Concentration Proteomics Sample Preparation**; Woodard Toni[1]; Zhe Wang[1]; Ma Hongyan[1]; Saurav Malla[1]; Si Wu[1]; *[1]University of Oklahoma, Norman, OK*

WP 489 **SPE Method Optimization and Transfer to an Automated Sample Preparation Platform for Low Level Catecholamine Analysis using LC-MS/MS**; Alan Edgington[1]; Adam Senior[1]; Lee Williams[2]; Victor Vandell[3]; Geoff Davies[1]; Helen Lodder[1]; Rhys Jones[1]; Steve Jordan[1]; Claire Desbrow[1]; Paul Roberts[1]; Dan Menasco[3]; *[1]Biotage GB Limited, Cardiff, UK; [2]Biotage GB Limited, Cardiff; [3]Biotage LLC, Charlotte, NC*

WP 490 **Dual Immobilized Enzyme Reactors for Peptide, Glycan, and Glycopeptide online LC-MS/MS Analysis**; Kerry Wooding[1]; Rui Zhu[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX*

WP 491 **Handy Devices for Quantitative Capillary Blood Microsampling**; Shinobu Kudoh[1]; Ippei Takeuchi[2]; *[1]Shimadzu Techno-Research, Inc., Ohta-Ku, Tokyo; [2]Shimadzu Corp, Kyoto, Japan*

WP 492 **Rapid, Efficient and Reproducible Sample Preparation for Quantitative Proteomics by a Surfactant-Aided Precipitation/On-Pellet Digestion Strategy**; Shichen Shen[1]; Bo An[1]; Jun Li[1]; Xiaomeng Shen[1]; Chengjian Tu[1]; Jun Qu[1]; *[1]University at Buffalo, Buffalo, NY*

WP 493 **A Quantitative LC-MS Method to Determine Lutein Levels in Whole Human Blood Using Dried Blood Spot Analysis (DBS)**; Carl Norén[1]; Todime Reddy[1]; Stefan Ehling[1]; *[1]Abbott Nutrition, Columbus, OH*

WP 494 **Fully Automated Evaluation of Dextrorphan Extraction Procedure by DBS In-Tips, analyzed with RTC-LC-MS/MS**; Sylvain R Letarte[1]; SERGE AUGER[2]; Pierre Picard[3]; *[1]Phytronix Instruments, Boisbriand, Canada; [2]Phytronix Technologies, Quebec, QC; [3]Phytronix Technologies, Quebec, Canada*

WP 495 **In-depth Proteomic Quantification of Cell Secretome in Serum-Containing Conditioned Medium**; Yejing Weng[1]; Zhigang Sui[1]; Yichu Shan[1]; Lihua Zhang[1]; Yukui Zhang[1]; *[1]Chinese Academy of Sciences, Dalian, China*

WP 496 **A Multiwell Magnetic Mixer for Automated Sample Preparation**; Chang Liu[1]; Don W Arnold[2]; Thomas R Covey[1]; *[1]SCIEX, Concord, ON; [2]SCIEX, Redwood City, CA*

WP 497 **Quantitative Analysis of low-Abundance Serological Proteins with Peptide Affinity-Based Enrichment and Pseudo-Multiple Reaction Monitoring by Hybrid Quadrupole Time-Of-Flight Mass Spectrometry**; Kwang Hoe Kim[1, 2]; Yeong Hee Ahn[3]; Eun Sun Ji[1]; Ju Yeon Lee[1]; Jin Young Kim[1]; Hyun Joo An[2]; Jong Shin Yoo[1, 2]; *[1]Korea Basic Science Institute, Chungbuk, South Korea; [2]Chungnam National University, Daejeon, South Korea; [3]Cheongju University, Cheongju, South Korea*

WP 498 **Advancing the MStern Blotting – PVDF Membrane-Based Peptide Fractionation in a 96 Well Format**; Sebastian Berger[1, 2]; Saima Ahmed[3]; Michaela Helmel[3]; Hanno Steen[3]; *[1]Boston Children's Hospital, Boston, MA; [2]Harvard Medical School, Boston, MA; [3]Boston Children's Hospital, Harvard Medical School Boston, MA*

WP 499 **Quantification of Celecoxib in Rat Skin using LC-MS/MS Method after Collagenase Digestion and Bead Lysis**; Raghupathi Aleti[1]; Ilayaraja Kalaikadhiban[1]; Sailakshmi Chennupati[1]; Devender Reddy Ajjala[1]; Ramakrishna Nirogi[1]; *[1]Suven Life Sciences Ltd, Hyderabad, Telangana*

WP 500 **Basic Reverse Phase Fractionation on OasisHLB-uElution Plates as a Fast Sample Preparation Technique for LCMSMS Analysis of Low Protein Amounts**; Robert N O'Meally[1]; Tatiana N. Boronina [1]; Maximilian Konig[1]; Felipe Andrade[1]; Robert N Cole[1]; *[1]Johns Hopkins University School of Medicine, Baltimore, MD*

WP 501 **LC/MS/MS Analysis with On-line Cartridge for Removal of Phospholipids from Protein Precipitation Biological Fluid Samples**; David S. Bell[1]; Xiaoning Lu[1]; Hillel K. Brandes[1]; Craig R Aurand[1]; Sara Smith[1]; Carmen T. Santasania[1]; *[1]MilliporeSigma, Bellefonte, PA*

WP 502 **Different Approach for Improvement of Low Recovery Dried Blood Spot Storage Sample and Its Application in Bioanalytical Assay**; Dawei Zhou[1]; John Ma[1]; Mohamed Osman[1]; Xinping Fang[1]; *[1]WuXi AppTec Co., Plainsboro, NJ*

WP 503 **Simultaneous Quantitation of Five Leachables in Lipid Emulsions by LC-MS/MS Using 2,2-Dimethoxypropane**; Yousheng Hua[1]; Jim Story[1]; Peifeng Hu[1]; Dennis Jenke[1]; Christopher M Jones[1]; *[1]Baxter Healthcare, Round Lake, IL*

WP 504 **A Conventional Procedure to Reduce Asn Deamidation Artifacts during Trypsin Peptide Mapping**; Yekaterina Kori[1, 2]; Rekha Patel[2]; Alyssa Neill[2]; Hongcheng Liu[2]; *[1]University of Massachusetts Amherst, Amherst, MA; [2]Alexion Pharmaceuticals, Cheshire, CT*

LIPIDS: PROFILE ANALYSIS
505 - 536

WP 505 **Optimization of Female Sex Hormone Extraction for Semi-Quantitative Analysis in Human Plasma by UHPLC/MS/MS**; Juan Aristizabal Henao[1]; Richard W Smith[1]; Ken D Stark[1]; *[1]University of Waterloo, Waterloo ON, Canada*

WP 506 **Lipidomic Profiling of Biological Samples using Off-Line Two-Dimensional High-Performance Liquid Chromatography-High Resolution Mass Spectrometry**; Monica Narvaez-Rivas[1]; Qibin Zhang[2]; *[1]University of North Carolina at Greensboro, Kannapolis, NC; [2]University of North Carolina Greensboro, Greensboro, NC*

WP 507 **UHPLC Combined with Ultra-high Resolution QTOF-MS for Rapid Lipidomic Profiling of Serum for Discovery of Lipid Biomarkers of Parkinson's Disease**; Jaspaul Tatlay[1]; Dorothea Mung[1]; Richard Camicioli[2]; Liang Li[1]; *[1]University of Alberta, Edmonton, Canada; [2]Neuroscience and Mental Health Institute, Department of Medicine, Edmonton, AB, Canada*

WP 508 **Environmental Lipidomics: Examining the Case of Pansteatitis in Mozambique Tilapia**; John Bowden[1]; Jeremy Koelmel[2]; Stephen E Somerville[3]; Timothy J Garrett[2]; Richard A Yost[2]; Robert Chapman[4]; Louis Guillette[3]; *[1]NIST, Charleston, SC; [2]University of Florida, Gainesville, FL; [3]Medical University of South Carolina, Charleston, SC; [4]South Carolina Department of Natural Resources, Charleston, SC*

WP 509 **Comprehensive Lipid and Protein Analysis of Size Fractionated Serum Lipoproteins in Normal versus Dyslipidemic Subjects**; Michael Gardner[1]; Zsuzsanna Kuklenyik[1]; David M Schieltz[1]; Bryan A Parks[1]; Jon Rees[1]; Lisa G McWilliams[1]; Yulanda Williamson[1]; Christopher Toth[1]; Jeffrey Jones[1]; Michael Andrews[1]; John R Barr[1]; *[1]Centers for Disease Control and Prevention, Atlanta, GA*

WP 510 **Reverse Phase LC–ESI-QTOF Methodology for the Analysis of Lipids in Whole Blood**; Ralph Hindle[1]; Ken D Stark[2]; Juan J Aristizabal Henao[2]; Richard W Smith[3]; Sheher Mohsin[4]; *[1]Vogon Laboratory Services, Alberta, Cochrane, Canada; [2]Department of Kinesiology, University of Waterloo, Waterloo ON, Canada; [3]University of Waterloo Mass Spectrometry Facility, University of Waterloo, Waterloo ON, Canada; [4]Agilent Technologies, Schaumburg, IL*

WP 511 **The Application of Lipidomics to the Study of Hepatocellular Carcinoma (HCC) Induced by Low Dose, High-Energy, High Charge Ions (HZE)**; Brooke L Barnette[1]; Shinji K Strain[1]; Cheryl F Lichti[1]; Yu Yongjia[1]; Robert Ullrich[1]; Mark R Emmett[1]; *[1]University of Texas Medical Branch at Galveston, Galveston, TX*

WP 512 **Analysis of Lipids in Spinal Cords of Experimental Autoimmune Encephalomyelitis (EAE) Mice using On-Line Photochemical Derivatization and Tandem Mass Spectrometry**; Leelyn Chong[1]; Xiaoxiao Ma[1]; Yu Xia[1]; Zheng Ouyang[1]; *[1]Purdue University, West Lafayette, IN*

WP 513 **Lipid Peroxidation Profiles in Acute Hepatic Ischaemia-Reperfusion Injury**; Michael Dunn[1]; Aimen Amer[2]; Margaret Knight[1]; Clair Roper[1]; Peter Blain[1]; Matthew Wright[2]; *[1]Medical Toxicology Centre, Newcastle University, Newcastle upon Tyne, UK; [2]Institute of Cellular Medicine, Newcastle University, Newcastle upon Tyne, UK*

WP 514 **The Comparison of Glycosphingolipids in an Epithelial Ovarian Cancer Cell Line and a Nontumorigenic Epithelial Ovarian Cell Line using MALDI-MS**; Krishani Kumari Rajanayake[1]; William Taylor[1]; Dragan Isailovic[1]; *[1]The University of Toledo, Toledo, OH*

WP 515 **Fatty Acid Re-Esterification in Adipose Tissue - Beneficial Futile Metabolite Cycling**; Ondrej Kuda[1]; Martina Rombaldova[1]; Jan Kopecky[1]; *[1]Institute of Physiology, CAS, Prague, Czech Republic*

WP 516 **Analysis of Phospholipids, Lipid A and Sterols from Outer Membrane Vesicles Shed by Acinetobacter baumanniiDU202**; Geul Bang[1]; Semin Park[1]; Sung-Ho Yun[2]; Seung Il Kim[2]; Man Ho Choi[3]; Yun-Gon Kim[4]; Young Hwan Kim[1]; *[1]Korea Basic Science Institute, Cheongju, Korea; [2]Korea Basic Science Institute, Daejeon, Korea; [3]Korea Institute of Science and Technology, Seoul, Korea; [4]Soongsil University, Seoul, Korea*

WP 517 **Differing Effects of Red-tide Exposure on the Lipidome of Phytoplankton Competitors**; Scott Hogan[1]; Remington Poulin[1]; Julia Kubanek[1]; Facundo M Fernandez[1]; *[1]Georgia Institute of Technology, Atlanta, GA*

WP 518 **Fusarium oxysporum f. spcubense Aggressiveness Investigated by MALDI-TOF-MS Lipid Profile**; Daniele F. O. Rocha[1]; Cristiane M. S. Cunha[2]; Katia R. A. Belaz[1]; Fabio N. dos Santos[1]; Robert H. Hinz[3]; Adriana Pereira[3]; Alexandre Visconti[3]; Ester Wicket[3]; Lidiane Maria de Andrade[4]; Claudio A. O. Nascimento[4]; Nogueira Marcos Eberlin[1]; *[1]Thomson Mass Spectrometry Laboratory-UNICAMP, Campinas, Brazil; [2]Flora Biotecnologia Ltda, Itajaí, Brazil; [3]Empresa de Pesquisa Agropecuária e Extensão Rural de Santa Catarina- EPAGRI, Itajaí, Brazil; [4]Chemical Engineering Department of Polytechnic School of University of São Paulo, São Paulo, Brazil*

WP 519 **Direct Analysis of Phospholipids in Biological Tissues Using Internal Extractive Electrospray Ionization Mass Spectrometry**; Haiyan Lu[1]; Jianyong Zhang[2]; Wei Zhou[3]; Yiping Wei[2]; Huanwen Chen[4]; *[1]East china university of Technology, Nanchang, China; [2]Second Affiliated Hospital of Nanchang University, Nanchang, China; [3]East China Institute of Technology, Nanchang, China; [4]East China University of Technology, Nanchang, Mainland*

WP 520 **Ambient Ionization Methods and Liquid Chromatography – Mass Spectrometry Analysis of Human Melanoma Biopsies**; Louis Searcy[1]; Candice Ulmer[2]; Matthew Kazaleh[2]; Michael Costanzo[2]; Nikolaus Gravenstein[2]; Richard A. Yost[2]; *[1]University of Florida, Gainesville, FL; [2]University of Florida, Gainesville, FL*

WP 521 ***In-situ* and *in-vitro* Regional Analysis of Lipids in Mammalian Vitreous Humor using MALDI-MS**; Abby Schnepf[1]; M. Cecilia Yappert[2]; Douglas Borchman[3]; *[1]Department of Chemistry, University of Louisville, Louisville, KY; [2]Department of Chemistry University of Louisville, Louisville, KY; [3]Department of Ophthalmology and Visual Sciences University of Louisville, Louisville, KY*

WP 522 **Tissue Identification by Rapid Evaporative Ionization Mass Spectrometry (REIMS) Based on Fragmentation Profile of Glycerophospholipids**; Richard Schäffer[1]; Tamas Juhasz[1]; Tamas Karancsi[1]; Steven D Pringle[2]; Zoltan Takats[3]; Julia Balog[1, 3]; *[1]Waters Research Center, Budapest, Hungary; [2]Waters, Wilmslow, UK; [3]Imperial College, London, UK*

WP 523 **Detection of Altered Brain Lipids by LC-MS and Imaging Mass Spectrometry in Demyelinating, Remyelinating and Dysmyelinating Mouse Models**; Xiaoping L. Hronowski[1]; Raj Maganti[1]; Brian T Wipke[1]; Robert Dunstan[1]; Peter Juhasz[1]; *[1]Biogen Inc., Cambridge, MA*

WP 524 **A General Normal Phase HPLC Separation Hyphenated with HR/AM – Tandem Mass Spectrometric Method for Whole Lipidomics Profiling**; Qifeng Zhang[1]; Michael J.O. Wakelam[1]; *[1]Babraham Institute, Cambridge, UK*

WP 525 **Comprehensive Profiling of Lipids in Chicken Skin by High Resolution Mass Spectrometry with Online Information Dependent Acquisition Workflow**; Yushi Pan[1]; Kevin zhang[2]; Huaidong Yu[3]; Yong Fang[4]; *[1]Pan YS, Nanjing, China; [2], Beijing, Beijing; [3]Yu HD, Beijing, China; [4]Fang Y, Nanjing, China*

WP 526 **Phospholipid Profiling by Two Distinct MRM Measurements to Identify Phospholipid's Class and Fatty Acid Composition**; Tsuyoshi Nakanishi[1]; Masaki Yamada[1]; Suzumi Tokuoka[2]; Yoshihiro Kita[2]; Takao Shimizu[2, 3]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]The University of Tokyo, Tokyo, Japan; [3]National Center for Global Health and Medicine, Tokyo, Japan*

WP 527 **Lipid Profiling of Madin-Darby Canine Kidney Cells and Its Lipid Changes Induced by Aristolochic Acid(I) using Two-Dimensional LC-MS**; Honggang Nie[1]; Liu Ranran[1]; Yang Youyou[2]; Liu Huwei[1]; Bai Yu[1]; *[1]Peking University, Beijing, China; [2]Chinese Oil & Foodstuffs Corporation (COFCO) Nutrition and Health Research Institute, Beijing, China*

WP 528 **High-Throughput Lipidomics Workflow for Identification and Quantification of >1000 Lipids in 13 Different Lipid Classes**; Richard John Robinson[1]; Fred Hubbard[1]; Philip Michael Charpia[1]; Alexandria Conner[1]; Anne Evans[2]; Luke Miller[1]; Steve Watkins[1]; Don Harvan[1]; *[1]Metabolon, Inc., Durham, NC; [2]Metabolon, Inc., Durham, NC*

WP 529 **Lipidomic Analysis of Cultured Cells Lines**; Finnur Freyr Eiriksson[1, 2]; Manuela Magnusdottir[2]; Halldorsson Skarpheðinn[2]; Ottar Rolfsson[2]; Helga M. Ogmundsdottir[2]; Margrét Thorsteinsdottir[1, 2]; *[1]ArcticMass, Reykjavik, Iceland; [2]University of Iceland, Reykjavik, Iceland*

WP 530 **Profiling Lipids in Plants Using Infusion and Chromatography Based High Resolution Mass Spectrometry Methods with Automated Data Processing**; Yelena A. Adelfinskaya[1]; Daniel J J Gachotte[1]; Jeffrey R Gilbert[1]; Jesse L Balcer[1]; Laura L Wayne[1]; *[1]Dow AgroSciences, Indianapolis, IN*

WP 531 **Lipid and Fatty Acid Analysis in Grape Seeds and Grape Seed Oil with High Resolution Mass Spectrometry**; Zareen Khan[1]; Akanksha Singh[2]; Ahammed Shabeer T.P.[1]; Manoj Pillai[3]; Kaushik Banerjee[1]; *[1]National Referral Laboratory, ICAR-National Research Centre for Grapes, Pune, Maharashtra, India; [2]SCIEX, Gurgaon, Haryana; [3]SCIEX, Gurgaon, Haryana India*

WP 532 **Methods to Analyze Beneath the Surface of Oil Seeds using Mass Spectrometry**; Suresh Annangudi[1]; Holly Henderson[2]; Callee Walsh[2]; Trust T Razunguzwa[2]; Jeffrey R Gilbert[1]; *[1]Dow AgroSciences, Indianapolis, IN; [2]Protea Biosciences, Inc. Morgantown, WV*

WP 533 **Accelerating Lipid Profiling Acquisition Strategies using Differential Mobility Spectrometry and SWATH® Data Collection**; Eva Duchoslav[1]; Brad T Patterson[2]; Larry J Campbell[1]; Yves J C LeBlanc[1]; *[1]SCIEX, Concord ON, Canada; [2]SCIEX, Melbourne VIC, Australia*

WP 534 **A Simple, Flexible, and Automated Infusion System for Lipidomic Analysis using Mass Spectrometry**; Jeff McDonald[1]; Steve Stiller[2]; *[1]UT Southwestern Medical Center, Dallas, TX; [2]LEAP Technologies, Carrboro, NC*

WP 535 **The Rapid Evaporative Ionisation Mass Spectrometry (REIMS) iKnife Identifies Gynaecological Tissue with Excellent Accuracy in the *ex-vivo* and *in-vivo* Setting**; David L Phelps[1]; Julia Balog[1, 2]; Louise Gildea[1]; Mona El-Bahrawy[1]; Abigail Speller[1]; Robert Brown[1]; Sadaf Ghaem-Maghami[1]; Zoltan Takats[3]; *[1]Imperial College, London, UK; [2]Waters Corporation, Budapest, Hungary; [3]Imperial College London, South Kensington Campus London, UK*

WP 536 **REIMS has the Potential to Improve Diagnostic of Hepatocellular Carcinoma Liver – Perspectives towards Intraoperative Molecular Diagnostics**; Tiffany Porta[1]; Julia Balog[2]; Flora Olivier[1]; Pierre-Maxence Vaysse[1]; Ulf P. Neumann[3]; Steven W.M. Olde Damink[4]; Thorsten Cramer[3]; Ron M.A. Heeren[1]; *[1]M4I Institute - Maastricht University, Maastricht, The Netherlands; [2]Waters Corporation, Wilmslow, UK; [3]RWTH Aachen, Aachen, Germany; [4]Maastricht University Medical Center +, Maastricht, The Netherlands*

METABOLOMICS: CLINICAL APPLICATIONS
537 - 549

WP 537 **Identifying "Sweet-spots" of Preeclamptic Urine Metabolomics with High Resolution and Accurate Mass Measurements**; Hongwu Jing[1]; Yu Cao[1]; Arpad Somogyi[1]; Guomao Zhao[2]; Michelle Axe[2]; Catalin S Buhimschi[1]; Irina A Buhimschi[2]; Vicki H Wysocki[1]; *[1]The Ohio State University, Columbus, OH; [2]Nationwide Children's Hospital, Columbus, OH*

WP 538 **Integrative Pathway Analysis of Metabolic Signature in Bladder Cancer: A Linkage to Cancer Genome Atlas Project and Prediction of Survival**; Nagireddy Putluri; *Baylor College of Medicine, Houston, TX*

WP 539 **Development of Highly Sensitive Quantification Method for Testosterone Human Serum by Liquid Chromatography–Tandem Mass Spectrometry**; Vasanta Putluri[1]; Sriramya Donepudi[1]; Feng Jin[1]; Andre Szczesniewski[2]; Vadiraja B Bhat[2]; J Peter Cook[1]; Dolores J Lamb[1]; Arun Sreekumar[1]; Nagireddy Putluri[1]; *[1]Baylor College of Medicine, Houston, TX; [2]Agilent Technologies, Wilmington, DE*

WP 540 **Targeted Metabolomics of Liver Donor Allografts: A Clinical Application**; Jeffrey A Culver[1, 2]; Andrew V Zelenin[1, 2]; Christopher Petucci[1, 2]; Stephen J Gardell[1, 2]; John B Seal[3]; *[1]Sanford Burnham Prebys Medical Discovery Institute, Orlando, FL; [2]Southeast Center For Integrated Metabolomics, Gainesville, FL; [3]Ochsner Medical Center, New Orleans, LA*

WP 541 **Metabolomics and Flux Analysis Informed on the Mechanism of Response of AML to IACS-10759, a Potent and Selective OXPHOS Inhibitor**; Pietro Morlacchi; *UT MD Anderson Cancer Center (IACS/CCCT), Houston, TX*

WP 542 **Use of a Novel C18-Based Stationary Phase for Human Urine Metabolite Profiling By UHPLC-High Resolution Accurate Mass Spectrometry (HRAM);** Alan P McKeown[1]; Catherine Ortori[2]; Geoffrey Faden[3]; *[1]Advanced Chromatography Technologies Ltd, Aberdeen; [2]The School of Pharmacy, University of Nottingham, Nottingham, UK; [3]MACMOD Analytical Inc., Chadds Ford, PA*

WP 543 **Discriminatory Ability of Ambient Ionisation Mass Spectrometry in Analysing Skin Secretions: A Non-Invasive Diagnostic Test of Lower Airway Infection?**; Emmanuelle Bardin[1]; Frances Bolt[1]; Eric Alton[1, 2]; Andrew Bush[1, 2]; Jane Davies[1, 2]; Zoltan Takats[1]; *[1]Imperial College London, South Kensington Campus London, UK; [2]Royal Brompton and Harefield NHS Foundation Trust, London, UK*

WP 544 **Comprehensive Cerebrospinal Fluid Metabolomic Profiling for Mechanism Study of Idiopathic Intracranial Hypertension**; Liang Zhao[1]; Xiali Zhong[1]; Abhay Moghekar[1]; Thomas Hartung[1]; *[1]Johns Hopkins University, Baltimore, MD*

WP 545 **Isotope-based Metabolomic Analysis of Human Samples**; Kevin Y Cho[1]; Ying-Jr Amanda Chen[1]; Nathaniel G Mahieu[1]; Gary Patti[1]; *[1]Washington University School of Medicine, St. Louis, MO*

WP 546 **Integrative Metabolomic and Proteomic Analysis Reveals Biomarkers Related to Oxidative Stress in Traumatic Brain Injury**; Veera Venkata Ratnam Bandaru[1]; Sartaj Ahmad Mir[1]; Frederick Korley[1]; Robert D Stevens[1]; Akhilesh Pandey[1]; *[1]Johns Hopkins University School of Medicine, Baltimore, MD*

WP 547 **Bioaccessible Phytochemicals from Black Raspberries after Interaction with Saliva – Determining Exposure in the Oral Cavity Using a Metabolomics Approach**; Ken M Riedl[1]; Jennifer Ahn-Jarvis[1]; Matthew Teegarden[1]; Thomas Knobloch[1]; Christopher Weghorst[1]; Purnima Kumar[1]; Steven Clinton[1]; Yael Vodovotz[1]; Steven J Schwartz[1]; *[1]The Ohio State University, Columbus, OH*

WP 548 **Studying Individual Differences in Cancer Drug Efficacy using Metabolomics of a Panel of Human Cell Lines**; Thomas Hankemeier[1]; Liewei Wang[2]; Ruud Berger[3]; Amy Harms[3]; Slavik Koval[3]; Sabine Bos[3]; Silvia Marin[4]; Marta Cascante[4]; Dick Weinshilboum[5]; Rima Kaddurah-Daouk[6]; *[1]Leiden University, Leiden, South Holland; [2]Clinical Pharmacology, Mayo Clinic, Rochester, MN; [3]Leiden University, Leiden, Netherlands; [4]University of Barcelona (UB); [5]Mayo Clinic, Rochester, MN; [6]Duke University Medical Center, Durham, NC*

WP 549 **Lipidomic Analysis of Endometriosis Foci by Direct Tissue-Spray Mass Spectrometry**; Vitaliy Chagovets[1]; Zhihao Wang[2]; Anna Borisova[1]; Vadim Lagutin[1]; Natalia Starodubtseva[1]; Andrey Kozachenko[1]; Konstantin Chingin[2]; Chen Huanwen[2]; Leila V Adamyan[1]; Vladimir Frankevich[1]; Gennady Sukhikh[1]; *[1]Research Center for Obstetrics, Gynecology and Perinatology of the Ministry of Healthcare of the Russian Federation, Moscow; [2]Jiangxi Key Laboratory for Mass Spectrometry and Instrumentation, East China University of Technology, Nanchang, China*

METABOLOMICS: UNTARGETED METABOLITE PROFILING (ANIMAL/HUMAN/OTHER)
550 - 574

WP 550 **Drosophila as a Model System for Microbiome Research - a GCMS Based Metabolomics Approach**; Bhavapriya Vaitheesvaran[1]; John McMullen[2]; Anthony Macherone[3]; Angela E Douglas[2]; Justin R Cross[1]; *[1]Memorial Sloan Kettering Cancer Center, New York, NY; [2]Cornell University, Ithaca, NY; [3]Agilent Technologies, Little Falls, DE*

WP 551 **Lipidome and Metabolome Analyses of Mouse Hippocampus in Response to Low-dose X-ray Irradiation using Liquid Chromatography-Mass Spectrometry**; Fereshteh Zandkarimi[1]; Jeffrey Morré[1]; Jacob Raber[2]; Claudia S Maier[1]; *[1]Oregon State University, Department of Chemistry Corvallis, OR; [2]OHSU, Dep. Behavioral Neuroscience, Neurology, & Radiation Medicine, ONPRC, Portland, OR*

WP 552 **Comparative High Resolution Metabolomics of Metastatic vs. Non-Metastatic Tumors in a Murine Medulloblastoma Model**; Danning Huang[1]; Martin R L Paine[1]; Jingbo Liu[2]; Sophia Banton[2]; Shuzhao Li[2]; Tobey MacDonald[2]; Facundo M Fernández[1]; *[1]Georgia Institute of Technology, Atlanta, GA; [2]Emory University School of Medicine, Atlanta, GA*

WP 553 **Caloric Restriction Improves Diabetes-Induced Nonalcoholic Fatty Liver Diseases by Changing Metabolism**; Youngae Jung[1]; Geum-Sook Hwang[1, 2]; *[1]Western Seoul Center, Korea Basic Science Institute, Seoul, Republic of Korea; [2]Department of Life Science, Ewha Womans University, Seoul, Republic of Korea*

WP 554 **Comprehensive HPLC-MS Metabolomics Analysis of Brain Tissue Reveals Age, Region, and Gender-Specific Effects of *Centella asiatica***; Parnian Lak[1]; Nora Gray[2]; Luisa Zini[3]; Phillip Seitzer[3]; Christopher Harris[2]; Joseph Quinn[2, 4, 5]; Amala Soumyanath[2]; Jan Fred Stevens[1]; Claudia Maier[1]; *[1]Oregon State University, Corvallis, OR; [2]Oregon Health and Sciences University, Portland, OR; [3]Proteome Software, Portland, OR; [4]PADRECC, Portland, OR; [5]Portland Veterans Affairs Medical Center, Portland, OR*

WP 555 **Global Lipid Profiling in Aging Mouse Model associated with Osteoporosis**; Eun-ha Kim[1]; Geum-Sook Hwang[1]; *[1]KBSI Western Seoul Center, Seoul, Republic of Korea*

WP 556 **Metabolomics Approach for Mice Serum Associated with Epidermal Growth Factor Receptorand BaP-induced Mouse Lung Tumor Genesis using Liquid Chroma**; Hui Ling Lee; *Fu Jen Catholic University, New Taipei, TAIWAN*

WP 557 **Global Metabolomic Profile Differentially Segregates with Calcium Supplementation in Mice Fed a High-Fat Western Style Diet**; Muhammad Aslam[1]; Li Zhang[2]; Christine Bassis[1]; Maureen Kachman[2]; Charles Burant[2]; Ingrid Bergin[3]; James Varani[1]; *[1]Department of Pathology, Internal Medicine, Medical of School, University of Michigan, Ann Arbor, MI; [2]Michigan Regional Comprehensive Metabolomics Resource Center; University of Michigan, Ann Arbor, MI; [3]Unit for Laboratory Animal Medicine, University of Michigan, Ann Arbor, MI*

WP 558 **LC-MS/MS Based Metabolomic Analysis of the Effect of Biogenic Amine in a LPS-induced Sepsis Mouse Model**; Yu-Min Liu[1]; Soo-Ray Wang[2]; Maw-Rong Lee[1]; *[1]National Chung-Hsing University, Taichung, Taiwan (R.O.C.); [2]Chung Shan Medical University, Taichung, Taiwan (R.O.C.)*

WP 559 **Diabetes Markers: Using Orbitrap HRAM and a New Workflow for Differential Analysis of Zucker Rat Plasma Metabolome**; Junhua Wang[1]; Maciej P Bromirski[2]; Ralf Tautenhahn[3]; David Peake[4]; Kiyonami Reiko[4]; Tina Settineri[4]; Ken Miller[4]; *[1]Thermo Fisher Scientific Inc, San Jose, CA; [2]Thermo Fisher Scientific, Bremen, DE; [3]Thermo Fisher Scientific, San Jose, CA; [4]ThermoFisher, San Jose, CA*

WP 560 **Effects of Dietary Different Doses of Copper and High Fructose Feeding on Rat Fecal Metabolome**; Biyun Shi[1, 2]; Ming Song[3]; Xiaoli Wei[1, 2]; Xinmin Yin[1, 2]; Dale Schuschke[4]; Imhoi Koo[1, 2]; Craig McClain[3, 5]; Xiang Zhang[1,2,5]; *[1]Department of Chemistry, University of Louisville, Louisville, KY; [2]Center for Regulatory and Environmental Analytical Metabolomics, University of Louisville, Louisville, KY; [3]Department of Medicine, University of Louisville, Louisville, KY; [4]Department of Physiology and Biophysics, University of Louisville, Louisville, KY; [5]Department of Pharmacology and Toxicology, University of Louisville, Louisville, KY*

WP 561 **Optimization of Tissue Extraction for GCMS Metabolomic Analysis Reveals Altered Metabolism of Barbiturates in a Polycystic Kidney Disease Model**; Hayley Abbiss[1, 2, 3]; Garth L. Maker[3, 4, 5]; Gabrielle C. Musk[4, 6]; Catherine Rawlinson[3, 4, 5, 7]; Joel P.A. Gummer[3, 4]; Patricia A. Fleming[4]; Jacqueline K. Phillips[8]; Mary C. Boyce[9]; John Moncur[2]; Robert D. Trengove[3, 4, 5]; *[1]Murdoch University, Perth, Western Australia; [2]SpectralWorks, Cheshire, UK; [3]Separation Science and Metabolomics Laboratory, Perth, Australia; [4]Murdoch University, Perth, Australia; [5]Metabolomics Australia, Western Australian Node, Perth, Australia; [6]The University of Western Australia, Perth, Australia; [7]Curtin University, Perth, Australia; [8]Macquarie University, Sydney, Australia; [9]Edith Cowan University, Perth, Australia*

WP 562 **Spatial -temporal Analysis of Metabolite Expression in Xenopus laevisembryos during Early Development.**; Jennifer Arceo[1]; Nicole M Schiavone[2]; Danielle A Boley[2]; Norman J Dovichi[2]; *[1]University of Notre Dame, Notre Dame, IN; [2]University of Notre Dame, Notre Dame, IN*

WP 563 **Capillary Zone Electrophoresis-Electrospray Ionization-Mass Spectrometry for Xenopus laevismetabolomic Analysis**; Nicole Schiavone[1]; Jennifer Arceo[1]; Danielle A Boley[1]; Norman J Dovichi[1]; *[1]University of Notre Dame, Notre Dame, IN*

WP 564 **Evaluating the Metabolic Impact of Feeding Baboons a High Fat, High Caloric Diet using an Accurate Mass GC/QTOF**; Mark Libardoni[1]; Matthew Curtis[2]; Stephan Baumann[2]; *[1]Southwest Research Institute, San Antonio, TX; [2]Agilent Technologies, Santa Clara, CA*

WP 565 **Profiling and Quantitative Analysis of Small Molecule Metabolites and Neurotransmitters in Crustacean Hemolymph/Neuronal Tissues Using Reversed-Phase and Mix-Mode LC-MS/MS**; Qinjingwen Cao[1]; Chuanzi OuYang[1]; Xuefei Zhong[2]; Lingjun Li[1, 2]; *[1]University of*

Wisconsin-Madison, Madison, WI; [2]School of Pharmacy, University of Wisconsin-Madison, Madison, WI

WP 566 **An Untargeted Metabolomics Approach for Determining Biomarkers Involved in Spontaneous Pre-Term Birth (sp-PTB) Delivery, using a Label-Free LC-DIA-MS Approach**; Shirish Yakkundi[1]; Lee Gethings[2]; James Langridge[2]; Louise Kenny[3, 4]; *[1]Cork University Maternity Hospital, Cork; [2]Waters, Wilmslow, UK; [3]Cork University Maternity Hospital, Cork, Ireland; [4]University College Cork, Cork, Ireland*

WP 567 **Global Metabolomics and Lipidomics of Non-Alcoholic Fatty Liver Disease and Non-Alcoholic Steatohepatitis in Human Plasma by LC-HRMS**; Allison J Levy[1]; Rainey E Patterson[1]; Jeremy P Koelmel[1]; Srilaxmi Kalavalapalli[2]; Nishanth Sunny[2]; Fernando Brill[2]; Kenneth Cusi[2]; Timothy J Garrett[3]; Richard A Yost[1, 3]; *[1]Chemistry Department, University of Florida, Gainesville, FL; [2]Department of Medicine, University of Florida, Gainesville, FL; [3]Department of Pathology, Immunology, and Laboratory Medicine, University of Florida, Gainesville, FL*

WP 568 **Comparative Evaluation of Open Access Software used in Liquid Chromatography-Mass Spectrometry Based Untargeted Metabolomics**; Stephanie Samra[1]; Benjamin Wancewicz[1]; Brian DeFelice[1]; Oliver Fiehn[1]; *[1]UC Davis, Davis, CA*

WP 569 **IMS-DIA-MS Characterisation and IMS-MRM QconCAT Quantitation of the Lipidome and Apolipoprotein Complements of Obesity and Diabetes Cohorts**; Lee A Gethings[1]; Johannes PC Vissers[1]; Jose Castro-Perez[2]; Yvonne Woolerton[3]; Lynn McLean[3]; Robert Beynon[3]; James I Langridge[1]; *[1]Waters, Wilmslow, UK; [2]Waters Corp., Milford, MA; [3]Centre for Proteome Research, Institute of Integrative Biology, University of Liverpool, Liverpool, UK*

WP 570 **Evaluation of Ion Mobility/ TOF Mass Spectrometry with Multiple LC Method Parameters for Enhanced Detectionin Metabolic Profiling**; Paul Rainville[1]; David Heywood[1]; Langridge James[2]; Robert Plumb[1]; Jose Castro-Perez[1]; *[1]Waters, Milford, MA; [2]Waters, Manchester, UK*

WP 571 **Profiling the Gut Microbiota Metabolome using HPLC coupled to Ion Mobility-Mass Spectrometry to Study Obesity**; James Poland[1]; Alexandra C Schrimpe-Rutledge[1]; Charles Robb Flynn[2]; John A McLean[1]; *[1]Vanderbilt Dept. of Chemistry, Nashville, TN; [2]Vanderbilt University, Nashville TN USA Nashville, TN*

WP 572 **Identification of Eicosanoids Mediating Thromboresistance using an Untargeted Metabolomics and Informatics Approach**; Patrizia B Stadler[1]; Shunyan Mo[1]; Phillip Seitzer[2]; Christopher M Colangelo[3]; Jeffrey J Rade[1]; Scott A Shaffer[1]; *[1]University of Massachusetts Medical School, Worcester, MA; [2]Proteome Software, Portland, OR; [3]Primary Ion, Old Lyme, CT*

WP 573 **Untargeted Profiling using GC-QTOF MS and Parallel EI and CI analysis to Identify Biomarker Panels to Stratify Patients for Treatment**; Robert Trengove[1, 2, 3]; Tom Dignan[2, 4]; Ben Hunter[2, 4]; Garth Maker[2, 4]; Hayley Abbiss[2, 4]; Joel Gummer[2, 3, 4]; *[1]Murdoch University, Murdoch , WA; [2]Separation Science and Metabolomics Laboratory, Perth, Australia; [3]Metabolomics Australia, WA Node, Murdoch, Australia; [4]1School of Veterinary and Life Sciences, Murdoch University, Murdoch, Australia*

WP 574 **Metabolomic Analysis of Melanoma Skin Tissues by Liquid Chromatography – Mass Spectrometry**; Matthew Kazaleh[1]; Candice Ulmer[1]; Louis Searcy[1]; Michael Costanzo[1]; Nikolaus Gravenstein[1]; Richard A Yost[1]; *[1]University of Florida, Gainesville, FL*

NANOSCALE AND MICROFLUIDIC SEPARATIONS AND MS
575 - 586

WP 575 **Segmented Flow Sampling with Push-Pull Theta Pipettes for Electrospray Ionization Mass Spectrometry**; Anumita Saha-Shah[1]; Curtis M Green[1]; David H Abraham[1]; Lane A Baker[1]; *[1]Indiana University Dept. Chemistry, Bloomington, IN*

WP 576 **Development of a Microfluidic Platform for High Throughput Validation of Candidate Disease Biomarkers**; I-Hsuan Chen[1]; Ning Bao[2]; Weiguo Andy Tao[1]; *[1]Purdue University, West Lafayette, IN; [2]Nantong University, Nantong, China*

WP 577 **Ionic Liquid Matrices for MALDI Analysis and CE Separation**; Leila Josefsson[1]; Johan Jacksen[1]; Åsa Emmer[1]; *[1]KTH Royal Institute of Technology, Stockholm, Sweden*

WP 578 **Sensitivity Gains using Microflow LC/MS for Oligonucleotide Analysis**; Michael Donegan[1]; James P Murphy[1]; *[1]Waters, Milford, MA*

WP 579 **Study of Ionization Efficiency on Silicon-Based, Micro-Fabricated Electrospray Nozzles for Micro Flow LC-ESI-MS appLications**; Christine Wang[1]; Simon J Prosser[1]; Jamey Jones[1]; Daniel Eikel[1]; *[1]Advion, Inc. Ithaca, NY*

WP 580 **Decreasing Cycle Time While Maintaining Analytical Sensitivity in Microflow LC/MS utilizing a Novel Valve Switching Algorithm**; Jay S. Johnson[1]; James P Murphy[2]; *[1]Water Corporation, Milford, MA; [2]Waters Corporation, Milford, MA*

WP 581 **Post-column Addition as a Tool to Enhance Performance in Microflow LC/MS**; Angela Doneanu[1]; Catherine Tremblay[1]; Michael P Donegan[1]; James P Murphy[1]; *[1]Waters, Milford, MA*

WP 582 **Increasing Operable Flow Range of a Nano-spray Source for High-Performance Microspray on a Curtain Gas Equipped Triple –Quadrupole API-MS**; Amanda Berg[1]; Helena Svobodova[2]; Gary A Valaskovic[2]; *[1]New Objective, Inc., Woburn, MA; [2]New Objective, Woburn, MA*

WP 583 **Picodroplet Mass Spectrometry for Miniaturized High Throughput Analysis of Synthetic Biology Clones**; Xin Li[1]; Murray J Brown[2]; Clive A Smith[1]; Gareth R Cooper[2]; Xin Liu[1]; Anthony Dossang[2]; Marian Rehak[1]; Angela Bridges[2]; Vinayaka Pawate[1]; Bill J Leavens[2]; *[1]Sphere Fluidics Limited, The Jonas Webb Building, Babraham Research Campus, Cambridge, UK; [2]GSK Medicines Research Centre, Gunnels Wood Road, Stevenage, Hertfordshire, UK*

WP 584 **High-throughput Enzymatic Characterization by Integration of Nanostructure-Initiator Mass Spectrometry and Droplet to Digital (D2D) Microfluidics**; Joshua Vance Heinemann[1]; Kai Deng[2, 3]; Steve C.C. Shih[2]; Jian Gao[1]; Markus de Raad[1]; Benjamin P Bowen[1, 3]; Paul D Adams[1, 3]; Anup K. Singh[2, 3]; Trent Northen[1, 3]; *[1]Lawrence Berkeley Nat'l Lab, Berkeley, CA; [2]Sandia National Laboratories, Albuquerque, NM; [3]Joint BioEnergy Institute, Emeryville, CA*

WP 585 **A Novel Targeted Metabolic Profiling Workflow for Simultaneous Reverse Phase and HILIC microflow LC-MS/MS Analysis**; Daniel M Warren[1]; Jeffery D Miller[1]; *[1]SCIEX, Redwood City, CA*

WP 586 **An Affordable and Simple-To-Use Snap-Chip-iMALDI Technology for Measuring Plasma Rennin Activity**; Huiyan Li[1, 2, 3]; Arya Tavakoli[2, 3]; Robert Popp[1]; Christoph H. Borchers[4, 5]; David Juncker[2, 3]; *[1]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [2]Biomedical Engineering Department, McGill University, Montreal, QC, Canada; [3]McGill University and Genome Quebec Innovation Centre, Montreal, QC, Canada; [4]University of Victoria - Genome BC Proteomics Centre, Victoria, BC; [5]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada*

PLANT 'OMICS'
587 - 613

WP 587 **Quantitative Analysis of Crosslinked Protein Complexes: A Novel Interactome Approach to Assess Pathogen-Triggered Unconventional Secretion in Arabidopsis**; Tricia Ho[1]; Kevin Blackburn[1]; John D Williamson[1]; Michael B Goshe[1]; *[1]North Carolina State University, Raleigh, NC*

WP 588 **Identification of Direct Substrates of MAP Kinases Activated by Environmental Stresses in Arabidopsis Thaliana through Protein Kinase Assay Linked-Phosphoproteomics**; Chuan-Chih Hsu[1]; Pengcheng Wang[2]; Chunzhao Zhao[2]; Jian-kang Zhu[2]; Weiguo Andy Tao[2]; *[1]Purdue University, West Lafayatte, IN; [2]Purdue University, West Lafayette, IN*

WP 589 **Chloroplast Protein Maturation, Regulation and Degradation**; Elden E. Rowland[1]; Jitae Kim[1]; Klaas J. van Wijk[1]; *[1]Cornell University, Ithaca, NY*

WP 590 **Emerging Role of Sirtuins and Lysine Acylation in the Regulation of Plant Metabolism**; Dana M Freund[1]; Jerry D Cohen[1]; Adrian D. Hegeman[1]; *[1]University of Minnesota at Twin Cities, Saint Paul, MN*

WP 591 **Label-free Quantitative Mass Spectrometry-Based Proteomic Approach for Comprehensive Analysis of Protein Complexes and Protein-Protein Interactions in Plants**; Uma Aryal[1]; Zachary McBride[2]; Donglai Chen[2]; Jun Xie[2]; Daniel Szymanski[2]; *[1]Purdue Proteomics Facility, Bindley Bioscience Center, West Lafayette, IN; [2]Purdue University, West Lafayette, IN*

WP 592 **Plant Proteomes Aplenty: Quantitative and Phylogenetic Analysis of Five Angiosperms, a Gymnosperm and a Bryophyte**; Harald Marx[1]; Alicia L Richards[1]; Dhileepkumar Jayaraman[1]; Jean-Michel Ané[1]; Joshua J Coon[1]; *[1]University of Wisconsin-Madison, Madison, WI*

WP 593 **Investigating the Expressed Kinome in *C. reinhardtii***; Emily Werth[1]; T.S. Karim Gilbert[2]; Lee M Graves[2]; Leslie M Hicks[1]; *[1]UNC Chapel Hill, Department of Chemistry Chapel Hill, NC; [2]UNC Chapel Hill, School of Medicine Chapel Hill, NC*

WP 594 **Quantitative Proteomics of Phaeodactylum tricornutuminPhosphate Limited Environment**; Shiang-Yu Tsai[1]; Pang-Hung Hsu[1]; *[1]Department of Bioscience and Biotechnology, National Taiwan Ocean University, Keelung, Taiwan*

WP 595 **UHPLC-HRMS Analysis of Herbal Plant Extracts to Screen for Small Molecule Drugs with Antibacterial Activity**; Gaganpreet Monga[1]; Anima Ghosal[1]; Dil Ramanathan[1]; *[1]Kean University, Union, NJ*

WP 596 **Comparative Protein Analysis of Oil Palm Mesocarp from Elaeis Guineensis and Elaeis oleifera to Investigate Acidification Process.**; Jessica K. A. Macêdo[1]; Jorge C. Rodrigues-Neto[1, 2]; Jéssica S. Barros[1, 3]; Letícia Jungmann[1]; Patrícia Verardi Abdelnur[4]; *[1]Embrapa Agroenergy, Brasilia, Brazil; [2]Federal University of Goiás, Goiânia, Brazil; [3]University of Brasília, Brasília, Brazil; [4]Embrapa Agroenergy, Brasilia, DF*

WP 597 **MALDI-Mass Spectrometric Imaging of Endogenous Peptides and Proteins in Medicago truncatula**; Caitlin Keller[1]; Erin Gemperline[1]; Junko Maeda[1]; Dhileepkumar Jayaraman[1]; Michael R Sussman[1]; Jean-Michel Ané[1]; Lingjun Li[1]; *[1]University of Wisconsin-Madison, Madison, WI*

WP 598 **iTRAQ 8-plex Labeling-Based Proteomics Analysis Reveals Difference of Protein Expression from Sorghum Root which was Treated by Aluminum**; Yong Yang; *USDA-ARS at Cornell University, Ithaca, NY*

WP 599 **Extracellular Proteomic Response of Thermally Stressed Symbiodinium: Implications for Symbiosis Breakdown during Bleaching**; Contessa Ricci[1]; Bren Ledbetter[1]; Tam Nguyen[1]; Saiful M Chowdhury[1]; Laura Mydlarz[1]; *[1]University of Texas at Arlington, Arlington, TX*

WP 600 **Deep Proteome Analysis of Gerontoplasts from the Inner Integument of Developing Seeds of Jatropha curcas**; Mohibullah Shah[1]; Emanoella L. Soares[1]; Magda alberto fernandez lima[1]; Camila B. Pinheiro[1]; Arlete A. Soares[1]; Gilberto B Domont[2]; Fabio CS Nogueira[3]; Francisco A. P. Campos[1]; *[1]Federal University of Ceará, Fortaleza, Brazil; [2]Federal University of Rio de Janeiro, Rio de Janeiro, Brazil; [3]UFRJ, Rio de Janeiro, Rio de Janeiro*

WP 601 **Quantitative Proteomics of Phaeodactylum tricornutumin Acidified Environment**; Tai-Yi Jiang[1]; Pang-Hung Hsu[1]; *[1]Department of Bioscience and Biotechnology, National Taiwan Ocean University, Keelung, Taiwan*

WP 602 **Standard-flow UHPLC Coupled with TripleQuad MS is a Versatile Platform for Both Targeted Metabolomics and Proteomics**; Daniel Vik[1]; Meike Burow[2]; Barbara Ann Halkier[2]; *[1]University of Copenhagen, Frederiksberg C, Denmark; [2]University of Copenhagen, Copenhagen, Denmark*

WP 603 **Stable Isotopic Labeling of Intact Plants for Molecular Turnover Measurement by HRMS: New Labeling Apparatus and Data Processing Approaches**; Calvin P Peters[1]; Dana M Freund[1]; Aaron K Rendahl[1]; Jerry D Cohen[1]; Adrian D. Hegeman [1]; *[1]University of Minnesota at Twin Cities, Saint Paul, MN*

WP 604 **Multi-OMICs Investigation of the Lignin Deposition Altering Enzyme Family of Arogenate Dehydratases in Arabidopsis and Poplar Tree**; Kim K. Hixson; *Washington State University, Richland, WA*

WP 605 **Qualification and Quantification of Cannabinoids and Terpenes in Extracts of Cannabis sativaby Gas Chromatography – Mass Spectrometry**; Allegra Leghissa[1]; Zacariah L. Hildenbrand[2]; Sean Jun[3]; Aaron L Hicks[3]; Kevin A Schug[1]; *[1]The University of Texas at Arlington, Arlington, TX; [2]Inform Environmental, LLC, Dallas, TX; [3]C4 Laboratories, LLC, Mesa, AZ*

WP 606 **Systemic Defense Induction and Post-Ingestive Rearrangement of Plant Toxins in Insects– a Metabolomics Approach Driven by Automated Compound Identification**; Sven Heiling[1]; Aiko Barsch[2]; Heiko Neuweger[3]; Emmanuel Gaquerel[4]; Ian T Baldwin[5]; *[1]Max-Planck-Society, Jena, Thüringen; [2]Bruker Daltonics Ltd, Bremen, DE; [3]Bruker Daltonics Ltd, Bremen, Germany; [4]Centre for Organismal Studies Heidelberg, Heidelberg, DE; [5]Max Planck Institute for Chemical Ecology, Jena, DE*

WP 607 **Metabolic Profiling of Stilbenes by LC-MS for Genetic Analysis in an F2 Interspecific Grapevine Hybrid Family**; Soon Li Teh[1]; Bety Rostandy[1]; Mani Awale[2]; Shanshan Yang[3]; Jonathan Fresnedo-Ramírez[3]; Qi Sun[3]; Matthew D. Clark[1]; Anne Y. Fennell[2]; James J. Luby[1]; Adrian D. Hegeman[1]; *[1]University of Minnesota at Twin Cities, Saint Paul, MN; [2]South Dakota State University, Brookings, SD; [3]Cornell University, Ithaca, NY*

WP 608 **Comprehensive Analysis of Tropical Flower Secondary Metabolites**; Elena Stashenko; *Universidad Industrial de Santander, Bucaramanga, Santander, Colombia*

WP 609 **Accounting for Complexity: A Procedure for the Targeted Analysis Of Primary- and Secondary-Metabolites, and Phytohormones from a Single Plant Extract**; Martin Schäfer[1]; Christoph Brütting[1]; Mario Kallenbach[1]; Gordon van 't Slot[2]; Paul Speir[3]; Ian T Baldwin[1]; *[1]Max Planck Institute for Chemical Ecology, Department of Molecular Ecology, Jena, Germany; [2]Bruker Daltonik GmbH, Bremen, Germany; [3]Bruker Daltonics, Inc., Billerica, MA*

WP 610 **Depth Profiling of Whole Soybean Nodules using Laser Ablation Electrospray Ionization Mass Spectrometry**; Christopher Anderton[1]; Sylwia A Stopka[2]; Beverly J Agtuca[3]; Rosalie K Chu[1]; David W Koppenaal[1]; Gary Stacey[3]; Akos Vertes[2]; Ljiljana Pasa-Tolic[1]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]George Washington University, Washington DC; [3]University of Missouri, Columbia, MO*

WP 611 **Identificacion of Metabolites Involved in the Color Reversion Process in Blackberry Fruit using LC-ESI-QTOF**; Victor Manuel Mondragon Olguin[1]; Georgina Alejandra Pérez Pérez[2]; Edmundo M. Mercado Silva[2]; Gelasio Perez[1]; *[1]Agilent Technologies Mexico, Mexico, DF; [2]Universidad Autonoma de Queretaro, Queretaro, QRO*

WP 612 **REIMS (Rapid Evaporative Ionization Mass Spectrometry) and Multi-Variant Statistics, Two Tools in Support of Weed Grass Speciation and Phenotype Characterization**; Sara Stead[1]; Jackson Pope[2]; Robert Edwards[3]; Melissa Brazier-Hicks[3]; Catherine Tetard-Jones[3]; Zoltan Takats[4]; *[1]Waters corp, Manchester, Lanc; [2]Waters, Wilmslow, UK; [3]University of Newcastle, Newcastle upon Tyne, UK; [4]Imperial College, London, UK*

WP 613 **DESI-MS Imaging with Ion Mobility and Multivariate Analysis for the Determination of Weed Grass Species and Surface Level Characteristics**; Philippa Jayne Hart[1]; Sara Stead[1]; Emmanuelle Claude[1]; Hernando Olivos[2]; Melissa Brazier-Hicks[3]; Catherine Tetard-Jones[3]; Robert Edwards[3]; *[1]Waters Corporation, Wilmslow, UK; [2]Waters Corporation, Beverly, Massachusetts; [3]Newcastle University, Newcastle upon Tyne, UK*

PROTEIN THERAPEUTICS: QUANTITATIVE ANALYSIS 614 - 650

WP 614 **Method Development of an Automated Hybrid LBA-LC/MS Assay for the Quantitative Bioanalysis of the Biotherapeutic Teriparatide in Human Plasma**; Jean-Nicholas Mess[1]; Daniel Villeneuve[1]; Georges Koudssi[1]; Anahita Keyhani[1]; *[1]Algorithme Pharma Inc., Laval, Canada*

WP 615 **Improving the Sensitivity for an Immunocapture LC-MS Assay of Infliximab in Rat Plasma Using Trap-and-Elute MicroLC-MS**; Remco van Soest[1]; Lei Xiong[1]; *[1]SCIEX, Redwood City, CA*

WP 616 **Development and Validation of an LC-MS/MS Method for the Quantitation of Linker-extended Cyanovirin-N in Rat Plasma**; Hui Hong[1]; Wenzhong Liang[1]; Xin Zhang[1]; Xinping Fang[1]; *[1]WuXi AppTec (Shanghai) Co. Ltd., Shanghai, China*

WP 617 **Quantitation of Insulin Glargine and Major Metabolites in Human Plasma Using Hybrid LBA-LC/MS with Automated Magnetic Particle Processing**; Kevork Mekhssian[1]; Jean-Nicholas Mess[1]; Anahita Keyhani[1]; *[1]Algorithme Pharma Inc., Laval, Canada*

WP 618 **Quantitation of a Modified Insulin in Rat Plasma Using Triple Quad 6500 LC-MS/MS**; Rong Huang[1]; Guangchun Zhou[1]; Joshua Froning[1]; Yong-Xi Li[1]; *[1]Medpace Bioanalytical Laboratories, Cincinnati, OH*

WP 619 **Automated Biotherapeutic Quantitation from Tissue**; Kristin Geddes[1]; Lisa A Vasicek[2]; Daniel S Spellman[2]; Kevin P Bateman[2]; *[1]Merck and Co, Inc, West Point, PA; [2]Merck & Co., Inc., West Point, PA*

WP 620 **Quantitative Bioanalysis of Rituximab and Reditux for Biosimilarity Assessment Comparing Triple Quadrupole and Hybrid Time-of-Flight Platforms**; Richard Lavallée[1]; Daniel Villeneuve[1]; Kevork Mekhssian[1]; Jean-Nicholas Mess[1]; Anahita Keyhani[1]; *[1]Algorithme Pharma Inc., Laval, Canada*

WP 621 **Using a Tandem Protein Precipitation/Immunoaffinity Purification Extraction to Resolve Specificity and Sensitivity Roadblocks: Bioanalysis of a PEGylated Human Protein Analog**; Jonathan R St-Germain[1]; Luca Genovesi[1]; Jean-Nicholas Mess[1]; Anthony T Murphy[2]; Selina Estwick[2]; Patricia L Brown-Augsburger[2]; Anahita Keyhani[1]; *[1]Algorithme Pharma Inc., Laval, Canada; [2]Eli Lilly and Company, Indianapolis, IN*

WP 622 **Comparison of Bottom-Up and Top-Down Analytical Methodologies for the Quantitative Bioanalysis of Large Therapeutic Peptides in Biological Matrix**; Georges Koudssi[1]; Jean-Nicholas Mess[1]; Anahita Keyhani[1]; *[1]Algorithme Pharma Inc., Laval, Canada*

WP 623 **Generic Quantitative LC-MS/MS Assay for Analysis of hIgG1 Based Therapeutic Proteins in Cynomolgus Monkey Serum Using Immunocapture with MSIA™-D.A.R.T.'S™**; Christian Lanshoeft[1, 2]; Olivier Heudi[1]; Sarah Cianférani[2]; Eric E Niederkofler[3]; Ravindra Chaudhari[3]; Andrew Paul Warren[1]; Franck Picard[1]; Olivier Kretz[1]; *[1]Novartis Institutes for Biomedical Research, Drug Metabolism and Pharmacokinetics, Basel, Switzerland; [2]Université de Strasbourg, Laboratoire de Spectrométrie de Masse BioOrganique, Institut Pluridisciplinaire Hubert Curien, Strasbourg, France; [3]Thermo Fisher Scientific, Tempe, AZ*

WP 624 **Applying Rapid Trypsin Digestion for Targeted Protein Quantitation in Rat Plasma by Liquid Chromatography/ Tandem Mass Spectrometry**; Moucun Yuan[1]; Morse Faria[1]; Jinlin Shen[1]; Song Zhao[1]; Eric Ma[1]; Elizabeth Dompkowski[1]; Michael Waldron[1]; Bruce Hidy[1]; William R. Mylott Jr.[1]; Rand Jenkins[1]; *[1]PPD, Richmond, VA*

WP 625 **Absolute Quantitation of Glycan and Site-Specific Glycoforms on Commercial mAbs using Multiple Reaction Monitoring**; Nari Seo[1]; Unyong Kim[2]; Hyun Joo An[1]; *[1]GRAST&AGRS, Chungnam National University, Daejeon, Republic of Korea; [2]Asia-Pacific Glycomics Reference Site (AGRS), Daejeon, Republic of Korea*

WP 626 **Improved Reagents and Software for Comparing Biosimilar and Originator Therapeutic Proteins: Accurate Analysis of Deamidation and Disulfide Bond Scrambling**; Wilfred H Tang[1]; Marshall Bern[1]; John St Skilton[1]; Eric Carlson[1]; Michael J Ford[2]; Karthik Pisupati[3]; Anna Schwendeman[3]; Chris Hosfield[4]; Sergei Saveliev[4]; Michael M Rosenblatt[4]; Marjeta Urh[4]; Chris Becker[1]; *[1]Protein Metrics Inc., San Carlos, CA; [2]MS Bioworks, LLC Ann Arbor, MI; [3]University of Michigan, Ann Arbor, MI; [4]Promega Corp, Madison, WI*

WP 627 **The Use of Generic Surrogate Peptides for the Quantitative Analysis of hIgG1 in Pre-Clinical Species with High-Resolution Mass Spectrometry**; Christian Lanshoeft[1, 2]; Thierry Wolf[1]; Olivier Heudi[1]; Sarah Cianférani[2]; Samuel Barteau[1]; Markus Walles[1]; Kelly B Doering[3]; Guillaume Bechade[4]; Franck Picard[1]; Olivier Kretz[1]; *[1]Novartis Institutes for Biomedical Research, Drug Metabolism and Pharmacokinetics, Basel, Switzerland; [2]Université de Strasbourg, Laboratoire de Spectrométrie de Masse BioOrganique, Institut Pluridisciplinaire Hubert Curien, Strasbourg, France; [3]Waters, Milford, MA; [4]Waters AG, Baden-Daettwil, Switzerland*

WP 628 **Host Cell Protein Analysis by microflow-LC High Resolution SWATH-MS of Vaccine Samples under Development**; Søren Heissel[1]; Milla Neffling[2]; Rikke Raaen Lund[3]; Thomas Kofoed[3]; Marie Grimstrup[3]; Nick Morrice[2]; Anne Fich Holmbjerg[4]; Max Per Kristiansen[4]; Ingrid Kromann[4]; Peter Højrup[1]; Ejvind Mørtz[3]; *[1]Department of Biochemistry and Molecular Biology, University of Southern Denmark Odense, Denmark; [2]SCIEX, Phoenix House Lakeside Drive Warrington Cheshire UK; [3]Alphalyse A/S, Odense M, DK; [4]Statens Serum Institut, Copenhagen, Denmark*

WP 629 **Highly Sensitivity and Reproducible MRM Based Quantitation of Follicle Stimulating Hormones (FSH) in Human Plasma using QTRAPTM 6500**; Faraz Rashid[1]; Rahul Baghla[2]; Prashant Kale[3]; Manoj Shukla[3]; Milin Shah[3]; Dipankar Malakar[2]; Anoop Kumar[2]; Manoj Pillai[2]; *[1]SCIEX, 121 Udyog Vihar Phase IV Gurgaon, India; [2]Sciex Gurgaon, Gurgaon, India; [3]Lambda Therapeutic Research Ltd, Ahmedabad, India*

WP 630 **Streamlining the Complete Sequence Variant Analysis Workflow for Biotherapeutics**; Andrew Dawdy[1]; Michelle English[2]; Mellisa Ly[2]; Andrew Saati[2]; Lisa A Marzilli[2]; Olga Friese[1]; Jason C Rouse[2]; Yong J Kil[3]; Marshall Bern[3]; Eric Carlson[3]; Chris Becker[3]; *[1]Pfizer, Inc. Chesterfield, MO; [2]Pfizer, Inc. Andover, MA; [3]Protein Metrics Inc., San Carlos, CA*

WP 631 **Comparison of First Dimension Fractionation Strategies for Directed MS Analysis of Host Cell Proteins**; Jordy Hsiao[1]; Te-Wei Chu[1]; Gregory O Staples[1]; Oscar Potter[1]; Hongfeng Yin[1]; Kevin Killeen[1]; *[1]Agilent Technologies, Santa Clara, CA*

WP 632 **Determination of Total Recombinant Human α-Galactosidase A in Plasma Samples by Liquid Chromatography-Tandem Mass Spectrometry (LC-MS/MS)**; Rick Hamler[1]; Kees Bronsema[2]; Peter Pruim[2]; Peter Bults[2]; Deborah Hilliard[1]; Russell Gotschall[1]; Franklin K Johnson[1]; Hung Do[1]; Kenneth Valenzano[1]; Nico van de Merbel[2]; Elfrida R Benjamin[1]; *[1]Amicus Therapeutics, Cranbury, NJ; [2]PRA Health Sciences, Assen, The Netherlands*

WP 633 **Herceptin Quantitation Using Universal and Signature Peptides by Hybrid LBA/LC-MS Method**; XI QIU[1]; Daniell Rowles[1]; Susan Zondlo[1]; John Kolman[1]; Zamas Lam[1]; *[1]QPS, Newark, DE*

WP 634 **Quantitative Analysis of Adalimumab using nano-Surface and Molecular-Orientation Limited (nSMOL) proteolysis and LC/MS/MS**; Deepti Bhandarkar[1]; Ravi Krovidi[2]; Rashi Kochhar[1]; Shailendra Rane[1]; Shailesh Damale[1]; Purushottam Sutar[1]; Anant Lohar[1]; Ashutosh Shelar[1]; Jitendra Kelkar[1]; Ajit Datar[1]; Pratap Rasam[1]; *[1]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India; [2]Lambda Therapeutic Research, Ahmedabad, India*

WP 635 **SSPaQ: A Subtractive Method for the Parallel Quantification of the Degree of Modification at Every Possible Site of a Protein**; Guillaume Gabant[1]; Alain Boyer[1]; Martine Cadene[1]; *[1]CBM CNRS UPR4301, Orleans, France*

WP 636 **Quantification of the Antibody Drug Conjugate, Trastuzumab Emtansine and the Monocolonal Antibody, Trastuzumab in Plasma Using a Generic Kit-Based Approach**; Hua Yang[1]; Mary E Lame[1]; Erin E Chambers[1]; Sherri Naughton[1]; *[1]Waters Technologies Corporation, Milford, MA*

WP 637 **Applying a Standardized, Kit-based Approach to Achieve 10 ng/mL Infliximab from 35 µL Plasma**; Mary E Lame[1]; Hua Yang[1]; Erin E Chambers[1]; Sherri Naughton[1]; *[1]Waters, Milford, MA*

WP 638 **Quantification of Host Cell Proteins in Biotherapeutics using Stable Isotope Labeled Chinese Hamster Ovary Proteins (SIL-CHOP) as an Internal Standard**; Pegah R Jalili[1]; Zhiyun Cao[1]; Kevin Ray[1]; Rong-Rong Zhu[2]; *[1]MilliporeSigma, Saint Louis, MO; [2]MilliporeSigma, Bedford, MA*

WP 639 **Host Cell Protein Analysis of Biopharmaceuticals using Automatic Offline Fractionation and LC/MS**; Alex Zhu[1]; Jing Chen[2]; Steve Murphy[2]; Jordy Hsiao[3]; *[1]Agilent Technologies, Wilmington, DE; [2]Agilent Technologies, Inc. Madison, WI; [3]Agilent Technologies, Santa Clara, CA*

WP 640 **Exploiting His-tags in Recombinant Protein Therapeutics to Introduce Metal Tracers for Tracking Biodistribution of Biopharmaceuticals *in vivo***; Chengfeng Ren[1]; Grégoire Bonvin[1]; Cedric Bobst[1]; Igor A Kaltashov[1]; *[1]University of Massachusetts Amherst, Amherst, Massachusetts*

WP 641 **Analysis of N-Glycans Released from Monoclonal Antibodies using an ESI-MS-friendly Fluorescent Tag**; Oscar Potter[1]; Gregory O Staples[1]; Hongfeng Yin[1]; Kevin Killeen[1]; *[1]Agilent Technologies, Santa Clara, CA*

WP 642 **Evaluation of Transferrin Metal Tracers using Native ESI-MS and *in-vitro* Model for Tracking Its Biodistribution with ICP-MS.**; Grégoire Bonvin[1]; Cedric Bobst[2]; Igor A Kaltashov[1]; *[1]University of Massachusetts Amherst, Amherst, Massachusetts; [2]University of Massachusetts-Amherst, Amherst, Massachusetts*

WP 643 **Comprehensive HCP Profiling by Targeted and Untargeted Analysis of DIA Mass Spectrometry Data with PRM qualification**; Simion Kreimer[1]; Yuanwei Gao[1]; Mi Jin[2]; Nesredin Mussa[2]; Alexander R. Ivanov[1]; Barry L. Karger[1]; *[1]Barnett Institute and Department of Chemistry and Chemical Biology, Northeastern University, Boston, MA; [2]Bristol-Myers Squibb, Devens, MA*

WP 644 **A Promising Alternative to SRM-Very-high-resolution selected-ion- Monitoring (vHR-SIM@500k) Enables Ultra-sensitive and Selective Biotherapeutics Quantification**; Yang Qu[1]; Bo An[1]; Ming Zhang; Xiaomeng Shen; Shichen Shen; Jun Li; Jun Qu; *[1]SUNY at Buffalo, Buffalo, NY*

WP 645 **Significant Throughput Increase in Peptide Mapping/MAM Analysis Using 2D-UPLC**; Cong Wu[1]; Hai Yue[1]; Sabrina Benchaar[1]; *[1]Amgen, Inc., Thousand Oaks, CA*

WP 646 **Sulfur-based Characterization of Protein Standards using Isotope Dilution Inductively Coupled Plasma Mass Spectrometry**; Hyun-Seok Lee[1, 2]; Sook Heun Kim[1]; Ji-Seon Jeong[1, 3]; Yong-Moon Lee[2]; Yong-Hyeon Yim[1, 3]; *[1]KRISS, Daejeon, Republic of Korea; [2]College of Pharmacy, Chungbuk National University, Cheongju, Korea; [3]Department of Analytical Sciences for Biology, University of Science and Technology (UST), Daejeon, Korea*

WP 647 **Bioanalysis of Radiolabeled Payload by Isotopic Pattern Deconvolution and LC-MS/MS to Investigate Tissue Distribution of Protein Drug Conjugates**; Weiqi Chen[1]; Wenying Li[1]; Jinping Gan[1]; *[1]Bristol-Myers Squibb Co., Princeton, NJ*

WP 648 **Site-Specific Glycosylation Quantitation of Bioengineered Recombinant Therapeutical Glycoproteins**; Muchena J. Kailemia[1]; Wanghui Wei[1]; Kalimuthu Karuppanan[1]; Jasmine M. Corbin[1]; Yanhong Li[1]; L My Phu[1]; Abhaya Dandekar[1]; Xi Chen[1]; Somen Nandi[1]; Karen McDonald[1]; Carlito Lebrilla[1]; *[1]University of California, Davis, Davis, CA*

WP 649 **Large-scale and Ultra-Sensitive Investigation of Biotherapeutics by A Novel Antibody-Free, Dual-Mechanism Enrichment Strategy**; Ming Zhang[1]; Bo An[1]; Yang Qu[1]; Shichen Shen[1]; Jun Qu[1]; *[1]SUNY at Buffalo, Buffalo, NY*

WP 650 **Novel Sample Treatment and LC/MS Strategies Achieved Highly Accurate and Sensitive Investigation of Tissue Distributions of Therapeutic**; Wei Fu[1]; Bo An[1]; Ming Zhang[1]; Yang Qu[1]; Jun Qu; *[1]SUNY at Buffalo, Buffalo, NY*

PROTEOMICS: NEW APPROACHES (GLOBAL)
651 - 674

WP 651 **ProteomeTools: Large Libraries of Synthetic Peptides, Spectra and Software for Facilitating Human Proteome Research**; Daniel Paul Zolg[1]; Mathias Wilhelm[1]; Peng Yu[1]; Karsten Schnatbaum[2]; Johannes Zerweck[2]; Tobias Knaute[2]; Ulf Reimer[2]; Holger Wenschuh[2]; Bernard Delanghe[3]; Thomas Moehring[3]; Andreas Huhmer[4]; Gina Tan[4]; Mohammed Abujarour[5]; Siegfried Gessulat[5]; Stephan Aiche[5]; Hans-Christian Ehrlich[5]; Bernhard Kuster[1, 6]; *[1]Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; [2]JPT Peptide Technologies GmbH, Berlin, Germany; [3]Thermo Fisher Scientific, Bremen, DE; [4]Thermo Fisher Scientific, San Jose, CA; [5]SAP SE, Innovation Center Potsdam Potsdam, Germany; [6]Bavarian Biomolecular Mass Spectrometry Center, Technical University of Munich, Freising, Germany*

WP 652 **Comprehensive Draft of the HeLa Proteome to a Depth of More than 13,000 Proteins**; Christian Dahl Kelstrup[1]; Dorte B Bekker-Jensen[1]; Tanveer S Batth[1]; Sara C Larsen[1]; Michael L Nielsen[1]; Jesper V Olsen[1]; *[1]CPR, University of Copenhagen, Copenhagen, Denmark*

WP 653 **Subtilisin for Large Scale (phospho)proteomcis – the Beginning of a Wonderful Love Story?**; Humberto Gonczarowska-Jorge[1, 2]; Stefan Loroch[1]; Margherita Dell'Aica[1]; René Zahedi[3]; *[1]ISAS, Dortmund, Germany; [2]CAPES Foundation, MinistryofEducationofBrazil Brasília-Brazil; [3]ISAS, Dortmund*

WP 654 **A New Approach to the Analysis of Intact Major Urinary Proteins (MUPs) from Mouse Urine by CESI-MS**; Stephen J. Lock[1]; Robert J. Beynon[2]; Guadalupe Gomez-Baena[2]; Edna Betgovargez[3]; *[1]SCIEX, Warrington, Cheshire; [2]Centre for Proteome Research, Institute of Integrative Biology, University of Liverpool, Liverpool, UK; [3]SCIEX, Concord ON, Canada*

WP 655 **Proteogenomics of HEK293 Cell Line: Identification of Variant Peptides using Deep Proteome Data from the Inter-Laboratory Studies**; Anna Lobas[1, 2]; Dmitry Karpov[3,4]; Arthur Kopylov[3]; Elizaveta Solovyeva[1, 2]; Mark Ivanov[1, 2]; Irina Ilina[3]; Vassily Lazarev[5]; Ksenia Kuznetsova[3]; Ekaterina Ilgisonis[3]; Victor Zgoda[3]; Mikhail V Gorshkov[1, 2]; Sergei Moshkovskii[3]; *[1]Institute for Energy Problems of Chemical Physics, Moscow, Russian Federation; [2]Moscow Institute of Physics and Technology, Dolgoprudny Moscow Oblast, Russia; [3]Institute of Biomedical Chemistry, Moscow, Russia; [4]Engelhardt Institute of Molecular Biology, Russian Academy of Sciences, Moscow, Russia; [5]Research Institute of Physico-Chemical Medicine, Federal Medico-Biological Agency, Moscow, Russia*

WP 656 **Novel Approaches in *de novo* Peptide Sequencing and Proteogenomics as Tools to Explore Uncharted Organisms**; Bernhard Blank-Landeshammer[1]; Karsten Bißt[1]; Laxmikanth Kollipara[1]; Vera Rieder[2]; Marleen Stuhr[3]; Tilman Schell[4]; René P Zahedi[1]; Markus Pfenninger[4]; Jörg Rahnenführer[2]; Hildegard Westphal[3]; Albert Sickmann[1]; *[1]Leibniz-Institut für Analytische Wissenschaften, Dortmund, Germany; [2]Fakultät Statistik, Technische Universität Dortmund, Dortmund, Germany; [3]Leibniz Center for Tropical Marine Ecology (ZMT), Bremen, Germany; [4]Biodiversity and Climate Research Centre (BiK-F), Frankfurt Am Main, Germany*

WP 657 **Proteomic Study of Rhizopus Microsporus Fungus Growing in Presence of Copper**; Meriellen Dias[1]; Lidiane Maria de Andrade[1]; Enrique Eduardo Rozas[1]; Mariana de Paula Eduardo[1]; Maria Anita Mendes[1]; *[1]University of São Paulo, São Paulo, SP*

WP 658 **Identification of Methylation and Phosphorylation in Arginine/Serine-Rich Domains by Electron Transfer Dissociation Mass Spectrometry**; Isaac Bishof[1]; Duc M. Duong[2]; Eric B. Dammer[2]; Nicholas T. Seyfried[2]; *[1]Emory University, Atlanta, GA; [2]Emory University School of Medicine, Atlanta, GA*

WP 659 **Capturing Protein Binders to Yeast Ribosome Biogenesis and Stress Response Genes Using Multiplexed HyCCAPP**; Yunxiang Dai[1]; Julia Kennedy-Darling[1]; Mark Scalf[1]; Audrey Gasch[1]; Lloyd M Smith[1]; *[1]University of Wisconsin-Madison, Madison, WI*

WP 660 **Elucidation of Dynamic Cell Surface Protein-Protein Interactions using Chemoproteomic Technologies**; Damaris Bausch-Fluck[1]; Maria P Pavlou[1]; Bernd Wollscheid[1]; *[1]Institute of Molecular Systems Biology, Dep. of Health Sciences and Technology, ETH Zürich, Zürich, Switzerland*

WP 661 **Development of an On-Slide-Digestion, MS Assay from Formalin-Fixed Paraffin Embedded (FFPE) Breast Tissue**; Ten-Yang Yen [1]; Moe Thein[2]; Roger Yen[2]; Leslie Timpe[2]; Bruce Macher[2]; *[1]San Francisco State University, San Francisco , CA; [2]San Francisco State University, San Francisco, CA*

WP 662 **Multi-omics Analysis for the Global Proteins and Metabolites in Experimental Autoimmune Myocarditis Rat Model**; Jin Woo Jung[1]; Jae Hun Jung[2]; Kwang Pyo Kim[2]; Geum-Sook Hwang[3]; Jungju Seo[1]; *[1]Korea Basic Science Institute, Deajeon, Republic of Korea; [2]Kyung Hee University, Yongin, Republic of Korea; [3]Korea Basic Science Institute, Seoul, Republic of Korea*

WP 663 **Multiplexing Targeted Proteomics: Increased Throughput of Targeted Biomarker Measurements using Isobaric Labels and Dedicated MS3 Analysis**; Robert Everley[1]; Brian K. Erickson[1]; Christopher M. Rose[1]; Steven P Gygi[1]; *[1]Harvard Medical School, Boston, MA*

WP 664 **Comparative Study on Chemical Derivatization of Lysines to mimic Arg-C digestion**; Vahid Golghalyani[1]; Michael Karas[1]; *[1]Goethe University, Frankfurt Am Main, Germany*

WP 665 **Developing an LC/MS/MS Method for the Identification of Key Secretome Proteins from Human Lung Spheroid Cells**; Dipti Paudel[1]; Phuong-Uyen Dinh[2]; Jhon Cores[3]; Robert Kevin Blackburn[3]; Ke Cheng[3]; Michael Goshe[3]; *[1]NCSU, Raleigh, NC; [2]North Carolina State University, Raleigh, NC; [3]North Carolina State University, Raleigh, NC*

WP 666 **Evaluation and Establishment of the Method for the Accurate Protein Quantification in the Subcellular Fraction**; Atsushi Sakamoto[1]; Akiko Matsui[1]; Asami Saito[1]; Gaku Morinaga[1]; Akiko Takamoto[1]; Naoki Ishiguro[1]; Shinobu Suzuki[1]; *[1]Nippon Boehringer Ingelheim, KOBE, JPN*

WP 667 **Fluorescence Complementation Mass Spectrometry (FCMS) for Identifying Direct Upstream Kinases**; Lingfei Zeng; *Department of MCMP, Purdue, West Lafayette, IN*

WP 668 **Protein Analysis Using a Combination of an Online Trypsin Immobilized Enzyme Reactor and CAD/ETD Tandem Mass Spectrometry**; Kun Cho[1]; Sang Eun Hong[2]; Kyung Ju Jang[2]; Kuk Ro Yoon[2]; Jong Shin Yoo[1]; *[1]KBSI, Cheongju-Si, S. Korea; [2]Hannam University, Daejeon, Korea*

WP 669 **Parrallel SUMO/Ubi Profiling Using an Optimized Peptide IP**; Frederic Lamoliatte[1]; Francis McManus[1]; Ghizlane Maarifi[2]; Mounira K. Chelbi-Alix[2]; Pierre Thibault[1]; *[1]IRIC-Université de Montréal, Montréal, QC; [2]INSERM Unité Mixte de Recherche S 1124, Université Paris Descartes, Paris, France*

WP 670 **Electron-Transfer/Higher-Energy Collision Dissociation (EThcD) Improves Spectral Quality while Retaining Quantitation Accuracy in Isobaric Tag-based Quantitative Proteomic Studies**; Yu Feng[1]; Qing Yu[1]; Lingjun Li[1]; *[1]University of Wisconsin-Madison, Madison, WI*

WP 671 **A New Digestion Method to Analyze Respiratory Complex I**; Stefan Schoenborn; *Department of Pharmaceutical Chemistry, Goethe University, Frankfurt, Germany*

WP 672 **The Establishment of Nano Mass Spectrometry Analysis Techniques for the Identification of Lead Ion Effect in Hemoglobin**; Ming-Hui Yang[1]; Yu-Chang Tyan [2]; *[1]Graduate Institute of Medicine, KMU, Kaohsiung, Taiwan; [2]Kaohsiung Medical University, Kaohsiung, Taiwan*

WP 673 **A Quantitative Tunable Digestion Approach Uncovers Novel Acetyl and Methyl Marks on Histones**; Chris Adams[1]; Nora Yucel[2]; Allis C Chien[2]; Ryan D Leib[2]; *[1]Stanford University, Stanford, CA; [2]Stanford University, Stanford, CA*

WP 674 **Identification of GHB-binding Proteins by Mass Spectrometry – (Chemo)proteomic Analysis of Synaptosomal Membrane Proteins**; Ulrike Leurs; *University of Copenhagen, Copenhagen, Sjaelland*

PROTEOMICS: QUANTITATIVE (LABELING/TAGGING/MS/ QUANTITATION)
675 - 704

WP 675 **Development of Dimethyl Pyrimidinyl Ornithines (DiPyrO) as Mass Defect-Based Tags for Quantitative Proteomics**; Amanda Rae Buchberger[1]; Dustin Frost[1]; Lingjun Li[1]; *[1]University of Wisconsin-Madison, Madison, WI*

WP 676 **Examining pH Specificity of Peptide N-terminal Amine Tagging Reagents for cPILOT Analysis**; Lindsay Osentoski[1]; Yaphet Geadion[1]; Joseph Dudenhoeffer[1]; Christina King[1]; Renã A.S. Robinson[1]; *[1]University of Pittsburgh, Pittsburgh, PA*

WP 677 **Application of SuperQuant to Obtain Quantitative Information of the Glioblastoma Proteome**; Thiago Verano-Braga[1]; Vladimir Gorshkov[1]; Sune Munthe[2]; Mia Dahl Soerensen[2]; Bjarne Winther Kristensen[2]; Frank Kjeldsen[3]; *[1]Department of Biochemistry and Molecular Biology, University of Southern Denmark Odense, Denmark; [2]Odense University Hospital, Odense, DK; [3]BMB, Odense M*

WP 678 **Combining of iTRAQ Labeled Peptides from HPLC Fractions: Where is the Limit for Peptides/Proteins Detected and Quantified?**; Trong Khoa Pham[1]; Kirsty Richards[2]; Jo Roobol[2]; Colin Robinson[2]; Phillip C. Wright[3]; *[1]Department of Chemical and Biological Engineering, The University of Sheffield, Sheffield, UK; [2]School of Biosciences, University of Kent, Canterbury, UK; [3]Faculty of Science, Agriculture and Engineering, Newcastle University, Newcastle upon Tyne, UK*

WP 679 **Increasing Protein Quantification in 6-plex TMT Experiments**; Jane Liu[1]; Michael Sweredoski[2]; Sonja Hess[2]; *[1]Pomona College, Claremont, CA; [2]California Institute of Technology, Pasadena, CA*

WP 680 **Evaluation of a Pulsed SILAC-TMT Multiplexing Strategy for Measurement of Proteome Dynamics**; Jana Zecha[1]; Chen Meng[1]; Mathias Wilhelm[1]; Susan Klaeger[1]; Bernhard Kuster[1, 2]; *[1]Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; [2]Bavarian Biomolecular Mass Spectrometry Center, Technical University of Munich, Freising, Germany*

WP 681 **Extended Mass Range QQQ for Routine Analysis of Large, Low-Charge State Peptide Ions**; Linfeng Wu[1]; Christine A Miller[1]; *[1]Agilent Technologies, Santa Clara, CA*

WP 682 **Pseudo-isobaric Fragment Ions Provide Accurate and Precise Proteome Quantification Results**; Yuan Zhou[1]; Jianhui Liu[1]; Zhigang Sui[1]; Lihua Zhang[1]; Yukui Zhang[1]; *[1]Key Laboratory of Separation Science for Analytical Chemistry; Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China*

WP 683 **Investigation of Q-TOF Instruments Advantages for label-free Proteome Analysis**; Stephanie Kaspar-Schoenefeld[1]; Markus Lubeck[1]; Annette Michalski[1]; Pierre-Olivier Schmit[2]; *[1]Bruker Daltonik GmbH, Bremen, Germany; [2]Bruker Daltonique S.A., Wissembourg, France*

WP 684 **Stable-isotope Maleic Anhydride Labeling-based Approach for Quantitative Proteomics**; Kai Zhang[1]; Shuzhen Zheng[2]; Shanshan Tian[3]; Zhenchang Guo[3]; Guijin Zhai[3]; *[1]Tianjin Medical University, Tianjin, Tianjin; [2]Nankai university, Tianjin, China; [3]Tianjin Medical University, Tianjin, China*

WP 685 **Intact Protein Quantitation up to a 1000-fold Using Protein Universal Pseudo-isobaric Dimethylation**; Zhixin Tian[1]; Houqin Fang[1]; Kaijie Xiao[1]; *[1]Department of Chemistry, Tongji University, Shanghai, Shanghai*

WP 686 **Evaluation of a Novel Tandem Quadrupole Mass Spectrometer for the Quantitative Analysis of Peptides using a Multi-Point Internal Calibration Method**; Billy Molloy[1]; Donald JL Jones[2, 3]; Donald P Cooper[4]; Johannes PC Vissers[4]; James I Langridge[4]; *[1]Waters, Wilmslow ; [2]Department of Cancer Studies, University of Leicester, UK, Leicester, UK; [3]Cardiovascular Research Centre, Glenfield Hospital, Leicester, UK, Leicester, UK; [4]Waters, Wilmslow, UK*

WP 687 **Comparison of Label-Free and TMT Quantification for Global Phosphoproteome Analysis of Apoptotic Cells**; Emmanuelle Lezan[1]; Christoph Schmutz[1]; Simon Josef Ittig[1]; Erik Ahrné[1]; Alexander Schmidt[1]; *[1]Biozentrum, University of Basel, Basel, Switzerland*

WP 688 **Examining Proton Transfer and Ion Scattering for Intact Proteins in a Triple Quadrupole Mass Spectrometer**; Evelyn H Wang[1]; Dananjaya Kalu Appulage[1]; Erin A. McAllister[2]; Kevin A Schug[1]; *[1]University of Texas at Arlington, Arlington, TX; [2]Shimadzu Scientific Instruments, Columbia, MD*

WP 689 **α- and β-tubulin Isotype Repertoire Quantification by LC-SRM in Blood Platelet and HeLa Cells**; Agnes Hovasse[1]; Magda Magiera[2]; Catherine Strassel[3]; Alain Van Dorsselaer[4]; Carsten Janke[2]; Francois Lanza[3]; Christine Schaeffer-Reiss[4]; *[1]Laboratoire de Spectrométrie de Masse BioOrganique, IPHC, UMR7178, Centre National de la Recherche Scientifique, Université de Strasbourg, Strasbourg, Alsace; [2]Institut Curie, Orsay, France; [3]UMR_S 949 Inserm, EFS-Alsace, Université de Strasbourg, Strasbourg, France; [4]Laboratoire de Spectrométrie de Masse BioOrganique, IPHC, UMR7178, Centre National de la Recherche Scientifique, Université de Strasbourg, Strasbourg, France*

WP 690 **Combination of Ultrasensitive Sample Preparation and NHS-chemistry Enables Sensitive Quantification of Lysine Acetylation and Large Proteome Coverage**; Christian Frese[1]; Özge Karayel[1]; Jeroen Krijgsveld[1]; *[1]DKFZ German Cancer Reserach Center, Heidelberg, Germany*

WP 691 **Combining Ion Mobility Enhanced DDA and DIA Workflows for Label-Free Quantitative Phosphoproteomics**; Ute Distler[1, 2]; Pedro Navarro[1]; Jennifer Hahlbrock[1]; Kuharev Jörg[1]; Stefan Tenzer[1]; *[1]Institute for Immunology, University Medical Center of the Johannes-Gutenberg University Mainz, Mainz, Germany; [2]Focus Program Translational Neuroscience (FTN), University Medical Center of the Johannes-Gutenberg University Mainz, Mainz, Germany*

WP 692 **Comprehensive Relative Quantification of the Cytochromes P450 by micro-LC and SWATH® Acquisition and Data Processing using Cloud Computing**; Rosalind E. Jenkins[1]; Sibylle Heidelberger[2]; Thomas Knapman[2]; Francesco Brancia[2]; Neil Kitteringham[1]; Kevin B Park[1]; Mark Carfazzo[3]; *[1]MRC Centre for Drug Safety Science, Liverpool, UK; [2]SCIEX, Phoenix House Lakeside Drive Warrington Cheshire UK; [3]Sciex, Redwood Shores, CA*

WP 693 **Interference-free Multiplexed Quantification with Complement Reporter Ions: Technological Advances and Application to Nucleocytoplasmic Partitioning**; Martin Wuehr[1, 2]; Graeme C McAlister[3]; Thomas Güttler[2]; Brian K. Erickson[2]; Matthew Sonnett[2]; Ramin R. Rad[2]; Keisuke Ishihara[2]; Leonid Peshkin[2]; Aaron C. Groen[2]; Marc Presler[2]; Elizabeth Van Itallie[2]; Wilhelm Haas[4]; Timothy J. Mitchison[2]; Steven P. Gygi[2]; Marc W. Kirschner[2]; *[1]Princeton University, Princeton, NJ; [2]Harvard Medical School, Boston, MA; [3]Thermo Fisher Scientific, San Jose, CA; [4]Massachusetts General Hospital, Boston, MA*

WP 694 **Veracity or Serendipity? Contradicting Conjectures in Protein Quantification**; Russell P Grant[1]; Christopher M Shuford[1]; Patricia L Holland[1]; *[1]Laboratory Corporation of America, Burlington, NC*

WP 695 **A New and Easy Approach for End-User Driven Quantification of SIL Peptide Solutions in Targeted Proteomics**; Karsten Schnatbaum[1]; Lars Hornberger[1]; Johannes Zerweck[1]; Tobias Knaute[1]; Lawrence Eckler[2]; Ulf

Reimer[1]; Holger Wenschuh[1]; *[1]JPT Peptide Technologies GmbH, Berlin, Germany; [2]JPT Peptide Technologies, Berlin, Germany*

WP 696 **PRM Method Optimization on a Q-Exactive Plus Using a Well-Defined Quantitative Proteomics Standard**; Zhiyun Cao[1]; James J Walters[2]; Kevin B Ray[2]; *[1]MilliporeSigma, St. Louis, Missouri; [2]MilliporeSigma, St. Louis, MO*

WP 697 **Optimizing Experimental Design for Ultra-deep Discovery Proteomics of Breast Cancer Patient Derived Xenografts with Isobaric Peptide Labeling**; Qiang Zhang[1]; Robert Sprung[1]; Petra Erdmann-Gilmore[1]; Yiling Mi[1]; Rose Connors[1]; Sherri Davies[1]; Shunqiang Li[1]; Reid Townsend[1]; *[1]Washington University School of Medicine, Saint Louis, MO*

WP 698 **Development of Robust, Reproducible, High-Throughput Quantitative Proteomic Assays for Cellulosic Biofuel Applications**; Yan Chen[1]; Leanne Jade G Chan[1]; Héctor García Martín[1]; Paul D Adams[1]; Christopher J Petzold[1]; *[1]Lawrence Berkeley National Laboratory, Berkeley, CA*

WP 699 **Highly Multiplexed MRM-based Peptide Quantitation in Human Plasma Using Two Different Stable Isotope Labeled Peptides for Calibration**; André LeBlanc[1]; Sarah Michaud[2]; Andrew Percy[1]; Darryl B Hardie[1]; Juncong Yang[1]; Nicholas Sinclair[1]; Jillaine Proudfoot[1]; Adam Pistawka[1]; Derek S Smith[1]; Christoph H. Borchers[3, 4]; *[1]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [2]MRM Proteomics, Inc., Victoria, BC, Canada; [3]University of Victoria - Genome BC Proteomics Centre, Victoria, BC; [4]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada*

WP 700 **Second Generation Combinatorial Mass Tag (CMT) Isobaric Reagents with Improved Quantitative Precision**; Craig Braun[1]; Brian Erickson[1]; Gregory Bird[2]; Steven P Gygi[1]; *[1]Harvard Medical School, Boston, MA; [2]Dana Farber Cancer Institute, Boston, MA*

WP 701 **Utilizing Synthetic Peptides and Skyline for Validating Quantitative Changes in Bacterial Proteomics**; Chia-Fang Lee[1]; Chen-Hsun Tsai[1]; Lydia M. Contreras[1]; Maria D. Person[1]; *[1]University of Texas at Austin, Austin, TX*

WP 702 **A Peptide-Retrieval Strategy Enables Significant Improvement of Quantitative Performance Without Compromising Confidence of Identification**; Chengjian Tu [1]; Shichen Shen[1]; Quanhu Sheng[2]; Yu Shyr[2]; Jun Qu[1]; *[1]University at Buffalo, Buffalo, NY; [2]Vanderbilt University, Nashville, TN*

WP 703 **Multiplexing Quantification of Proteins by Single-Cell CE-μESI-HRMS Finds Translational Cell Heterogeneity in the 16-cell Frog (Xenopus) Embryo**; Camille Lombard-Banek[1]; Sally A Moody[1]; Peter Nemes[1]; Sushma Reddy[1]; *[1]The George Washington University, Washington, DC*

WP 704 **Secretome Profiling of Antibody-Producing CHO Cells using Non-Natural Amino Acid Crosslinking Pull Down and Mass Spectrometry**; Carlo Martins[1]; Raghothama Chaerkady[1]; Michael Bowen[1]; Deniz Baycin-Hizal[1]; *[1]MedImmune, Gaithersburg, MD*

SMALL MOLECULES: QUANTITATIVE ANALYSIS (PART 1) 705 - 728

WP 705 **Dilute and Shoot FI-MS/MS for Quantification of Glycocholic Acid in Human Bile using Standard Addition Method**; Raghavi Kakarla[1]; Ramakrishna reddy Voggu[1]; Janet R Donaldson[2]; Baochuan Guo[1]; *[1]Cleveland State University, Cleveland, OH; [2]Mississippi State University, Starkville, MS*

WP 706 **Development of Cost-Effective Liquid Chromatography-Tandem Mass Spectrometry Method for Polar Drugs and Metabolites**; Xiaodong Zhu[1]; Jingguo Hou[1]; Jerry Gardella[1]; Melvin Tan[1]; Tom Lloyd[1]; Edward Wells[1]; *[1]Worldwide Clinical Trials Drug Development Solution, Austin, TX*

WP 707 **Development and Validation of an Ultra Sensitive and Automated LC-MS/MS Method for the Measurement of Naloxone, Buprenorphine and Norbuprenorphine**; Nick Peng[1]; Ben Gaboury[1]; Nichole Boice[1]; Dan Pederson[1]; Ardeshir ardeshir khakang[1]; *[1]Axis Clinicals, Dilworth, MN*

WP 708 **Development and Validation of a Simple, Rugged and Automated LC-MS/MS Method for the Determination of Mesalamine in Human Plasma**; Nick Peng[1]; BEN GABOURY[1]; Sarah Maasjo[1]; Ardeshir Khadang[1]; *[1]Axis Clinicals, Dilworth, MN*

WP 709 **Simultaneous Determination of Tamsulosin and Solifenacin in Human Plasma by Ultra-High Performance Liquid Chromatography with Tandem Mass Spectrometry**; Jin Sun Woo[1]; Hwa Suk Kim[1]; Seo Hyun Yoon[1]; Joo-Youn Cho[1]; *[1]Seoul National University College of Medicine, Seoul, South Korea*

WP 710 **Applications of Improved GCMS Method for Fatty Acid Analysis in Samples from Bariatric Patients and Mice Fed Omega-3 Fatty Acids**; Kazimierz Surowiec[1]; Nadeeja N. Wijayatunga[1]; Latha Ramalingam[1]; Valerie G. Sams[2]; Gregory J. Mancini[2]; Matthew L. Mancini[2]; Yehia Mechref[1]; Naima Moustaid-Moussa[1]; *[1]Texas Tech University, Lubbock, TX; [2]University of Tennessee Medical Center, Knoxville, TN*

WP 711 **A Two-dimensional Liquid Chromatography (2D-LC) to Separate an Interference Peak from Norfentanyl for Its Successful Bioanalysis**; Moo-Young Kim[1]; Brendan Laing[1]; Fumin Li[1]; *[1]PPD, Middleton, WI*

WP 712 **Development and Validation of a LC-MS/MS Method for the Simultaneous Quantitation of Carboplatin and Etoposide in Human Plasma and Ultrafiltrate**; Jessica Sima[1]; Ganesh S Moorthy[2]; Athena Zuppa[2]; Elizabeth Fox[2]; *[1]Children's Hospital of Philadelphia, Philadelphia, PA; [2]Children's Hopsital of Philadelphia, Philadelphia, PA*

WP 713 **Highly Accurate Sample Collection, Handling and LCMSMS Bioanalysis of Liposomal Amphotericin B Plasma Samples**; Jason Bilodeau[1]; François Viel[1]; Nadine Boudreau[1]; Clark Williard[1]; *[1]inVentiv Health, Québec, Canada*

WP 714 **Determination of Unconjugated Naloxone, Conjugated Naloxone and Total Naloxone in Human Plasma by LCMSMS**; Louis-Charles Boisvert[1]; Nicolas Jean[1]; Guy Havard[1]; Philippe Belanger[1]; Marie-Josée Marcoux[1]; Sylvain Lachance[1]; Nadine Boudreau[1]; Clark Williard[1]; *[1]inVentiv Health, Québec, Canada*

WP 715 **Trace Level Quantitative Determination of Phthalates from High Risk Dosage Pharmaceutical Formulations using LC/MS/MS**; Purushottam Sutar[1]; Rashi Kochhar[1]; Deepti Bhandarkar[1]; Shailendra Rane[1]; Shailesh Damale[1]; Anant Lohar[1]; Ashutosh Shelar[1]; Jitendra Kelkar[1]; Pratap Rasam[1]; Ajit Datar[1]; *[1]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India*

WP 716 **Highly Sensitive Multiplexed Analysis of Levosalbutamol from Plasma using LC/MS/MS**; Ashutosh Shelar[1]; Shailesh Damale[1]; Shailendra Rane[1]; Purushottam Sutar[1]; Anant Lohar[1]; Deepti Bhandarkar[1]; Rashi Kochhar[1]; Pratap Rasam[1]; Jitendra Kelkar[1]; Ajit Datar[1]; *[1]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India*

WP 717 **Robust, Sensitive and Accurate Determination of Different Opioids in Human Plasma by LCMSMS**; Genevieve Emond[1]; Marc Fournier[1]; Marie-Claude Théberge[1]; Nathalie Pelletier[1]; Marie-Josée Marcoux[1]; Sylvain Lachance[1]; Nadine Boudreau[1]; Clark Williard[1]; *[1]inVentiv Health, Québec, Canada*

WP 718 **Simultaneous Assay of Multiple Synthetic Contraceptive Hormones in Human Serum by LCMS-MS**; Steven W Blue[1]; Rachel Lieberman[2]; David W Erikson[1]; Christopher Gilles[2]; *[1]Oregon National Primate Research Center, Beaverton, OR; [2]Shimadzu Scientific Instruments, Columbia, MD*

WP 719 **Highly Sensitive Automated Assay for the Determination of Oxytocin in Human Plasma by LC-MS/MS**; Nicolas Jean[1]; Philippe Bélanger[1]; Carine Lévesque[1]; Marie-Claude Théberge[1]; Nadine Boudreau[1]; Clark Williard[1]; Hermes Licea-Perez[2]; Jonathan Kehler[2]; Thomas Mencken[2]; *[1]inVentiv Health, Québec, Canada; [2]GlaxoSmithKline, Upper Merion, PA*

WP 720 **Quantification of Tenofovir and Emtricitabine in Human Plasma using High Throughput LDTD-MS/MS**; Jean Lacoursiere[1]; Annie-Claude Bolduc[2]; Alex Birsan[1]; Serge Auger[1]; Pierre Picard[1]; *[1]Phytronix Technologies, Inc. Quebec, Canada; [2]Université Laval, Québec, Canada*

WP 721 **A Sensitive LC-MS/MS Method for Quantitation of Naltrexone and 6ß-Naltrexol in Human Plasma (1 pg/mL)**; Dawei Zhou[1]; Shaoting Zhang[1]; Mohamed Osman[1]; Xinping Fang[1]; *[1]WuXi AppTec Co., Plainsboro, NJ*

WP 722 **Quantification of N-Hydroxy Riluzole Metabolite in Human Plasma: The Investigation of the Stability of the Analyte**; Luc Bouchard[1]; Nathalie Pelletier[1]; Sylvain Lachance[1]; Nadine Boudreau[1]; Clark Williard[1]; *[1]inVentiv Health, Québec, Canada*

WP 723 **Ultra-Sensitive LCMSMS Determination of Teriparatide in Human Plasma**; Philippe Bélanger[1]; Marie-Josée Marcoux[1]; Nadine Boudreau[1]; Clark Williard[1]; *[1]inVentiv Health, Québec, Canada*

WP 724 **Development of an Ultrasensitive Assay for Quantification of Free Ticagrelor in Plasma using Equilibrium Dialysis and LC-MS/MS**; Ann-Sofie Sandinge[1]; Annika Janefeldt[1]; *[1]AstraZeneca R&D, Gothenburg, Sweden*

WP 725 **Bioanalytical LC/MS/MS Method for the Determination of a Vitamin E analog in Human Plasma**; Jeff Jeppson[1]; Elizabeth Dibbern[1]; Ridha Nachi[1]; *[1]Celerion, Lincoln, NE*

WP 726 **Comparison of the Quantitation of Bile Acids using Full Scan and Targeted SIM Mode on using UPLC/HRAM MS**; Brandon Wilcock[1]; Lijuan Fu[1]; Nan Zhao[1]; Cassidy Hatch[1]; Nidhi Jaiswal[1]; Min Meng[1]; Troy Voelker[1]; Scott Reuschel[1]; *[1]Covance, Salt Lake City, UT*

WP 727 **A Selective and Ultra-Sensitive LC-MS/MS Method for Simultaneous Quantitation of Norgestrel and Norgestimate in Human Plasma**; Shuyu Hou[1]; Sheth Raj[1]; Hongkun Liang[1]; Yuan-Shek Chen[1]; Hsu Ben[1]; *[1]QPS, LLC, Newark, DE*

WP 728 **Rapid Analysis of Ceftriaxone in Human Intestinal Chyme, Human Plasma, and Dog Plasma by HPLC/MS/MS**; Todd Lusk[1]; John F Kokai-Kun[2]; Michael Schlosser[3]; Stacey Zeman[1]; Sara Brady[1]; Daniel 1 Mulvana[4]; Thad Yousey[5]; *[1]Q² Solutions Bioanalytical and ADME Labs, Ithaca, NY; [2]Synthetic Biologics, Inc., Rockville, MD; [3]MSR Pharma Services, Inc., Lincolnshire, IL; [4]Q² Lab Solutions Bioanalytical and ADME Labs, Ithaca, NY; [5]Quintiles, Ithaca, NY*

Set up all Thursday posters .....7:30 – 8:00 am
Odd-numbered posters present .....10:30 am – 1:00 pm
Even-numbered posters present .....12:00 – 2:30 pm
Remove all Thursday posters .....2:30 – 3:00 pm

AMBIENT IONIZATION: FUNDAMENTALS AND INSTRUMENTATION (DART/PLASMA, LASER, SAWN) 001 - 030

ThP 001 **Dopant-Assisted Direct Analysis in Real Time (DART) Ionization with Argon Gas**; Robert B. Cody[1]; A. John Dane[1]; *[1]JEOL USA Inc., Peabody, MA*

ThP 002 **Method Development of High Throughput Lipid Analysis in Foods by Direct Analysis in Real Time Mass Spectrometer (DART-MS)**; Jun Watanabe[1]; Sakakura Motoshi[2]; Shiota Teruhisa[2]; *[1]Shimadzu Corporation, Kyoto; [2]AMR Inc., Tokyo, Japan*

ThP 003 **Acoustically Levitated Drops: A Containerless Microreactor Coupled with Ambient Ionization Mass Spectrometry**; Elizabeth A Crawford[1]; Cemal Esen[2]; Dietrich A Volmer[1]; *[1]Saarland University, Saarbrücken, Germany; [2]Ruhr-University Bochum, Bochum, Germany*

ThP 004 **Application of Direct Analysis in Real Time-Mass Spectrometry to the Study of Oxidation of Skin Oil Components with Indoor Ozone**; Shouming Zhou[1]; Matthew Forbes[2]; Jonathan P D Abbatt[1]; *[1]University of Toronto, Toronto ON, Canada; [2]Department of Chemistry, University of Toronto, Toronto, ON*

ThP 005 **Development of a Flavor Release Analysis Method on Volatile Compounds of Citrus Fruits by DART MS**; Sagawa Takehiko[1]; Matsumoto Keiko[2]; Watanabe Jun[2]; Takei Chikako[3]; Sakakura Motoshi[4]; Shiota Teruhisa[4]; Matsufuji Hiroshi[5]; *[1]S & B Foods Inc., Tokyo, Japan; [2]Shimadzu Corporation, Kyoto, Japan; [3]Bio Chromato, Inc. Fujisawa, Japan; [4]AMR Inc., Tokyo, Japan; [5]Nihon University, Fujisawa, Japan*

ThP 006 **Direct Quantification Technique for Natural Moisturizing Factor (NMF) in Stratum Corneum by Direct Analysis in Real Time Mass Spectrometry (DART-MS)**; Katsuyuki Maeno[1]; Yasuo Shida[2]; Haruo Shimada[1]; *[1]Shiseido Global Innovation Center, Yokohama, Japan; [2]University of Yamanashi, Kofu, Japan*

ThP 007 **Accurate Quantification of Urinary Creatinine by Stable Isotope Dilution and DART Coupled to Quadrupole Time-of-Flight Mass Spectrometry**; Ning Zhang[1, 2]; Yuanyuan Song[1]; Meiling Lu[3]; Weibing Zhang[2]; Hailin Wang[1]; Xiaokun Duan[4]; Charles C. Liu[4]; *[1]Research Center for Eco-Environmental Sciences, Beijing, China; [2]East China University of Science and Technology, Shanghai, China; [3]Agilent Technologies (China) Limited, Beijing, China; [4]ASPEC Technologies LTD, Beijing, China*

ThP 008 **Research of Real-Time Monitoring Method for Volatiles in Chinese Liquor (Baijiu) Tasting**; Ming Liu[1]; Zijing Xu[2]; Jianghao Lu[1]; Yi Zhang[2]; Qiding Zhong[1]; Xiaomei Yuan[1]; Zhenghe Xiong[1]; Xiaokun Duan[3]; Kai Liu[3]; *[1]China National Research Institute of Food & Fermentation Industries, Beijing, China; [2]Sichuan Jiannanchun Group Co. Ltd, Mianzhu, Sichuan; [3]ASPEC Technologies LTD, Beijing, China*

ThP 009 **Screening Analysis of Primary Aromatic Amines in Textiles using DART-MS**; Yamamura Yutaro[1]; Maeda Kengo[2]; Jun Watanabe[3]; Sakakura Motoshi[4]; Shiota Teruhisa[4]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]Shimadzu Co., Kyoto, Japan; [3]Shimadzu Corporation, Kyoto; [4]AMR Inc., Tokyo, Japan*

ThP 010 **A Study of DART® as a Technique for Ambient Surface Analysis of Polymers**; Dana Reed[1]; Katri Huikko[1]; Steven Pachuta[1]; Ali Rafati[1]; *[1]3M Corporation, St. Paul, MN*

ThP 011 **On-line Coupling of Surface Plasmon Resonance to Ambient Mass Spectrometry**; Huwei Liu[1]; Yiding Zhang[2]; Yu Bai[2]; *[1]Peking University, Beijing; [2]Peking University, Beijing, China*

ThP 012 **An Interface for Online Coupling Surface Plasmon Resonance with Mass Spectrometry using Dielectric Barrier Discharge Ionization**; Yiding Zhang[1]; Yu Bai[1]; Huwei Liu[1]; *[1]Peking University, Beijing, China*

ThP 013 **Determination of Peroxide Explosives and Related Compounds by Dielectric Barrier Discharge Ionization-Mass Spectrometry (DBDI-MS)**; Sebastian Hagenhoff[1]; Heiko Hayen[1]; *[1]University of Muenster, Muenster, Deutschland*

ThP 014 **Surface Erosion and Analysis of Polymer Sample via Micro Dielectric Barrier Plasma Jet Mass Spectrometry**; Songyue Shi[1]; Xiaoxia Gong[1]; Xinyue Liang[1]; Gerardo Gamez[1]; *[1]Texas Tech University, Lubbock, TX*

ThP 015 **Low Temperature Plasma Desoption/Ionization Mass Spectrometry for Quantitative Analysis of Exhaled Breath Collected on Filter Substrates**; Xiaoxia Gong[1]; Songyue Shi[1]; Xinyue Liang[1]; Mohammad Choudhury[1]; Gerardo Gamez[1]; *[1]Texas Tech University, Lubbock, TX*

ThP 016 **Effects of Molecular Gas Addition on a Helium Flowing Atmospheric-Pressure Afterglow (FAPA) Ambient Desorption/Ionization (ADI) Source**; Sunil Badal[1]; Jacob T. Shelley[1]; *[1]Department of Chemistry and Biochemistry, Kent State University, Kent, OH*

ThP 017 **Reactive Ambient Mass Spectrometry with Flowing Atmospheric Pressure Afterglow**; Gerardo Gamez[1]; Xiaoxia Gong[1]; Xinyue Liang[1]; Songyue Shi[1]; Mohammad Choudhury[1]; *[1]Texas Tech University, Lubbock, TX*

ThP 018 **A Microwave Plasma for Simultaneous Molecular and Atomic Ambient Ionization of Solids**; Kenyon Evans-

Nguyen[1]; Jon Gerling[2]; Ashley Windom[3]; *[1]University of Tampa, Tampa, FL; [2]Gerling Applied Engineering, modesto, CA - California; [3]The University of Tampa, Tampa, FL*

ThP 019 **Automatic Analyte Ion Recognition and Background Removal for Ambient Mass Spectrometry Data Based on Cross Correlation**; Yi You[1]; Sunil P. Badal[1]; Jacob T. Shelley[1]; *[1]Department of Chemistry and Biochemistry, Kent State University, Kent, OH*

ThP 020 **Characterization of Chemical Noise in AP MALDI using LTQ and Orbitrap Mass Spectrometer**; eugene Moskovets[1]; Vladimir M Doroshenko[2]; Shelley N Jackson[3]; Amina S Woods[3]; *[1]MassTech Inc, Columbia , MD; [2]MassTech, Inc Columbia, MD; [3]NIDA-IRP, NIH Baltimore, MD*

ThP 021 **Magnetic-Field-Assisted Laser-Ablation Ambient Mass Spectrometry**; Yao Lu[1]; Yun Shen Zhou[1]; Lei Liu[1]; Xi Huang[1]; Yongfeng Lu[1]; *[1]Department of Electrical and Computer Engineering, University of Nebraska-Lincoln, Lincoln, NE*

ThP 022 **Sensitivity Improvement of Infrared Laser Atmospheric Pressure Ionization Mass Spectrometry by Synchronizing a Q-TOF Mass Spectrometer and the Laser Pulse**; Hashiya Homare[1]; Iguchi Yasunari[2]; Hazama Hisanao[2]; Awazu Kunio[2]; *[1]Osaka University, Suita; [2]Osaka University, Suita, Japan*

ThP 023 **Coaxial Gas Flow Enhances Sample Plume Transfer Efficiency for Remote Laser Ablation Electrospray Ionization Mass Spectrometry**; Jarod Fincher[1]; Brent Reschke[2]; Nicholas Morris[2]; Akos Vertes[1]; *[1]The George Washington University, Washington, DC; [2]Protea Biosciences, Inc. Morgantown, WV*

ThP 024 **Using Rapid Evaporative Ionisation Mass Spectrometry (REIMS) to Identify Microorganisms at Species Level from Pure and Mixed Cultures**; Simon Cameron[1]; Frankie Bolt[1]; Adam Burke[1]; Zsolt Bodai[1]; Alvaro Perdones-Montero[1]; Julia Balog[2]; Tamas Karancsi[2]; Daniel Simon[2]; Richard Schaffer[2]; Tony Rickards[3]; Kate Hardiman[1]; Monica Rebec[3]; Zoltan Takats[1]; *[1]Imperial College London, London, UK; [2]Waters Research Center, Budapest, Hungary; [3]Imperial College Healthcare NHS Trust, London, UK*

ThP 025 **Surface Acoustic Wave Nebulization Sample Introduction for Vacuum-Assisted Plasma Ionization**; Stephen Zambrzycki[1]; Matthew C Bernier[2]; Joel Keelor[2]; Sung Hwan Yoon[3]; David R Goodlett[3]; Facundo M Fernandez[2]; *[1]Georgia Institute of Technology, Atlanta, Georgia; [2]Georgia Institute of Technology, Atlanta, GA; [3]University of Maryland School of Pharmacy, Baltimore, MD*

ThP 026 **Surface Acoustic Wave Nebulization – Mass Spectrometry: A Tool for Rapid Analysis of Food Products**; Gloria S Yen[1]; Thomas Schneider[2]; Benjamin L Oyler[2]; Sung Hwan Yoon[2]; Tao Liang[2]; David P A Kilgour[3]; Erik Nilsson[1]; David R Goodlett[1, 2]; *[1]Deurion LLC, Seattle, WA; [2]University of Maryland, School of Pharmacy, Baltimore, MD; [3]Nottingham Trent University, School of Science & Technology, Nottingham, UK*

ThP 027 **Performance Characterization of Surface Acoustic Wave Nebulization for Lipid A Mass Spectrometric Analysis**; Tao Liang[1]; Thomas Schneider[2]; Sung Hwan Yoon[2]; Benjamin L Oyler[2]; Andrew Dennison[3]; Gloria S Yen[4]; Yue Huang[4]; Adam A Stokes[5]; Anthony J Walton[3]; Robert K Ernst[6]; Erik Nilsson[4]; David R Goodlett[2, 4]; *[1]University of Maryland School of Pharmacy, Baltimore, MD; [2]School of Pharmacy, University of Maryland Baltimore, MD; [3]School of Chemistry, The University of Edinburgh, Edinburgh, UK; [4]Deurion LLC, Seattle, WA; [5]School of Engineering The University of Edinburgh, Edinburgh, UK; [6]University of Maryland Baltimore School of Dentistry, Baltimore, MD*

ThP 028 **Surface Acoustic Wave Nebulization – Mass Spectrometry on a TripleTOF Mass Spectrometer**; Thomas Schneider[1]; Benjamin L Oyler[1]; Larry J Campbell[2]; Yves J C LeBlanc[3]; Tom Covey[3]; Gloria S Yen[4]; Erik Nilsson[4]; David R Goodlett[1]; *[1]University of Maryland School of Pharmacy, Baltimore, MD; [2]AB SCIEX, Concord, Canada; [3]AB SCIEX, Concord ON, Canada; [4]Deurion LLC, Seattle, WA*

ThP 029 **Rapid Identification of Adulterated Edible Oils by DART-QTOF system**; Tanxi Cai[1]; Xiaokun Duan[2]; Peng Wu[3]; Lili Niu[3]; Fuquan Yang*[3]; Charles C. Liu[2]; *[1]Institute of Biophysics, CAS, Beijing, China; [2]ASPEC Technologies LTD, Beijing, China; [3]Institute of Biophysics, CAS beijing, China*

ThP 030 **Analysis of Metallocene using Atmospheric Pressure Chemical Ionization and Atmospheric Pressure Photo Ionization Coupled with Ion Mobility Mass Spectrometry**; Mathilde Farenc[1, 2, 3]; Budagwa Assumani[1,3]; Carlos Afonso[2, 3]; Pierre Giusti[1, 3]; *[1]TOTAL Refining and Chemicals, TRTG Gonfreville l'Orcher, France; [2]Normandie Univ, CNRS UMR 6014 COBRA Mont St Aignan, France; [3]TOTAL RC - CNRS Joint Laboratory C2MC :Complex Matrices Molecular Characterization, France*

BIOMARKERS: DISCOVERY (PART 2)
031 - 058

ThP 031 **Non-Target Urinary and Serum Metabonomic Study of Radix Astragali Treated on Rheumatoid Arthritis Rats Using UPLC-Q-TOF-HDMS**; Zhiqiang Liu[1]; Tengfei Xu[1]; *[1]Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun, CN*

ThP 032 **Potential Diagnostic Biomarkers and Pathway Analysis of Ovarian Cancer by Lipidomics**; Yangyang Zhang; *Institute of Chemistry,Chinese Academy of Sciences, Beijing, China*

ThP 033 **Death Domain Associated Protein DAXX May Regulate a Distinct Lipid Metabolism Signature in Breast Cancer**; Iqbal Mahmud[1]; Timothy J Garrett[1]; Daiqing Liao[1]; *[1]University of Florida, Gainesville, FL*

ThP 034 **Identification of Unusual Bile Acids as Biomarkers for Niemann-Pick C Disease Using Charge-Remote Fragmentation of N-(4-Aminomethylphenyl)Pyridinium Derivatives**; Xuntian Jiang[1]; Laurel Mydock[1, 2]; Fong-Fu Hsu[1]; Douglas Covey[1]; David E Scherrer[1]; Rohini Sidhu[1]; Forbes D Porter[3]; Nicole M Yanjanin[3]; Dennis J Dietzen[1]; Jean Schaffer[1]; Daniel Ory[1]; *[1]Washington University in St. Louis, St. Louis, MO; [2]Washington University in St. Louis, St Louis, MO; [3]NIH/NIAID, Bethesda, MD*

ThP 035 **Human Plasma Lipidome Variations in Active Tuberculosis**; Huipeng Neo[1, 2, 3]; Shanshan Ji[4]; Federico Torta[4]; Anne K Bendt[4]; Cynthia Chee[5]; Yee Tang Wang[5]; Pavanish Kumar[6]; Bhairav Paleja[6]; Amit Singhal[6]; Gennaro De Libero[6]; Markus R Wenk[4]; *[1]NUS Singapore, Singapore, Singapore; [2]Agilent Technologies Pte Ltd, Singapore, Singapore; [3]Department of Biological Sciences, Singapore, Singapore; [4]National University of Singapore, Singapore, Singapore; [5]Tuberculosis Unit, Tan Tock Seng Hospital, Singapore, Singapore; [6]Singapore Immunology Network (SIgN), A*STAR, Singapore, Singapore*

ThP 036 **Mass Spectrometry-Based Metabolomics for Biomarker Discovery after Angioplasty**; Yatao Shi[1]; Bowen Wang[1]; Xudong Shi[1]; Lian-Wang Guo[1]; K. Craig Kent[1]; Lingjun Li[1]; *[1]University of Wisconsin-Madison, Madison, WI*

ThP 037 **Lysophosphatidylinositol: A Novel Biomarker of Ischemia and a Potential Prognostic Indicator of Cardiac Arrest**; Koichiro Shinozaki[1]; Tai Yin[1]; Junhwan Kim[1]; *[1]The Feinstein Institute for Medical Research, Manhasset, NY*

ThP 038 **Following Biomarkers of Central Metabolism in Muscles from Diabetic Mouse Model: Metabolic Pathway Imaging**; Juliette Masure[1]; Gregory Hamm[1]; Philippe Delataille[2]; Corinne Foucart[2]; David Bonnel[1];

Carole Belanger[2]; Raphael Darteil[1]; Jonathan Stauber[1]; *[1]ImaBiotech, MS Imaging Dept. LOOS, France; [2]Genfit, Loos, France*

ThP 039 **Analysis of Volatile Organic Compounds in Pleural Effusions by HS-SPME-cryo-trap-GC/MS**; Zhongping Huang[1]; Jie Zhang[1]; Huijun Liu[1]; Lili Wang[1]; *[1]Zhejiang University of Technology, Hangzhou, China*

ThP 040 **Controlling the Misuse of Anabolic Steroids by Steroidal Biomarkers Profiling**; Kin-Sing Wong[1]; George H.M. Chan[1]; Emmie N.M. Ho[1]; Terence S.M. Wan[1]; *[1]Racing Laboratory, The Hong Kong Jockey Club, Hong Kong, China*

ThP 041 **Serum Total Fatty Acids as Potential Biomarkers for Differentiate Benign Lung Diseases from Lung Cancer**; Junling Ren[1]; Zhili Li[2]; *[1]Institute of Basic Medical Sciences, CAMS & PUMC, Bejing, CN; [2]IBMS, CAMS&PUMC, Beijing*

ThP 042 **Modeling the Exposome Paradigm: Exposure Analysis of the Western Honey Bee**; Chloe Wang[1]; Malia Wenny[1]; Robert L Broadrup[1]; Christopher Mayack[2]; Anthony Macherone[3, 4]; *[1]Haverford College, Haverford, PA; [2]Swarthmore College, Swarthmore, PA; [3]Agilent Technologies, Wilmington, DE; [4]Johns Hopkins University School of Medicine, Baltimore, MD*

ThP 043 **Proteomics of Human Plasma in Heart Failure with Preserved Ejection Fraction (HFpEF) using Novel Chemical Affinity, Mixed Mode Matrix (M3)**; Richard Mbasu[1]; Donald DL Jones[2]; Liam M Heaney[2]; Leong L Ng[2]; Sandhu K Jatinderpal[2]; Paulene Quinn[2]; Daniel C Chan[2]; *[1]University of Leicester, Leicester, Leicestershire; [2]University of Leicester, Leicester, UK*

ThP 044 **Mass Spectrometry Based Proteomics to Investigate and Characterize the Jumping Translocation Breakpoint (JTB) Protein using Cancer Cell Lines**; Devika Channaveerappa[1]; Kangning Li[1]; Costel C. Darie[1]; *[1]Clarkson University, Potsdam, NY*

ThP 045 **Label-free Shotgun Proteomics Identifies Markers of Inflammation from Fetal Fibroblasts**; Owen E Branson[1]; Brian C Wulff[1]; Miranda L Gardner[1]; Traci A Wilgus[1]; Michael A. Freitas[1]; *[1]Ohio State University, Columbus, OH*

ThP 046 **Mass Spectrometry Based Proteomic Investigation of Plasma Samples from Children with Autism Spectrum Disorder (ASD) and Matched Controls**; Kelly Wormwood[1]; Megan M Borland[1]; Emmalyn J Dupree[1]; Alisa G Woods[1]; Blythe Corbett[2]; Costel C Darie[1]; *[1]Clarkson University, Potsdam, NY; [2]Vanderbilt University, Nashville, TN*

ThP 047 **Using LC-MS/MS and Stable Isotope Tracers to Explore Circulating Biomarkers for the Kinetics of Liver Fibrosis** ; Haihong Zhou[1]; Yangqing Kan[2]; Ying Chen[2]; Ye Tian[2]; Yongcheng Huang[2]; Yonghua Zhu[2]; Taro Akiyama[2]; David Kelley[2]; Stephen Previs[2]; Shirly Pinto[2]; *[1]Merck & Co., Inc., Kenilworth, NJ; [2]Merck & Co, Kenilworth, NJ*

ThP 048 **Quantitative Proteomic Analysis of Serum Exosomes from Patients with Pancreatic Cancer Reveals the Differentially Expressed Proteins after Chemo-/Radio-Treatment**; Mingrui An[1]; Zhijing Tan[2]; Jianhui Zhu[2]; Jing Wu[2]; Jun Cao[2]; Rui Yang[2]; Xiucong Pei[2]; David M. Lubman[2]; *[1]University of Michigan, Ann Arbor, MI; [2]University of Michigan Medical Center, Ann Arbor, MI*

ThP 049 **Development of an Integrated and Effective Pipeline for Profiling Microbial Proteins from Mouse Fecal Samples by LC-MS/MS**; Jing Wu[1]; Jianhui Zhu[1]; Haidi Yin[1]; Mingrui An[1]; Nicholas Pudlo[1]; Eric Martens[1]; Grace Chen[1]; David M Lubman[1]; *[1]University of Michigan Medical Center, Ann Arbor, MI*

ThP 050 **CD90 Expression is Associated with Pancreatic Intraepithelial Neoplasias**; Xiucong Pei[1]; Jianhui Zhu[1]; Rui Yang[1]; Jiaqi Shi[2]; Zhijing Tan[1]; Mingrui An[1]; David M Lubman[1]; *[1]University of Michigan Medical Center, Ann Arbor, MI; [2]University of Michigan Medical School, Ann Arbor, MI*

ThP 051 **Facilitate Biomarker Discovery using Integrated "Omics" Differential Analysis with High Resolution Accurate LC/MS Approach**; Reiko Kiyonami[1]; Julian A Saba[2]; Sergei I Snovida[3]; David Peake[2]; Devin Drew[2]; Andreas Huhmer[2]; Ken Miller[2]; *[1]ThermoFisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific, Rockford, IL*

ThP 052 **Proteomic Analysis of Minute Amount of Colonic Biopsy Samples from Patients by Enteroscopy for Biomarker Discovery**; Xing Liu[1]; Zhou Hu[1]; Xu Yanli[2]; *[1]Chinese Academy of Sciences, Shanghai, China; [2]Fuyang People's Hospital, Fuyang, China*

ThP 053 **Early Diagnostic Biomarkers for Acute Liver Transplantation Rejection**; Su Jung Kim[1]; Ji Hyun Kim[1]; Na Young Kim[1]; Shin Hwang[2]; Hyun Ju Yoo[3]; *[1]Asan Institute for Life Sci, Asan Medical Center Seoul, South Korea; [2]Dep. Liver Transplantation and Heptobiliary Surgery, Asan Medical Center, Seoul, Republic of Korea; [3]Biomedical Research Center, Asan Institute for Life Sciences, Asan Medical Center, Seoul, Seoul*

ThP 054 **The Identification of Biomarkers of Normobaric Hypoxia and Recovery via Exhaled Breath**; Sean Harshman[1]; Brian Geier[2]; Leslie Drummond[3]; Laura Flory[2]; Maomian Fan[4]; Jeffrey Phillips[3]; Darrin Ott[5]; Claude Grigsby[4]; *[1]UES Inc, Air Force Research Laboratory, WPAFB, OH; [2]UES, WPAFB, OH; [3]Naval Medical Research Unit-Dayton, WPAFB, OH; [4]Air Force Research Laboratory, WPAFB, OH; [5]US AF School of Aerospace Medicine, WPAFB, OH*

ThP 055 **Integration of Tissue and Urine Proteomes for Biomarker Discovery and Verification of Renal Cell Carcinoma**; Yi-Ting Chen[1, 2, 3]; Chien-Lun Chen[4, 5]; Jau-Song Yu[2, 3]; Pei-Chia Wang[2]; Hsiao-Wei Chen[2]; Ying-Hsu Chang[6, 7]; Yu-Sun Chang[2, 3]; Ting Chung[2]; Tsung-Shih Lin[2]; *[1]Department of Biomedical Sciences, College of Medicine, Chang Gung University, Taoyuan, Taiwan; [2]Molecular Medicine Research Center, College of Medicine, Chang Gung University, Taoyuan, Taiwan; [3]Graduate Institute of Biomedical Sciences, College of Medicine, Chang Gung University, Taoyuan, Taiwan; [4]Department of Urology, Chang Gung Memorial Hospital, Taoyuan, Taiwan; [5]School of Medicine, College of Medicine, Chang Gung University, Taoyuan, Taiwan; [6]Division of Urology, Department of Surgery; LinKou Chang Gung Memorial Hospital, Taoyuan, Taiwan; [7]Graduate Institute of Clinical Medical Sciences, College of Medicine, Chang Gung University, Taoyuan, Taiwan*

ThP 056 **N-terminal Endogeneous Fragments of Tau in Human Cerebrospinal Fluid**; Gunnar Brinkmalm[1]; Claudia Cicognola[1]; Erik Portelius[1]; Henrik Zetterberg[1, 2]; Kaj Blennow[1]; Kina Höglund[1, 3]; *[1]University of Gothenburg, Mölndal, Sweden; [2]UCL Institute of Neurology, London, UK; [3]Karolinska Institutet, Huddinge, Sweden*

ThP 057 **Developing a Lysosomal Panel for Biomarker Discovery in Neurodegenerative Diseases using PRM**; Simon Sjödin[1]; Gunnar Brinkmalm[1]; Annika Öhrfelt[1]; Henrik Zetterberg[1, 2]; Kaj Blennow[1]; Ann Brinkmalm[1]; *[1]University of Gothenburg, Mölndal, Sweden; [2]UCL Institute of Neurology, London, UK*

ThP 058 **Longitudinal Profiling of Type 1 Diabetes Human Plasma Using TMT10-based Quantitative Proteomics Approach**; Chih-Wei Liu[1]; Lisa Bramer[2]; Bobbie-Jo Webb-Robertson[2]; Kathleen Waugh[3]; Marian J Rewers[3]; Qibin Zhang[1]; *[1]University of North Carolina at Greensboro, Greensboro, NC; [2]Pacific Northwest National Laboratory, Richland, WA; [3]University of Colorado School of Medicine, Aurora, CO*

BIOMARKERS: QUANTITATIVE ANALYSIS (SMALL MOLECULES & METABOLITES) 059 - 089

ThP 059 **Profiling of Medium-to-Long Chain acyl-CoAs Converted from Metabolism of Exogenous Fatty Acids in Mammalian Cells using LC-MS/MS**; Xiangkun Yang; *University of Georgia, Athens, GA*

ThP 060 **A Validated Multiplex Assay for the Quantification of Tryptophan and Four of Its Catabolites in Human Plasma and Cerebrospinal Fluid**; Joachim Hoke[1]; Andre Liesener[2]; Stefan Blech[1]; *[1]Boehringer Ingelheim Pharma GmbH & Co KG, Biberach, Germany; [2]Boehringer Ingelheim Pharma GmbH & Co. KG, Biberach an der Riss, Germany*

ThP 061 ***In vivo* Metabolic Profiling of the TCA Cycle**; Stephanie Dale[1]; Sheerin Shahidi-Latham[1]; E. Ellen Jones[1]; Cristine Quiason[1]; *[1]Genentech Inc, South San Francisco, CA*

ThP 062 **Comprehensive Profiling of Neurotransmitters in Cerebrospinal Fluid by LC-MS/MS**; Kanta Horie[1]; Yoshiaki Sato[1]; Takashi Kosasa[1]; Takeyasu Tomioka[1]; Motohiro Shiotani[1]; Makoto Ogo[1]; Yoshiya Oda[2]; *[1]Eisai Co. Ltd., Tsukuba, Japan; [2]Eisai Inc, Woodcliff Lake, NJ*

ThP 063 **Development of a Quantitative LC-MS Assay to Evaluate Depletion of Wall Teichoic Acid in Staphylococcus Aureus.**; Olga Berejnaia; *Merck & Co., Inc., Rahway, NJ*

ThP 064 **Validation of a High-Throughput Assay for the Quantification of Unbound and Total Desmosine and Isodesmosine in Human Plasma**; Andre Liesener[1]; Joachim Hoke[2]; Stefan Blech[2]; *[1]Boehringer Ingelheim Pharma GmbH & Co. KG, Biberach an der Riss, Germany; [2]Boehringer Ingelheim Pharma GmbH & Co KG, Biberach, Germany*

ThP 065 **Rapid Quantitative Analysis of 15 Major Bile Acids in Human Serum by UPLC-Tandem Mass Spectrometry**; Tian-Sheng Lu[1]; Aiping Zhu[1]; Wanqing Lu[1]; Emily Epure[1]; Yong-Xi Li[1]; *[1]Medpace Bioanalytical Laboratories, Cincinnati, OH*

ThP 066 **A Simultaneous Quantification Method Oftricarboxylic Acid Cycleprecursors and Intermediates**; Paul Rainville[1]; Robert Plumb[1]; Jose Castro-Perez[1]; James Langridge[1]; *[1]Waters, Milford, MA*

ThP 067 **Challenges in Development of LC-MS Methods for Highly Polar, Low Molecular Weight Compounds: A Quantitative Assay for Quinolinic Acid**; Regina Oliveira[1]; Asoka Ranasinghe[1]; Joelle M Onorato[1]; Celia D'Arienzo[1]; Petia A Shipkova[1]; *[1]Bristol-Myers Squibb, Princeton, NJ*

ThP 068 **Development and Validation of a Method for the Determination of Total Plasma Cholesterol Levels to Support 4β-Hydroxycholesterol Biomarker Studies**; Mark Leahy[1]; Matt Byers[1]; Victoria Jennings[2]; Joanne Hanson[2]; *[1]Covance, Madison, WI; [2]Covance, Harrogate, UK*

ThP 069 **Chiral Chromatography-Stable Isotope Dilution-Multiple Reaction Monitoring Mass Spectrometry for Characterization and Quantification of Complex Lipids in Human Biological Matrices**; Reza Nemati Josheghani[1]; Christopher Dietz[1]; Emily Anstadt[2]; Robert Clark[2]; Michael Michael Smith[1]; Frank Nichols[2]; Xudong Yao[1]; *[1]University of Connecticut, Storrs, CT; [2]University of Connecticut, Farmington, CT*

ThP 070 **Simultaneous Determination of Dehydroepiandrosterone (DHEA) and 17-Hydroxyprogesterone (17-OHP) in Human Plasma using LC-MS/MS**; Guangnong Zhang[1]; Gaungchun Zhou[1]; Feng Yin[1]; Morgan Byrd[1]; Tian-Sheng Lu[1]; Yong-Xi Li[1]; *[1]Medpace Bioanalytical Laboratories, Cincinnati, OH*

ThP 071 **Quantitative Analysis of Serum 2-Hydroxyglutarate using Gas Chromatography-Mass Spectrometry**; Salil Kumar Bhowmik[1, 2]; Nagireddy Putluri[1, 3]; Arun Sreekumar[1,2,4]; *[1]Dept. of Molecular and Cell Biology, Baylor College of Medicine, Houston, TX; [2]Alkek Center for Molecular Discovery, Baylor College of Medicine, Houston, TX; [3]Advanced Technology Core, Baylor College of Medicine, Houston, TX; [4]Verna and Marrs McLean Department of Biochemistry, Baylor College of Medicine, Houston, TX*

ThP 072 **Scaling Up: Improving Automated, High Throughput Measurement of Tobacco-Specific Nitrosamines in Urine by Liquid Chromatography-Atmospheric Pressure Ionization Tandem Mass Spectrometry**; Baoyun Xia[1]; Christina R Brosius[2]; Yang Xia[1]; Tonya Guillot[1]; John Lee[1]; Keegan J Nicodemus[2]; Dana Freeman[2]; Justin Lamar Brown[2]; Li Zhang[3]; Lanqing Wang[1]; *[1]Centers for Disease Control and Prevention, Atlanta, GA; [2]ORISE Centers for Disease Control and Prevention, Atlanta, GA; [3]Battelle Memorial Institute, Atlanta, GA*

ThP 073 **A Simple, Robust Method for Quantitative Analysis of Bile Acid Biomarkers in Human, Monkey, Dog, Mouse, and Rat Plasma Samples**; Angela Qi Shen[1]; Alyssa Kabat[1]; Wenlin Yuan[1]; Ritika Kurian[1]; Brittany Perley[1]; Steven Wiltshire[1]; *[1]Agilux Laboratories, Worcester, MA*

ThP 074 **Quantitation of 2-Hydroxyglutarate and α-Ketoglutarate: Impact of Matrix Selection**; Vikki M Tsefrikas[1]; Kyle S. Goodsell[1]; Dylan S. Bennett[1]; David Brigham[1]; Allysen Meymaris[1]; *[1]Agilux Laboratories, Worcester, MA*

ThP 075 **Identification of Plasma Phospholipids that Distinguish Normal Subjects from Asthma Patients and Separating Patients of Lower Airway Diseases**; Hay-Yan J. Wang[1]; Zhi-Fu Zheng[2]; Kuan-Lun Su[2]; Chau-Chyun Sheu[3]; Shau-Ku Huang[4]; *[1]National Sun Yat-Sen University, Kaohsiung , Taiwan; [2]National Sun Yat-Sen University, Kaohsiung, Taiwan; [3]Kaohsiung Medical University Hospital, Kaohsiung, Taiwan; [4]National Health Research Institutes, Miaoli, Taiwan*

ThP 076 **Quantitation of the Organic Acid Biomarkers Pyruvate and Lactate in Biological Matrices**; Dylan Bennett[1]; Allysen Meymaris[1]; Vikki Tsefrikas[1]; *[1]Agilux Laboratories, Worcester, MA*

ThP 077 **Quantitative Analysis of Short Chain Fatty Acids and Ketone Bodies in Plasma and Tissues as Oximes Derivatives by LC-MS/MS** ; Huachuan Marc Cao[1]; Mingfei Zeng[1]; *[1]Eli Lilly and Company, Shanghai, China*

ThP 078 **Quantitation of (C22:6)-bis(monoacylglycerol) phosphate and Profiling of Additional BMPs in Rat Urine as Markers of Phospholipidosis**; Joelle Onorato[1]; Petia Shipkova[2]; Mike Reily[3]; Yan He[2]; David Nelson[2]; Lois Lehman-McKeeman[2]; *[1]Bristol-Myers Squibb, Princeton, NJ; [2]Bristol-Myers Squibb Co., Princeton, NJ; [3]Bristol Myers Squibb, Princeton, NJ*

ThP 079 **Identification and Quantification Method for 2AG, 1AG and Arachidonic Acid in Plasma, CSF and Brain by LC-MS/MS:** ; Shakey Quazi; *Pfizer, Andover, MA*

ThP 080 **Quantitative Analysis of D-Alanine in Cerebral Spinal Fluid Using a Chiral HPLC Coupled with High Resolution Mass Spectrometry**; Brendan Tierney[1]; Christopher Holliman[1]; Hongying Gao[1]; *[1]Pfizer, Inc., Groton, CT*

ThP 081 **High Throughput UPLC-MS/MS Method for the Profiling of 11 Hydrosoluble Vitamins in Human Plasma**; Oksana Lavrynenko[1]; Serge Rezzi[1]; *[1]NIHS, Molecular Nutrition Group, Lausanne, CH*

ThP 082 **Detection of Aromatic Amines in Human Urine at ppt Level: a Semi-Automated Hamilton STAR/GC/MS/MS Method**; Tiffany Seyler[1]; Elizabeth Cowan[1]; Susan Pyatt[2]; Aaron Danberry[3]; Kyle Emer[1]; *[1]CDC, Atlanta, GA; [2]Former Associate Fellow, Atlanta, GA; [3]Former ORISE Fellow, Atlanta, GA*

ThP 083 **LC-MS/MS Quantitative Analysis of the Biomarkers Tryptophan, Kynurenine, and Kynurenic Acid in Mouse and Rat Plasma and Brain**; Alyssa Kabat[1]; Brittany Perley[1]; Steven Wiltshire[1]; *[1]Agilux Laboratories, Worcester, MA*

ThP 084 **Bioactivation of Heterocyclic Aromatic Amines by UDP Glucuronosyltransferases**; Tingting Cai[1]; Lihua Yao[1]; Robert Turesky[1]; *[1]University of Minnesota at Twin Cities, Minneapolis, MN*

ThP 085 **Urine Steroid Metabolite Profiling Using LC-HRAMS for Diagnosing Adrenal Cortical Carcinoma**; Jolaine Hines[1]; Irina Banocs[1]; Robert L Taylor[1]; Raman Deep Singh[1]; Aditya V Avula[1]; Stefan K Grebe[1]; Ravinder J Singh[1]; *[1]Mayo Clinic, Rochester, MN*

ThP 086 **Quantification of Lathosterol in Human Plasma Using UPLC-MS/MS System**; Guangchun Zhou[1]; Tian-Sheng Lu[1]; Nicole Greer[1]; Yong-Xi Li[1]; *[1]Medpace Bioanalytical Laboratories, Cincinnati, OH*

ThP 087 **Determination of Amino Acids and Biogenic Amines in Plasma and Urine in Cri Du Chat Disease by Mass Spectrometry**; Danielle Zildeana Furtado[1]; Leticia Dias Lima Jedlicka[1]; Heron Domingues Silva[1]; Nilson Antonio Assunção[1, 2]; *[1]UNIFESP, São Paulo, Brasil; [2]The Scripps Research Institute, La Jolla, CA*

ThP 088 **Multiplex Quantitative Localized Analysis of Metal-Tagged Antibodies using Event-By-Event Cluster Secondary Ion Mass Spectrometry**; Dmitriy Verkhoturov[1]; Kyungjin Son[2]; Stanislav V Verkhoturov[1]; Michael J Eller[1]; Alexander Revzin[2]; Emile A Schweikert[1]; *[1]Texas A&M University, College Station, TX; [2]University of California-Davis, Davis, CA*

ThP 089 **Improvements in LFQ for Reproducible Quantification of Proteomic Experiments: How DDA Outperforms DIA**; Ignacio Ortea[1]; Michael Blank[2]; Romain Huguet[2]; David M Horn[2]; Daniel Lopez Ferrer[3]; Andreas Huhmer[2]; *[1]IMIBIC, Cordoba, Spain; [2]Thermo Fisher Scientific, San Jose, CA; [3]ThermoFisher, Palo Alto, CA*

DRUG METABOLISM: QUANTITATIVE ANALYSIS
090 - 107

ThP 090 **Anti-Cancer Drug Detection at the Single Cell Level**; Shawna Standke[1]; Ning Pan[1]; Naga Rama Kothapalli[1]; Zhibo Yang[1]; Anthony W. Burgett[1]; *[1]University of Oklahoma, Dept. of Chem & Biochem Norman, OK*

ThP 091 **Comparative Studies on Intrinsic Clearance Predication of Low Turnover Compounds Using the Regular and Relay Cryopreserved Hepatocyte Methods**; Min Jiang[1]; Zhican Wang[2]; Dan Rock[2]; *[1]Amgen, South San Francisco, CA; [2]Amgen, Inc. South San Francisco, CA*

ThP 092 **Evaluation of QTOF HRMS Platform for Highly Sensitive Analysis of Raltegravir in Plasma in Support of Human Microdosing**; Li Sun[1]; Kevin Bateman[1]; Sukhdev Bangar[2]; Yun W Alelyunas[3]; Mark Wrona[3]; Sheila Breidinger[1]; Eric Woolf[1]; *[1]Merck & Co., Inc., West Point, PA; [2]Waters Corporation, Beverly, MA; [3]Waters, Milford, MA*

ThP 093 **Characterization of Ketamine Metabolism in Liver S9 Fractions from Aging Sprague Dawley Rats by Liquid Chromatography Tandem Mass Spectrometry**; Raphaël Santamaria[1]; Marie-Chantal Giroux[1]; Pascal Vachon[1]; Francis Beaudry[1]; *[1]Université de Montréal, St-Hyacinthe, QC*

ThP 094 **Methods for Analysis of Hydroxywarfarin Regio- and Stereoisomers in Bioanalytical Samples**; Karin Keller[1]; Laura Drake[1]; Crystal D Sergent[1]; Edward Wells[1]; Steve E Unger[1]; *[1]Worldwide Clinical Trials, Austin, TX*

ThP 095 **Determination of Cariprazine and Metabolites in Human Plasma by LC-MS/MS**; Jing Ke[1]; Guiyan Chen[1]; Allan Xu[1]; *[1]Keystone Bioanalytical Inc, North Wales, PA*

ThP 096 **Characterization of clozapine-N-oxide using LC-MS/MS**; Jeffrey F Kuhn[1]; Yu-wei Chen[1]; Patricia Jensen[1]; Leesa Deterding[1]; *[1]NIEHS, RTP, NC*

ThP 097 **Development and Validation of a Novel Enzyme Inhibition Assay for Determination of Statin Acid in Human Plasma using LC-MS/MS**; Yanjun Hu[1]; Huafang Jiang[1]; Junxian Zhao[2]; Wanhui Liu[2]; Xinping Fang[1]; Xin Zhang[1]; Wenzhong Liang[3]; *[1]WuXi AppTec (Shanghai) Co. Ltd., Shanghai, China; [2]Luye Pharma Group Co., Ltd, Yantai, China; [3]WuXi AppTec (Shanghai) Co. Ltd., Shanghai, Shanghai*

ThP 098 **Development and Validation of the Determination of Total CRS3123 in Human Urine by High Performance Liquid Chromatography Tandem Mass Spectrometry**; X. Steven Yan[1]; Marsha L. Luna[1]; ChenYu Chung[1]; Julie Showalter[1]; Yansheng Liu[1]; Matthew E Hinz[2]; *[1]KCAS Bioanalytical & Biomarker Services, Shawnee, KS; [2]DynPort Vaccine Company, Frederick, MD*

ThP 099 **LC-MS/MS Method for the Quantification of Fingolimod and Fingolimod Phosphate in Rat blood with Storage Stability**; Rajesh Kumar Boggavarapu[1]; Nagasurya Prakash Padala[1]; Praveen kunduru[1]; Devender Reddy Ajjala[1]; Ramakrishna Nirogi[1]; *[1]Suven Life Sciences Ltd, Hyderabad, Telangana*

ThP 100 **Testing the Ability of UBP-310 to Diffuse into Mouse Brain via LC-MS/MS (QQQ) Quantification**; Sandy Stayte[1]; Russell Pickford[2]; Justin Nash; Bryce Vissel[1]; *[1]Garvan Institute, Sydney, Australia; [2]University of New South Wales, Sydney, Australia*

ThP 101 **Solving the Enigma of Nitrate Tolerance with a Stable Isotope-Assisted, Multi-Platform Work Flow**; Elizabeth Axton[1]; Eleonso Cristobal[1]; Fred Stevens[1]; *[1]Oregon State University, Corvallis, OR*

ThP 102 **Using Triplicate Calibration Curves and Weighted Least Squares Regression to Reduce Experimental Error**; Kenneth Anderson[1]; Kevin P Bateman[2]; *[1]Merck & Co, Inc., West Point, PA; [2]Merck & Co., Inc., West Point, PA*

ThP 103 **Systematic Investigation of the Failure of One Analyte during Method Transfer and Cross Check of a 4-in-1 LC-MS/MS Method**; Bian Chao[1]; Daniel Neddermann[2]; Lihua Qiao[1]; Yixin Yang[1]; Liang Wenzhong[1]; Xin Zhang[1]; *[1]WuXi AppTec (Shanghai) Co. Ltd., Shanghai, China; [2]Novartis Pharma AG, Basel, Switzerland*

ThP 104 **Ionization Efficiency of Oligopeptides and Small Hydrophilic Molecules in ESI/MS**; Piia Liigand[1]; Karl Kaupmees[1]; Anneli Kruve[1]; *[1]University of Tartu, Institute of Chemistry, Tartu, Estonia*

ThP 105 ***In-vitro* Metabolic Stability and Profiling of Ponatinib, Vandetanib and Masitinib using Liquid Chromatography Tandem Mass Spectrometry**; Sawsan M Amer[1]; Adnan A. Kadi[2]; Hany W Darwish[1, 2]; Mohamed W. Attwa[1, 2]; *[1]College of Pharmacy, Cairo University Cairo, Egypt; [2]College of Pharmacy, King Saud University Riyadh, Saudi Arabia*

ThP 106 **Unusual Matrix Effects Observed during Quantitative LC-MS/MS Methods Development**; Yuyong ke[1]; Nicki Hughes[1, 2]; Fernand Labrie[2]; *[1]Bioanalytical Laboratory Services, a Division of LifeLabs LP, Toronto, Ontario; [2]EndoCeutics, Quebec City, QC*

ThP 107 **Evolution, Development, and Application of a Dynamic, High-Throughput, Enterprise-Level Autosampler for High-Performance LC/MS/MS Bioanalysis**; Brendon Kapinos[1]; John S Janiszewski[1]; Hui Zhang[1]; Mary Piotrowski[1]; Jianhua Liu[1]; Wayne Lootsma[2]; Steven Ainley[2]; *[1]Pfizer, Groton, CT; [2]Sound Analytics, Niantic, CT*

FOOD SAFETY: OTHER CONTAMINANTS (PART 2)
108 - 141

ThP 108 **Food Safety Detection of Targeted and Unknown Compounds Using OrbitrapTMLC-MS/MS System**; Charles T. Yang[1]; Dipankar Ghosh[1]; Jamie Humphries[2]; Nick Duczak[2]; Caroline Ding[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Austin, TX*

ThP 109 **A Multi-Residue Liquid Chromatography\Tandem Mass Spectrometry Method for the Analysis of Macrolides in Food Matrices**; Pavel Metalnikov [1]; Ilia Batov[2]; Renat

Selimov[2]; Ksenia Batova[2]; Alexander Komarov[2]; *[1]VGNKI, Moscow , Moscow; [2]VGNKI, Moscow, Moscow*

ThP 110 **Determination of Wilfordine and Wilforine in Honey using Liquid Chromatography with Tandem Mass Spectrometry** ; Chen Jianli; *Shimadzu, Wuhan , China*

ThP 111 **Determination and Quantification of Perchlorate in a Fruit Matrix Using Accelerated Solvent Extraction and IC-MS**; Kyle Renfrew; Amanda Hartman[1]; Nicholas Santiago; *[1]Thermo Fisher Scientific, Austin, TX*

ThP 112 **Determination of Papaverine and Other Alkaloids in Hot Pot Condiment by Direct Analysis in Real Time Mass Spectrometry**; Yi Li[1]; Weixia Wang[1]; Xiaohui Xiong[1]; Jiehui Hu[2]; Charles C. Liu[2]; *[1]Nanjing Tech University, Nanjing, Jiangsu; [2]ASPEC Technologies Limited, Beijing, BeiJing*

ThP 113 **Use of Ambient Ionization Mass Spectrometry for the Rapid Authentication of Food and Dietary Supplements**; Kari Organtini[1]; Gareth Cleland[1]; Beth Loecken[1]; Adam Ladak[1]; *[1]Waters, Milford, MA*

ThP 114 **Accessible and Efficient Screening of Multiclass Contaminants in Food**; Eimear McCall[1]; Ramesh Rao[1]; Adam Ladak[2]; Jennifer Burgess[2]; *[1]Waters, Wilmslow, UK; [2]Waters, Milford, MA*

ThP 115 **Authentication and Chemical Standardization of Licorice Dietary Supplements Using UHPLC-MS/MS**; Guannan Li[1, 2]; Charlotte Simmler[1, 2]; Dejan Nikolic[1, 2]; Shao-Nong Chen[1, 2]; Guido F. Pauli[1, 2]; Richard B. van Breemen[1, 2]; *[1]UIC/NIH Center for Botanical Dietary Supplements Research, Chicago, IL; [2]Department of Medicinal Chemistry and Pharmacognosy, University of Illinois College of Pharmacy, Chicago, IL*

ThP 116 **Analysis of Phosphodiesterase Type 5 Inhibitors Extracted from Herbal Preparations by DSA-TOF MS**; Robert J. Seward[1]; Jason Weisenseel[1]; Craig Young[1]; Wilhad M. Reuter[1]; *[1]PerkinElmer, Waltham, MA*

ThP 117 **Simultaneous Determination of Multiple Plant Growth Regulators in Bean Sprouts using Ultra-Performance Liquid Chromatography Tandem Mass Spectrometry**; Cheng Zheng[1]; Qiaoyuan Cheng[1]; Weifang Ni[1]; Chengyuan Cai[2]; Jingchao Lin[2]; Yongming Xie[2]; *[1]Zhejiang Institute of Food and Drug Control, Hangzhou, China; [2]PerkinElmer Management (Shanghai) Co., Ltd, Shanghai, China*

ThP 118 **High Sensitive Analysis of Peanut Allergen in Cumin and Spice Mix**; Clifford Robert[1]; Tairo Ogura[1]; *[1]Shimadzu Scientific Instruments, Columbia, MD*

ThP 119 **Simultaneous Determination of Hormones in Edible Bird's Nest using Ultra-Performance Liquid Chromatography Tandem Mass Spectrometry**; Dunming Xu[1]; Liping Zhong[1]; Sanmei Zeng[1]; Lizhong Yang[2]; Chengyuan Cai[2]; Jingchao Lin[2]; Yongming Xie[2]; *[1]Xiamen Entry-Exit Inspection and Quarantine Bureau, Xiamen, China; [2]PerkinElmer Management(Shanghai)Co., Ltd, Shanghai, China*

ThP 120 **Mass Spectrometry Based Methods to Detect the BoNTE in Catfish Specimen**; Tibor Pechan[1]; Olga Pechanova[2]; Jennifer Arnold[3]; *[1]Mississippi State University, Mississippi State, MS; [2]Mississippi State University, Starkville, MS; [3]Edward Via College of Osteopathic Medicine - Carolinas Department of Biomedical Science, Spartanburg, SC*

ThP 121 **Rapid Screening and Quantitation of Domoic Acid in Shellfish Homogenates using Laser Ablation Electrospray Ionization Mass Spectrometry (LAESI-MS)**; Pamela S. Cantrell[1]; Callee M. Walsh[2]; Haddon E. Goodman[2]; Pearse McCarron[3]; Kelley Reeves[3]; Wade A. Rourke[4]; Sinead O'Brien[5]; Daniel G. Beach[3]; *[1]Protea Biosciences, Morgantown, WV; [2]Protea Biosciences, Inc. Morgantown, WV; [3]National Research Council Canada, Halifax, Nova Scotia, Canada; [4]Canadian Food Inspection Agency, Dartmouth, Nova Scotia, Canada; [5]Marine Institute, Galway, Ireland*

ThP 122 **Analysis of Diarrhetic Shellfish Poisoning and Azaspiracid Shellfish Poisioning Toxins by Liquid Chromatography-Tandem Mass Spectrometry**; Li Yang[1]; Randy Self[1]; James Stuart[1]; Theodore Lapainis[1]; Daniel Rice[1]; Wen-Hsin Wu[1]; James Hungerford[1]; *[1]Food and Drug Administration, Bothell, WA*

ThP 123 **Multi-analyte Investigation in Relation to the Illicit Treatment of Fish Food with Hydrogen Peroxide**; Claudio Medana[1]; Riccardo Aigotti[1]; Federica Dal Bello[1]; Valentina Santoro[1]; Claudio Baiocchi[1]; *[1]University of Turin, Torino, Italy*

ThP 124 **Origin Determination of Eastern Oyster (Crassostrea virginica) by Combination of Heavy Metal Concentrations, Whole-Body Bulk and Compound Specific Isotope Analyses**; Mayara P. V. Matos[1]; Marc E Engel[2]; Glen P Jackson[3, 4]; *[1]Department of Biology, West Virginia University, Morgantown, WV; [2]Florida Department of Agriculture and Consumer Service, Tallahassee, FL; [3]Department of Forensic and Investigative Science, West Virginia University, Morgantown, WV; [4]C. Eugene Bennett Department of Chemistry, West Virginia University, Morgantown, WV*

ThP 125 **Quantitative Determination of Veterinary Drug Residues in Eggs by UPLC-MS/MS Using a Simple, Rapid and Effective Cleanup Approach**; Sujie Xla[1]; Dimple Shah[2]; Jeremy C Shia[2]; Michael S Young[2]; Adam Ladak[2]; Laura Suhadolnik[2]; *[1]Shanghai Institute for Food and Drug Control, Shanghai, China; [2]Waters, Milford, MA*

ThP 126 **Targeted Veterinary Drugs Screening in Food Matrix using EMR QuEChERS and Newly Developed Triple Quadrupole Mass Spectrometer**; Yanan Yang[1]; Dan-Hui Yang[2]; *[1]Agilent Technologies, Inc, Santa Clara, CA; [2]Agilent Technologies, Santa Clara, CA*

ThP 127 **Development of Multi-Class, Multi-Residue UHPLC MS/MS Method for Screening/Quantification of Veterinary Drugs in Complex Food Metrices and Related Products**; Azeem Hasan[1]; Hui Zhao[1]; John Zulkoski[1]; Barb Mitchell[1]; Thomas Vennard[1]; Katerina Mastovska[1]; *[1]Covance, Madison, WI*

ThP 128 **Extending the Linear Dynamic Range for Measurements Targeting Veterinary Drug Residues in Animal Feed by UPLC-laminar Flow HSID-MS/MS**; Jason Kong[1]; Frank Kero[2]; Joshua Ye[3]; Lisa Cousins[3]; Craig Young[2]; Sharanya Reddy[2]; *[1]Ohio Department of Agriculture, Reynoldsburg, OH; [2]PerkinElmer, Shelton, CT; [3]Ionics Mass Spectrometry Group, Bolton, Canada*

ThP 129 **Mass Spectrometry Reveals Distinct Extracellular Proteins of Food-Borne *Escherichia coli* O157:H7 and O104:H4**; Nazrul Islam[1]; Attila Nagy[2]; Garrett M. Wesley[3]; Xiangwu Nou[2]; Bret Cooper[4]; Dan Shelton[2]; *[1]University of Maryland, Colleg, College Park, MD; [2]Environmental Microbial and Food Safety Laboratory, USDA-ARS, Beltsville, MD; [3]Animal Biosciences and Biotechnology Laboratory, USDA-ARS, Beltsville, MD; [4]Soybean Genomics and Improvement Laboratory, USDA-ARS, Beltsville, MD*

ThP 130 **Meat Species Identification by Protein Profiling and Spectral Fingerprinting using MALDI-TOF-MS**; Man On So; *The Hong Kong University of Science and Technology, Hong Kong SAR, HK*

ThP 131 **Dispersive Liquid Liquid Microextraction of Beta-agonist Residues from Bovine Muscle and Their Determination using ESI-LC-MS/MS**; Phomolo Kgothi[1]; Simiso Dube[2]; Mathew Muzi Nindi[3]; *[1]Botswana National Veterinary Laboratory, Gaborone, Botswana, Gaborone, Botswana; [2]University of South Africa, , Florida Park, Roodepoort, Gauteng; [3]University of South Africa, Department of Chemistry, College of Science Engineering and Technology, Unisa Science Campus, Florida Park, Roodepoort, South Africa*

ThP 132 **Quantification of Brominated Fatty Acids in Rat Tissues and Serum using Isotope Dilution UPLC/ESI/MS/MS**; Kellie Woodling[1]; Priyanka Chitranshi[1]; Goncalo Gamboa da Costa[1]; *[1]FDA/NCTR, Jefferson, AR*

ThP 133 **Matrix-Standardization and Post-Extraction Addition of Internal Standard to Overcome Challenges during LC/MS/MS Quantification of Neomycin and Oxytetracycline in Rabbit Tissues**; Aimin Tan[1]; Xuan Susan Gui[2]; Molly Wong[2]; Gordon Bolger[2]; Albert Licollari[2]; John C Fanaras[2]; *[1]Nucro-Technics, Scarborough, ON; [2]Nucro-Technics, Scarborough ON, Canada*

ThP 134 **Determination of Meat Authenticity using a Comprehensive Proteomic Strategy, Data-Independent Acquisition and High-Resolution Mass Spectrometry**; Alberto Ruiz Orduna[1]; Erik Husby[2]; Claudia P. Martins[2]; Dipankar Ghosh[2]; Francis Beaudry[1]; *[1]Université de Montréal, St-Hyacinthe, QC; [2]Thermo Fisher Scientific, San Jose, CA*

ThP 135 **A Green Sample Preparation Method for the Determination of Chloramphenicol and Its Metabolite Residues in Meat and Milk using ESI-LCMS/MS**; Ompelege E Kemokgatla[1]; Simiso Dube[2]; Mathew Muzi Nindi[3]; *[1]Botswana National Veterinary Laboratory, Gaborone, Botswana, Gaborone, Botswana; [2]University of South Africa, , Florida Park, Roodepoort, Gauteng; [3]Department of Chemistry, College of Science Engineering and Technology, Unisa Science Campus, Florida, Rooderport , Republic of South Africa, Florida Park, Roodepoort, South Africa*

ThP 136 **Direct Quantitative Analysis of Lean Meat Essence in Pork Tissues using Internal Extractive Electrospray Ionization Mass Spectrometry**; Yipo Xiao[1]; Haiyan Lu[1]; Jianyong Zhang[2]; Yiping Wei[2]; Huanwen Chen[3]; *[1]East China Institute of Technology, Nanchang, China; [2]Department of Cardiothoracic Surgery to Second Affiliated Hospital of Nanchang University, Nanchang, China; [3]East China University of Technology, Nanchang, Mainland*

ThP 137 **DART-HRMS and MS/MS of Spectra of Sweeteners for Screening Beverages**; Luke K Ackerman[1]; Romina Shah[1]; *[1]FDA/CFSAN, College Park, MD*

ThP 138 **Direct Determination of Four Pyrazole Fungicidesin Grape Wines by Paper Spray Mass Spectrometry**; Han Chao[1, 2]; Fan Pu[3]; Wenpeng Zhang[2]; Zheng Ouyang[2, 3]; *[1]Wenzhou Entry-Exit Inspection and Quarantine Bureau, Wenzhou, China; [2]Weldon School of Biomedical Engineering, Purdue University, West Lafayette, IN; [3]Purdue University-Department of Chemistry, West Lafayette, IN*

ThP 139 **Assay of Resveratrol in Red Wine by Paper Spray Tandem Mass Spectrometry and Isotope Dilution**; Fabio Mazzotti [1]; Domenico Taverna[2]; Leonardo Di Donna[2]; Lucia Bartella[2]; Anna Napoli[2]; Giovanni Sindona[2]; *[1]Dipartimento di Chimica e Tecnologie Chimiche Università della Calabria, Rende, Italy; [2]Dipartimento di Chimica e Tecnologie Chimiche, Università della Calabria, Rende, Italy*

ThP 140 **Rapid Assay of Multi-Class Antimicrobials Residues in Food of Animal Origin by Paper Spray Mass Spectrometry**; Yuan Su[1]; Zheng Ouyang[1]; *[1]Purdue University, West Lafayette, IN*

ThP 141 **Weight-loss Herbal Medicine Control Quality and Authenticity by Paper Spray Ionization Mass Spectrometry**; Géssica A Vasconcelos[1]; Verônica Carvalho[1]; Carla Freitas[1]; Igor da Silva[1]; Ricardo Borges[2]; Wanderson Romão[3, 4]; Boniek Gontijo Vaz[5]; *[1]Federal University of Goiás, Goiânia, Brazil; [2]Brazilian Federal Police, Brasília, Brazil; [3]Federal Institute of Espirito Santos, Vilha Velha, Brazil; [4]Federal University of Espirito Santo, Vitoria, Brazil; [5]Federal University of Goiás, Goiânia, GO*

GCMS: INSTRUMENTATION AND APPLICATIONS (APPLICATIONS)
142 - 171

ThP 142 **Determination of Pesticide Residues in Traditional Chinese Medicinal Materials Milkvetch Root**; Xizhi Wang[1]; Shiheng Luo[1]; Feifei Tian[1]; Guixiang Yang[1]; Jun Fan[2]; Taohong Huang[2]; Shin-ichi Kawano[2]; Yuki Hashi[2]; *[1]Shimadzu (China) Co., Beijing, China; [2]Shimadzu (China) Co., Shanghai, China*

ThP 143 **Efficient Headspace Extraction of Plasticizers from Aqueous and Ethanolic Extracts**; Douglas Doster; *Aspen Research Corporation, New Germany, MN*

ThP 144 **Analysis of Isomeric Metabolites by GC-EI/PI/FI-MS**; Takeshi Furuhashi[1]; Koji Okuda[2]; Akihiko Kusai[2]; Takemichi Nakamura[3]; *[1]Ryukyu University, Okinawa, Japan; [2]JEOL Ltd., Akishima, Japan; [3]RIKEN, Wako, Japan*

ThP 145 **Determination of Tobacco-Specific N-nitrosamines in Mainstream Cigarette Smoke using in-pipette-tip Solid-Phase Extraction**; Yan-bo Luo[1]; Xiao-Jing Chen[1]; Hong-Fei Zhang[1]; Xing-Yi Jiang[1]; Xue Li[1]; Xiang-Yu Li[1]; Feng-Peng Zhu[1]; Yong-Qiang Pang[1]; Hong-Wei Hou[1]; *[1]China National Tobacco Quality Supervision and Test Center, Zhengzhou, China*

ThP 146 **Substance Characterization of Polyenthylene Polyamine by EI GC/MS**; O. David Sparkman[1]; Kirill Ttretyakov[2]; Patrick Batoon[3]; Itsuko Iwai Iwai[4]; Terry L. Ramus[4]; *[1]University of the Pacific, Antioch, CA; [2]Dakota Consulting Inc., Silver Springs, MD; [3]University of the Pacific, Stockton, CA; [4]Diablo Analytical, Antioch, CA*

ThP 147 **Multi Pesticides Residue Analysis in Ayurvedic Cough Syrup by GCMS/MS using QuEChERS' Extraction Method**; Durvesh Sawant[1]; Ankush Bhone[1]; Dheeraj Handique[1]; Prashant Hase[1]; Sanket Chiplunkar[1]; Jitendra Kelkar[1]; Ajit Datar[1]; Pratap Rasam[1]; Tina Kukreja[2]; *[1]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India; [2]G.N.I.R.D., G.N. Khalsa College Mumbai, India*

ThP 148 **Study of the Electron Ionization Fragmentation Patterns of 1-Alkoxycyclohexenes**; Krege M Christison[1, 2]; O. David Sparkman[1]; Patrickhenry Batoon[1]; Sven Hackbush[1]; Andreas H Franz[1]; *[1]University of the Pacific, Stockton, CA; [2]Chevron, Richmond, CA*

ThP 149 **Identification of Leachable Impurities from Pharmaceutical Container Closure Materials using Orbitrap Based GC-MS**; Dominic Roberts[1]; Andrew Feilden[2]; Richard Barlow[2]; Jason Cole[3]; Paul Silcock[1]; Kyle D'Silva[1]; Alexander Semyonov[4]; *[1]Thermo Fisher Scientific, Runcorn, UK; [2]Smithers Rapra, Shawbury, UK; [3]Thermo Fisher Scientific, Ausitn, TX; [4]Thermo Fisher Scientific, Austin, TX*

ThP 150 **Determination of Ceramides using GC/Q-TOF with a Novel High Efficiency Source**; Jennifer Sanderson[1]; Viorica Lopez-Avila[1]; Sofia Nieto[1]; *[1]Agilent Technologies, Santa Clara, CA*

ThP 151 **Differentiation between Type of Dialkyl Phthalates Based on their EI Mass Spectra**; O. David Sparkman[1]; Jianhua Ren Ren[2]; Patrickhenry Batoon[2]; Krege Christison[2]; *[1]University of the Pacific, Antioch, CA; [2]University of the Pacific, Stockton, CA*

ThP 152 **Quantitative Determination of Dioxins in Drinking Water by Isotope Dilution Triple Quadrupole GC-MS/MS**; Jackie Jackie[1]; Chong Chiew Mei[1]; Yeong Hui Xian Crystal[1]; Lahey Cynthia Melanie[1]; Loo Lai Chin[1]; *[1]Shimadzu (Asia Pacific) Pte Ltd, Singapore*

ThP 153 **GC/MS Metabolomics: Metabolic Mapping of Prostate Cancer Cell Lines**; Jan Crowley[1, 2]; Kristopher Kirmess[3]; Jeffrey Arbeit[1]; Kevin Yarasheski[1, 2]; Joseph Ippolito[1]; *[1]Washington University, St Louis, MO; [2]Department of Medicine, Washington University St. Louis, MO; [3]Washington University in St. Louis, St. Louis, MO*

ThP 154 **Characterization of Little Cigar Smoke Tar by GC-MS**; Steven Reeber[1]; Arunava Ghosh[1]; Robert Tarran[1]; Gary L. Glish[1]; *[1]The University of North Carolina at Chapel Hill, Chapel Hill, NC*

ThP 155 **Development and Validation of an Analytical Method to Quantitate Sulfolane in Rodent Plasma by GC/MS**; veronica Robinson[1]; Teruyo Uenoyama[2]; Brenda Fletcher[2]; Stephen Cooper[2]; Melanie R. Rehder Silinski[2]; Reshan Fernando[2]; Suramya Waidyanatha[1]; *[1]NIEHS / NIH, RTP, NC; [2]RTI International, RTI Int Research Triangle Park, NC*

ThP 156 **Fast and Accurate Analysis of Fluorotelomer Alcohols and Acrylates using Triple Quadrupole GC-MS/MS**; Cynthia Melanie Lahey[1]; Guo Wei Elgin Ting[2]; Hui Xian Crystal Yeong[1]; Jackie Jackie[1]; Chiew Mei Chong[1]; Lai Chin Loo[1]; *[1]Shimadzu (Asia Pacific) Pte Ltd, Singapore; [2]Nanyang Technological University, Division of Chemistry and Biological Chemistry, School of Physical and Mathematical Sciences, Singapore*

ThP 157 **Evolved Hydrogen Gas Analysis from the Industrial Materials using a Quadrupole Mass Spectrometer**; Masahiro Hashimoto[1]; Koji Okuda[1]; Makoto Okano[1]; Tetsuo Higuchi[1]; Akihiko Kusai[1]; *[1]JEOL Ltd., Akishima, Japan*

ThP 158 **Quantitative Determination of Aromatic Amines Formed from Azo Dyes in Textile using GCMS/MS**; Ankush Bhone[1]; Durvesh Sawant[1]; Dheeraj Handique[1]; Prashant Hase[1]; Sanket Chiplunkar[1]; Ajit Datar[1]; Jitendra Kelkar[1]; Pratap Rasam[1]; *[1]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, INDIA*

ThP 159 **Chemical Profiling of Whiskies using Orbitrap GC-MS**; Roberts Dominic[1]; Jana Hajslova[2]; Michal Stupák[2]; Jana Pulkrabova[2]; Jason Cole[3]; Paul Silcock[1]; *[1]Thermo Fisher Scientific, Runcorn, UK; [2]Institute of Chemical Technology, Prague, Czech Republic; [3]Thermo Fisher Scientific, Ausitn, TX*

ThP 160 **Analysis of Volatile Organic Compounds in Crude Oil using High Resolution Orbitrap GC/MS**; Aikaterini Kondyli[1]; Wolfgang Schrader[1]; *[1]Max-Planck Inst für Kohlenforschung., Mülheim / Ruhr, Germany*

ThP 161 **Metabolic Profiling of Arabidopsis Tissue Extract using GC-MS/MS Technology** ; Feroza Choudhury[1]; Amit Gujar[2]; Amith Reddy[1]; Ron Mittler[1]; Vladimir Shulaev[1]; *[1]University of North Texas, Denton, TX; [2]Thermo Fisher Scientific, Austin, TX, USA*

ThP 162 **Analysis of Trimethylsilyl Derivatives of Cyanogenic Glycosides from Flaxseed (Linum usitatissimum) by GC/MS**; Tao Fan[1]; Véronique J. Barthet[2]; *[1]Canadian Grain Commission, Winnipeg, Manitoba; [2]Canadian Grain Commission, Winnipeg, Canada*

ThP 163 **Gas Chromatography- & Liquid Chromatography-Mass Spectrometry-Based Metabolomics: Effects of Altered Extracellular pH on Cancer Metabolism**; Kristopher Kirmess[1]; Jan R Crowley[1]; Kevin Yarasheski[1]; Joseph Ippolito[1]; *[1]Washington University in St. Louis, St. Louis, MO*

ThP 164 **Quantitative GC-MS/MS Analysis of Bisphenols with Oxycarbonyl Derivatization**; Fred Bjorn Lih[1]; Deirdre K Tucker[1]; Sue E Fenton[1]; Leesa J Deterding[1]; *[1]NIEHS / NIH, RTP, NC*

ThP 165 **Detecting Toxic Byproducts from Pyrotechnic Reactions via Pyrolysis/Gas Chromatography/Mass Spectrometry Techniques**; Douglas Papenmeier[1]; Steven C. Weddle[1]; Eric J. Miklaszewski[2]; Caroline K. Wilharm[2]; Matthew A. Neiswinger[3]; Jonathan M. Dilger[2]; *[1]Special Warfare and Expeditionary Systems Department, Naval Surface Warfare Center, Crane Division, Crane, IN; [2]Spectrum Warfare Systems Department, Naval Surface Warfare Center, Crane Division, Crane, IN; [3]Science Applications International Corporation (SAIC), Crane, IN*

ThP 166 **A Novel Ladder Approach for the Characterization of Diisonoyl Phthalate using GC-MS**; Ian W. Shaffer[1]; Josh Allen Wilhide[1]; William R. LaCourse[1]; *[1]University of Maryland, Baltimore County Baltimore, MD*

ThP 167 **Transition Metal Catalyzed Lignin Hydrotreatment and Determination of Products by GC-MS and Thermal Carbon Analysis**; Honza Bilek; *University of North Dakota, Grand Forks, ND*

ThP 168 **Rapid On Site Analysis of BTEX Aromatics with a Miniaturized Field Portable Gas Chromatograph-Mass Spectrometer**; Alan Gallaspy[1]; Frank Kero[2]; *[1]PerkinElmer, Oak Brook, IL; [2]PerkinElmer, Waltham, MA*

ThP 169 **Isobutane Made Practical as a Reagent Gas for Chemical Ionization Mass Spectrometry**; G. Asher Newsome[1]; F. Lucus Steinkamp[2]; Braden C. Giordano[3]; *[1]Nova Research, Inc, Alexandria, VA; [2]National Research Council, Washington, DC; [3]U.S. Naval Research Laboratory, Washington, DC*

ThP 170 **Comparison of Headspace Methods for GC/MS Analysis of Foods**; Adam J. Patkin[1]; Sharanya Reddy[1]; David Scott[1]; Leeman Bennington[1]; Lee Marotta[1]; *[1]PerkinElmer, Shelton, CT*

ThP 171 **Unambiguous Identification of Reaction Products from Conversion of Nitric Oxide over Novel Photocatalyst Surfaces**; Ian G. M. Anthony[1]; Matthew R Brantley[1]; Adam R Floyd[1]; Abayomi D. Olaitan[1]; Deniz A Erdogan[2]; Emrah Özensoy[2]; Touradj Solouki[1]; *[1]Baylor University, Waco, TX; [2]Bilkent University, Bilkent University 06800 Bilkent Ankara, Turkey*

H/D EXCHANGE: PROTEIN STRUCTURE/FUNCTION (PART 2) 172 - 195

ThP 172 **Lamin A (LmnA)-induced Conformational Changes of AIMP3 (aminoacyl-tRNA Synthetases-Interacting Multifunctional Proteins) Revealed by H/D Exchange FT-ICR MS**; Yeqing Tao[1]; Pengfei Fang[2]; Nicolas L Young[3]; Min Guo[2]; Alan G Marshall[1, 3]; *[1]Florida State University, Tallahassee, FL; [2]The Scripps Research Institute, Jupiter, Florida; [3]NHMFL, Tallahassee, Fl*

ThP 173 **Insights into Dynamics of SufBC2D Fe-S Scaffold Complex by Hydrogen Deuterium Exchange Mass Spectrometry**; Siqi Guan[1]; Guanchao Dong[2]; Wayne Outten[2]; Patrick Frantom[1]; *[1]University of Alabama, Tuscaloosa, AL; [2]University of South Carolina, Columbia, SC*

ThP 174 **HDX-MS Reveals Co-Regulation of Vitamin D Receptor/ Retinoic X Receptor Alpha Heterodimer Activation by Selective VDR Modulator and VDRE Sequence Specificity**; Jie Zheng[1]; Bruce D Pascal[1]; Scott Novick[1]; Ruben D Garcia-Ordonez[1]; Pat Griffin[1]; *[1]The Scripps Research Institute, Jupiter, FL*

ThP 175 **Probing the Structural Dynamics of the Prokaryotic Amino Acid Transporter LeuT by Hydrogen/Deuterium Exchange Mass Spectrometry**; Patrick Sascha Merkle[1]; Kamil Gotfryd[2]; Ulrik Gether[2]; Claus Juul Løland[2]; Kasper Dyrberg Rand[1]; *[1]Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark; [2]Department of Neuroscience and Pharmacology, University of Copenhagen, Copenhagen, Denmark*

ThP 176 **pH Modulation of Myristate Exposure in the Human Immunodeficiency Virus Type-1 Matrix Protein: A Hydrogen Deuterium Exchange Mass Spectrometry Study**; Ioannis Karageorgos[1, 2]; Kerry Bauer[1, 2]; Jeffrey W Hudgens[1, 2]; *[1]National Institute of Standards & Technology, Rockville, MD; [2]Institute for bioscience and Biotechnology Research, Rockville, MD*

ThP 177 **Calcium-Mediated Interactions of S100A11 with Annexin Peptides Probed by HDX-MS and MD Simulations**; Yiming Xiao[1]; Gary S. Shaw[2]; Lars Konermann[2]; *[1]University of Western Ontario, London, ON; [2]University of Western Ontario, London, Ontario (ON)*

ThP 178 **Gas-phase Hydrogen Deuterium Exchange as a Structural Probe: Assessing Similarities in Gas- and Solution-Phase Peptide Structures**; Mahdiar Khakinejad[1]; Samaneh Ghassabi-Kondalaji[1]; stephen J Valentine[1]; *[1]West Virginia University, Morgantown, WV*

ThP 179 **HDX-MS to Map the Allosteric Site for Efavirenz, a Drug that Stimulates Cholesterol-Metabolizing P450 CYP46A1 Activity**; Kyle W Anderson[1, 2]; Natalia Mast[3]; Jeffrey W Hudgens[1, 2]; Joseph Lin[3]; Illarion V Turko[1, 2]; Irina A Pikuleva[3]; *[1]National Institute of Standards and Technology, Gaithersburg, MD; [2]Institute for Bioscience and Biotechnology Researc, Rockville, MD; [3]Case Western Reserve University, Cleveland, OH*

ThP 180 **Characterization of Conformation of Therapeutic Antibody Aggregation with Optimized Hydrogen/ Deuterium Exchange Mass Spectrometry**; Shanhua Lin[1]; Terry Zhang[2]; David M Horn[2]; Stephane Houel[2]; Xiaodong Liu[1]; Jonathan L Josephs[2]; *[1]Thermo Fisher Scientific, Sunnyvale, CA; [2]Thermo Fisher Scientific, San Jose, CA*

ThP 181 **Rapid Mapping of Antigen-Antibody Binding Sites utilizing Oxidative Footprinting and New Software**; Yining Huang[1]; Ke Sherry Li[1]; Manolo D. Plasencia[1]; Henry W Rohrs[1]; Michael L Gross[1]; Yong J Kil[2]; Marshall W. Bern[2]; Eric Carlson[2]; Chris Becker[2]; *[1]Washington University in St. Louis, St. Louis, MO; [2]Protein Metrics Inc., San Carlos, CA*

ThP 182 **Conformational Characterization of Nerve Growth factor-β and the Impact of Its Regulatory Pro-Part Domain**; Esben Trabjerg[1, 2]; Fredrik Kartberg[2]; Søren Christensen[2]; Kasper D. Rand[1]; *[1]Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark; [2]H. Lundbeck A/S, Valby, Denmark*

ThP 183 **Time-Resolved Hydrogen Deuterium Exchange Reveals the Structural Basis of Amyloidogenesis Inhibition by Alzheimer's Drug Candidates**; Shaolong Zhu[1]; Bin Deng[2]; Braden Sweeting[3]; Marcy Taylor[3]; Mark Reed[3]; Derek J. Wilson[2]; *[1]York University, Toronto, Ontario; [2]York University, Toronto, Canada; [3]Treventis Corporation, Toronto, Canada*

ThP 184 **Equilibrated and Kinetic Epitope Mapping for Therapeutic Antibodies by Time-Resolved ElectroSpray Ionization Hydrogen Deuterium eXchange (TRESI-HDX) Mass Spectrometry**; Bin N/A Deng[1]; Shaolong N/A Zhu[1]; Cristina N/A Lento[1]; Derek J. Wilson[1]; *[1]York University, Toronto, Canada*

ThP 185 **Conformational Changes in the Regulatory Domains of the Tec-family Tyrosine Kinase Btk upon Lipid Interaction**; Thomas E. Wales[1]; Raji E. E Joseph[2]; Amy H. H Andreotti[2]; John R. R Engen[1]; *[1]Northeastern University, Boston, MA; [2]Iowa State University, Ames, IA*

ThP 186 **Probing Protein Surface Chemistry and Unfolding Pathways by Coupling Gas-Phase HDX and Native MS**; Shane A Chandler[1]; Todd H Mize[1]; Michael R Morris[2]; Justin L. P. Benesch[1]; *[1]Oxford University, Oxford, UK; [2]Waters, Wilmslow, UK*

ThP 187 **Deprotection by Interaction in HXMS: A Glimpse into a Highly Dynamic Cellulolytic System**; Alan Kadek[1, 2]; Daniel Kavan[1, 2]; Roland Ludwig[3]; Petr Halada[1]; Petr Man[1, 2]; *[1]Institute of Microbiology CAS, Prague, Czech Republic; [2]Faculty of Science, Charles University in Prague, Prague, Czech Republic; [3]University of Natural Resources and Applied Life Sciences (BOKU), Vienna, Austria*

ThP 188 **HDX/MS of the *E. coli* Replicative DNA Polymerase Identifies Stabilizing Interactions between the DNA Sliding Clamp, Exonuclease and Clamp Loader**; Rafael Fernandez Leiro[1]; Sarah Louise Maslen[1]; Meindert H Lamers[1]; Mark Skehel[2]; *[1]MRC Laboratory of Molecular Biology, Cambridge, UK; [2]Medical Research Council, Cambridge, Cambridgeshire*

ThP 189 **Protein Footprinting and Mass Spectrometry Map the Interface of Marburg virus VP24 interacting with Keap1**; Jing Li[1]; Britney Johnson[2]; Daisy W Leung[2]; Christopher F Basler[3]; Gaya K Amarasinghe[2]; Michael L Gross[1]; *[1]Washington University in St. Louis, St. Louis, MO; [2]Washington University School of Medicine, St. Louis, MO; [3]Mount Sinai School of Med, New York, NY*

ThP 190 **HDX-MS Characterization of Selective Modulators for Retinoic-acid Receptor-related Orphan Receptor RORγt in Protective Immune Therapy**; Venkat Dharmarajan[1]; Scott Novick[2]; Mi Ra Chang[2]; Christelle Doebelin[2]; Ruben Garcia-Ordonez[2]; Ted Kamenecka[2]; Pat Griffin[2]; *[1]The Scripps Research Institute, Jupiter, Florida, Jupiter, FL; [2]The Scripps Research Institute, Jupiter, FL*

ThP 191 **Probing Cadherin Adhesive Interactions by Hydrogen/ Deuterium Exchange with Positive Electrospray 14.5 T FT-ICR Mass Spectrometry**; Peilu Liu[1]; Samantha Davila[2]; Susan Diane Pedigo[2]; Alan G Marshall[3, 4]; *[1]National High Magnetic Field Lab, Tallahassee, Florida; [2]Department of Chemistry and Biochemistry, University of Mississippi, University, MS; [3]National High Magnetic Field Laboratory, Tallahassee, FL; [4]Florida State University, Tallahassee, FL*

ThP 192 **Conformation-specific Interactions with Tomm34 Modulate Hsp70 Folding and ATPase Activities**; Jiri Hausner[1, 2]; Michal Durech[3]; Filip Trcka[3]; Dominika Coufalova[3]; Daniel Kavan[1, 2]; Petra Dvorakova[3]; Lenka Hernychova[3]; Elizabeth A. Blackburn[4]; Petr Man[1, 2]; Petr Muller[3]; Borivoj Vojtesek[3]; *[1]Institute of Microbiology CAS, Prague, Czech Republic; [2]Faculty of Science, Charles University in Prague, Prague, Czech Republic; [3]RECAMO, Masaryk Memorial Cancer Institute, Brno, Czech Republic; [4]Edinburgh Centre for Chemical Biology, University of Edinburgh, Edinburgh, UK*

ThP 193 **Beyond Structure Characterization: Structure Dynamics (Hydrogen deuterium exchange) Guided Biocatalyst Improv**; Susie Dai; *Office of the Texas State Chemist, Department of V, College Station , TX*

ThP 194 **Structure and Dynamics of RNA Binding to the Non-Canonical RNA Recognition Motif (RRM2) in Human La Protein**; Kerene Brown[1]; Mark Bayfield[2]; Derek Wilson[2]; *[1]York University, Toronto, Ontario; [2]York University, Toronto, Canada*

ThP 195 **Determination of Site-specific Protein-Ligand Binding Affinities using Protein Ligand Interaction Mass Spectrometry Titration and Hydrogen Deuterium Exchange (PLIMSTEX) Strategy**; Jagat Adhikari[1]; Don L. Rempel[2]; Michael L Gross[2]; *[1]Washington University in St. Louis, St Louis, MO; [2]Washington University in St. Louis, St Louis, MO*

IMAGING MS: METHOD DEVELOPMENT (MALDI)
196 - 215

ThP 196 **Regional Analysis of Anacardic Acids on the Surface of Pelargonium xhortorum (Geranium) Leaves using MALDI-MSI with a New Stable Matrix**; Marta Yappert[1]; Bryan Wessel[1]; David Schultz[2]; *[1]Department of Chemistry, University of Louisville, Louisville, KY; [2]Department of Biology, University of Louisville, Louisville, KY*

ThP 197 **Method Development for Imaging Mass Spectrometry on Dense Mineralized Tissue of Mouse Incisors**; Madeline Colley[1]; Yong-Hee Patricia Chun[2]; Stephan BH Bach[1]; *[1]University of Texas at San Antonio, San Antonio, TX; [2]UT Health Science Center at San Antonio, San Antonio, TX*

ThP 198 **MALDI-MSI for the Study of Flow-Cell and Agar Bound Microbial Biofilms**; Bin Li[1]; Sage Dunham[2]; Tong Si[2]; Ning Yang[2]; Clint Arnett[3]; Sweedler Jonathan[2]; *[1]University of Illinois at Urbana-Champaign, Urbana, IL; [2]University of Illinois at Urbana-Champaign, Urbana-Champaign, IL; [3]Engineer Research and Development Center-Construction Engineering Research Laboratory (ERDC-CERL), Champaign, IL*

ThP 199 **Microscopic MALDI-imaging Mass Spectrometry in Intestinal Tumors of Apc Mutant Mice using Two-Step Matrix Application**; Shuichi Shimma[1, 2]; Satoko Osawa[2, 3]; Masahiro Aoki[2, 4]; Yasushi Kojima[2, 4]; Tomoyoshi Soga[2, 5]; *[1]Osaka Univerisity, Suita, Osaka; [2]AMED-CREST, Tokyo, Japan; [3]Osaka University, Suita, Japan; [4]Aichi Cancer Center, Nagoya, Japan; [5]Keio University, Tsuruoka, Japan*

ThP 200 **Imaging of Lipids using 2,6 Dihydroxyacetophone Matrix with an AP-MALDI Source**; Ludovic Muller[1]; Shelley N Jackson[1]; Aurelie Roux[2]; Berk Oktem[3]; Vladimir M Doroshenko[3]; Amina S Woods[1]; *[1]NIH/NIDA-IRP, Baltimore, MD; [2]All Children's Hospital Johns Hopkins Medicine, Saint Petersburg, FL; [3]MassTech, Inc. Columbia, MD*

ThP 201 **Enhanced On-Tissue Analyte Derivatization with Electrospray Deposition of Reagents for MALDI MS Imaging of Neurotransmitters** ; Qian Wu[1]; Stanislav S. Rubakhin[1]; Troy J. Comi[1]; Jonathan V. Sweedler[1]; *[1]University of Illinois at Urbana-Champaign, Urbana-Champaign, IL*

ThP 202 **MALDI FTICR-IMS of a Mouse Lung for 3D Imaging and Reconstruction**; E. Ellen Jones[1]; Stephanie Dale[1]; Katherine A Kellersberger[2]; Christian Berg[2]; Cristine Quiason[1]; Sheerin Shahidi-Latham[1]; *[1]Genentech Inc, South San Francisco, CA; [2]Bruker Daltonic, Billerica, MA*

ThP 203 **From 2D to 3D MALDI Imaging Mass Spectrometry - Reconstruction of a Multimodal Imaged Epididymis**; Regis Lavigne[1]; Blandine Guevel[1]; Michael Becker[2]; Janine Beckmann[2]; Dennis Trede[3]; Herbert Thiele[4]; Melanie Lagarrigue[1]; Charles Pineau[1]; *[1]Protim, Irset, Inserm U.1085, Rennes, France; [2]Bruker Daltonic GmbH, Bremen, Germany; [3]SCiLS GmbH, Bremen, Germany; [4]Fraunhofer MEVIS Project Group Image Registration, Lübeck, Germany*

ThP 204 **Quantitative MALDI-MS Imaging of Tumour Spheroids** ; Rebecca Day[1]; Laura Cole[1]; Ieva Palubeckaite[1]; David Smith[1]; Neil Cross[1]; Malcolm R Clench[1]; *[1]Sheffield Hallam University, Sheffield, UK*

ThP 205 **MALDI Directed – Infrared Laser Ablation Sample Transfer for Spatially Resolved Biomolecule Analysis**; Kelin Wang[1]; Fabrizio Donnarumma[1]; Kermit K Murray[1]; *[1]Louisiana State Univeristy, Baton Rouge, LA*

ThP 206 **In-parallel MS and MS/MS MALDI Imaging without Sacrificing Spatial Resolution**; Rebecca Hansen[1, 2]; Young Jin Lee[1, 2]; *[1]Iowa State University, Ames, IA; [2]Ames Laboratory-US DOE, Ames, Iowa*

ThP 207 **MALDI Imaging-Driven Microproteomics Workflow for Biomarker Discovery Assays**; Deborah Alberts[1]; Rémi Longuespée[2]; Charles Pottier[3]; Nicolas Smargiasso[4]; Gabriel Mazzucchelli[5]; Dominique Baiwir[6]; Philippe Delvenne[3]; Fabien Pamelard[7]; Gaël Picard de Muller[7]; Edwin De Pauw[4]; *[1]Mass Spectrometry Laboratory, University of Liege, Liège, Belgium; [2]Proteopath GmbH, Trier, Germany; [3]Department of pathology, University of Liège Liège, BELGIUM; [4]Mass Spectrometry Laboratory, University of Liege, Liege, Belgium; [5]Mass Spectrometry Laboratory, University of Liege, Liege, Belgium; [6]GIGA Proteomics Facility, University of Liège Liège, Belgium; [7]ImaBiotech, Lille, France*

ThP 208 **Method Development on a MALDI Orbitrap Platform to Achieve High Throughput *in situ* DDA Analysis via Multiplex Mass Spectrometric Imaging**; Chuanzi Ouyang[1]; Bingming Chen[1]; Lingjun Li[1]; *[1]University of Wisconsin Madison, Madison, WI*

ThP 209 **A Rapid, Cell Culture-Based Method for Biomarker Discovery and Drug Screening by MALDI-MSI**; Courtney E Chandler[1]; Alison J Scott[1]; George A. Belov[2]; David R Goodlett[1]; Shane Ellis[3]; Robert K Ernst[1]; *[1]University of Maryland Baltimore, Baltimore, MD; [2]University of Maryland, College Park College Park, MD; [3]Maastricht University, Maastricht, NL*

ThP 210 **Histology-Directed Lipid Identification: Advanced Imaging Mass Spectrometry and Liquid Extraction Technologies Enable Spatially Specific Tandem Mass Spectrometry**; Daniel Ryan[1]; Boone Prentice[1]; Raf Van de Plas[2]; Jeffrey Spraggins[1]; Richard M Caprioli[1]; *[1]Vanderbilt University, Nashville, TN; [2]Delft University of Technology, Delft, Netherlands*

ThP 211 **Bottom-up Imaging of Prostate-Cancer Protein Biomarkers by MCAEF (Matrix Coating Assisted by an Electric Field)-LDI/FTMS**; Teesha C Baker[1]; Jun Han[2]; Darryl B Hardie[2]; Christoph H. Borchers[1, 3]; *[1]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada; [2]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [3]University of Victoria - Genome BC Proteomics Centre, Victoria, BC*

ThP 212 **MALDI Imaging for the Quantification of Small Molecules and the Understanding of Toxicity Mechanisms**; Melanie Lagarrigue[1]; Régis Lavigne[2]; Andrew Palmer[3]; Charles Pineau[4, 5]; *[1]Protim, Rennes, Brittany; [2]Protim - Irset Inserm U 1085, Rennes, France; [3]EMBL, Heidelberg, Germany; [4]Protim, IRSET Inserm U1085, Rennes, France; [5]University Rennes 1, Rennes, France*

ThP 213 **An Investigation of MALDI Imaging with Higher Speed Sample Stage "Rastering" from an Ion Mobility Enabled Q-TOF Mass Spectrometer**; Towers Mark[1]; Paul Murray[1]; Migas Lukasz[2]; Claude Emmanuelle[1]; Hoyes Emmy[1]; Chapman Richard[1]; *[1]Waters, Wilmslow, UK; [2]University of Manchester, Manchester, UK*

ThP 214 **High-Throughput Single Cell Analysis using High Spatial Resolution and High Sensitivity Imaging Mass Spectrometry**; Bo Yang[1]; Jeffrey M Spraggins[1]; Richard M Caprioli[1]; Jeremy L Norris[1]; *[1]Vanderbilt University MSRC, Nashville, TN*

ThP 215 **Loblolly Pine Seedling Imaging Analysis by DESI-MS and MALDI-MS**; Michelle Reid[1]; Gary F Peter[1]; Richard A Yost[1]; *[1]University of Florida, Gainesville, FL*

IMAGING MS: SMALL MOLECULES
216 - 247

ThP 216 **Exploring the Chemical Ecology of Fungi via Secondary Metabolite Distribution**; Vincent Sica[1]; Huzefa Raja[1]; Cedric Pearce[2]; Nicholas H Oberlies[1]; *[1]UNC - Greensboro, Greensboro, NC; [2]Mycosynthetix, Hillsborough, NC*

ThP 217 **Microbial Metabolite and Lipid Analysis by Imaging Laser Desorption Ionization Mass Spectrometry on Silicon Nanopost Array Platforms**; Rachelle Jacobson[1]; Akos Vertes[1]; *[1]George Washington University, Washington, District of Columbia*

ThP 218 **Optimizing the Production of Fungal Epipolythiodioxopiperazine Alkaloids Facilitated by Rapid Analysis via the droplet-LMJ-SSP Coupled with UPLC-PDA-HRMSMS/MS**; Soumia Amrine[1]; Huzefa Raja[1]; Cedric Pearce[2]; Nicholas Oberlies[1]; *[1]UNC Greensboro, Greensboro, NC; [2]Mycosynthetix, Hillsborough, NC*

ThP 219 **Profiling Secondary Metabolites from a Culture Evaluation of Penicillium restrictum with Droplet-Liquid Microjunction Surface-Sampling Probe**; Diana Kao; *University of North Carolina at Greensboro, Greensboro, NC*

ThP 220 **MALDI-FTMS Imaging Reveals Secondary Metabolites Produced during Interaction of Micro-Organisms with Higher Organisms**; Dirk Wunderlich[1]; Jens Fuchser[2]; Stephanie Grond[3]; Florian Zubeil[3]; Dorothee Wiesbrod[3]; *[1]Bruker Daltonics, Bremen, Bremen; [2]Bruker Daltonic GmbH, Bremen, Germany; [3]Eberhard Karls University Tübingen, Tübingen, Germany*

ThP 221 **Mass Spectrometry Imaging of Curtobacteriumsp. ER1/6, an Endophytic Bacterium with Potential Biocontrol against Citrus-Variegated Chlorosis**; Francisca D. S. Araújo[1]; Daiene S. Santos[2]; Welington L.

Araujo[2]; Marcos N Eberlin[1]; *[1]Unicamp, Campinas, SP; [2]University of São Paulo, São Paulo, SP*

ThP 222 **Imaging Mass Spectrometry of S-containing Metabolites in Asparagus officinalis**; Ryo Nakabayashi[1]; Tetsuya Mori[1]; Hiroshi Sudo[2]; Kiminori Toyooka[1]; Kazuki Saito[1, 3]; *[1]RIKEN Center for Sustainable Resource Science, Yokohama, Japan; [2]Hoshi University, Shinagawa, Japan; [3]Chiba University, Chiba, Japan*

ThP 223 **MALDI Imaging Mass Spectrometry Revealed the Different Distribution Patterns of Anthocyanin Species in Strawberry**; Hirofumi Enomoto[1]; Ryosuke Sato[1]; Hisakazu Yamane[1]; Fumiaki Yoshizawa[2]; *[1]Teikyo University, Utsunomiya, Japan; [2]Utsunomiya University, Utsunomiya, Japan*

ThP 224 **Three-Dimensional Visualization of Membrane Phospholipid Heterogeneity in Arabidopsis thaliana seeds by MALDI-MS Imaging**; Drew Sturtevant[1, 2]; Maria Dueñas[3, 4]; Young Jin Lee[3, 4]; Kent D. Chapman[1, 2]; *[1]University of North Texas, Denton, TX; [2]Center for Plant Lipid Research, Denton, TX; [3]Iowa State University, Ames, IA; [4]Ames Laboratory-US DOE, Ames, IA*

ThP 225 **Spatial Distribution of Lipids in Coffee Leaves (Coffea arabica) using MALDI Imaging Mass Spectrometry**; Karen T. Henández-Osorio[1]; Jeferson A. Valencia-Dávila[1]; Cristian Blanco-Tirado[1]; Marianny Y. Combariza[1]; *[1]Universidad Industrial de Santander, Bucaramanga, Santander, Colombia*

ThP 226 **Localization of the Salvinorin A diterpenoid Pathway in Savia divinorum by MALDI-FTICR-MS Imaging**; Jeong Jin Park[1]; Xiaoyue Chen[1]; Anna Berim[1]; Jing Wang[1]; David R. Gang[1]; *[1]Washington State University, Pullman, WA*

ThP 227 **Imaging Non-uniform Spatial Distribution of Energy Dense Metabolites for Efficient Capture and Chemical Storage of Solar Energy by Plants**; Bo Xie[1]; Liza Alexander[1, 2]; Jennifer Chmielowski[2]; Basil J. Nikolau[1, 2]; *[1]Ames Laboratory-US DOE, Ames, IA; [2]Iowa State University, Ames, IA*

ThP 228 **Imaging Mass Spectrometry Revealed Distributions of Anthocyanin Species in Haskap**; Takahiro Hayasaka[1]; Miwako Sugawara[2]; Masafumi Kudo[2]; Hitoshi Chiba[3]; Shu-Ping Hui[3]; *[1]Hokkaido University, Sapporo, Hokkaido; [2]Northern Advancement Center for Science & Technology, Sapporo, Japan; [3]Hokkaido University, Sapporo, Japan*

ThP 229 **Maldi Imaging of Alkaloids in Catharanthus roseusLeaves**; Lorenzo Caputi[1]; Gerhard Saalbach[1]; Sarah E. O'Connor[1]; *[1]John Innes Centre, Norwich, UK*

ThP 230 **Development of Laser Ablation Direct Analysis in Real Time Imaging Mass Spectrometry (LADI-MS)**; Rabi Musah[1]; Kristen L Fowble[1]; *[1]University at Albany-SUNY, Albany, NY*

ThP 231 **Mass Spectrometry Imaging Enhances Biochemical Pathway Elucidation**; David Gang[1]; Park Jeong-Jin[1]; Willis Mark[1]; Jing Wang[1]; *[1]Washington State University, Pullman, WA*

ThP 232 **Matrix Assisted Laser Desorption Ionization Mass Spectrometry Imaging of Glycosphingolipids in Rat Eye Tissue: Method Development and Optimization**; Gargey B. Yagnik[1]; Mandy Cromwell[2]; Alexander Brezzani[2]; Kelly Keefe[2]; Mark Bree[3]; Dinesh Bangari[4]; Petra Oliva[5]; Thomas O'Shea[1]; Hanlan Liu[1]; *[1]Drug Metabolism and Pharmacokinetics, Sanofi, Waltham, MA; [2]Rare Disease Pharmacology, Sanofi, Waltham, MA; [3]Preclinical Toxicology, Sanofi, Waltham, MA; [4]Pathology, Sanofi, Framingham, MA; [5]Biological Mass Spectrometry, Sanofi, Framingham, MA*

ThP 233 **Sub Micrometric 3D Analysis of Mosquito Ovaries using TOF-SIMS Imaging**; Quentin Vanbellingen[1]; Anthony Castellanos[1]; Marcela Nouzova[1]; Fernando G. Noriega[1]; Francisco Fernandez-Lima[1]; *[1]Florida International University, Miami, FL*

ThP 234 **Three Dimensional MALDI-MS Imaging of a Single Cell Zebrafish Embryo**; Maria Emilia Dueñas[1, 2]; Adam Feenstra[1, 2]; Jeffrey Essner[1]; Young Jin Lee[1, 2]; *[1]Iowa State University, Ames, IA; [2]Ames Laboratory-USDOE, Ames, IA*

ThP 235 **The Embryome: Molecules in Space and Time During the Early Stage Development**; Laszlo Mark[1, 2, 3]; Janos Schmidt[1, 3]; *[1]Department of Analytical Biochemistry, Institute of Biochemistry and Medical Chemistry, Medical School, University of Pecs, Pecs, Hungary; [2]PTE-MTA Human Reproduction Research Group, Pecs, Hungary; [3]Imaging Center for Life and Material Sciences, University of Pecs, Pecs, Hungary*

ThP 236 **Optimisation of Matrix Condition for theAnalysis of the Antifungal Agent (Terbinafine hydrochloride) in a Living Skin Equivalent Model**; Cristina Russo[1]; Malcolm R Clench[2]; Neil Bricklebank[2]; Catherine Duckett[2]; Stephen Mellor[3]; Stephen Rumbelow[4]; *[1]Sheffield Hallam University, Sheffield ; [2]Sheffield Hallam University, BMRC Sheffield, UK; [3]Croda Europe Ltd, Snaith, UK; [4]Croda Inc, New Castle, DE*

ThP 237 **Benchmarking New GCIB-SIMS Technology against MALDI and Applying GCIB-SIMS to Study Myocardial Infarction**; Amir Saeid Mohammadi[1]; Sanna Sämfors[1]; Andrew G Ewing[1, 2]; John Fletcher[2]; *[1]Chalmers University of Technology, Gothenburg, Sweden; [2]University of Gothenburg, Gothenburg, Sweden*

ThP 238 **Mass Spectrometric Imaging of a Three-Dimensional Osteosarcoma Model**; Ieva Palubeckaite[1]; Neil Cross[1]; Malcolm R Clench[1]; Christine Le Maitre[1]; *[1]Sheffield Hallam University, Sheffield, UK*

ThP 239 **The Effects of Diets on rat Brain Regional Lipid Composition using GCIB-SIMS**; Amir Saeid Mohammadi[1]; Alastair Ross[1]; John S Fletcher[2]; Andrew G Ewing[1, 2]; *[1]Chalmers University of Technology, Gothenburg, Sweden; [2]University of Gothenburg, Gothenburg, Sweden*

ThP 240 **Specific Isotopic Pattern of Brominated Pyrylium Salts Facilitates Mass Spectrometry Imaging and Identification of Derivatized Small Molecule Neuroactive Compounds**; Mohammadreza Shariatgorji[1]; Anna Nilsson[1]; Per E Andren[1]; *[1]Uppsala University, Uppsala, Sweden*

ThP 241 **MALDI Imaging with High Spatial Resolution for the Direct Analysis of Phospholipids in Rat Brain Tissue**; Simona Salivo[1]; Yuzo Yamazaki[2]; Omar Belgacem[3]; Peter Quinto Tranchida[1]; Luigi Mondello[1]; *[1]University of Messina, Messina, Italy; [2]Shimadzu Corporation, Kyoto, Japan; [3]Shimadzu, Kratos Manchester, UK*

ThP 242 **MALDI-TOF Imaging Mass Spectrometry Reveals a Massive Loss of Polyunsaturated Cardiolipins after Traumatic Brain Injury**; L.J. Sparvero[1]; Andrew A Amoscato[2]; Arthur B. Fink[2]; Tamil Anthonymuthu[2]; Simon Watkins[2]; Valerian E. Kagan[2]; Hulya Bayir[2]; *[1]University of Pittsburgh, Pittsburgh , PA; [2]University of Pittsburgh, Pittsburgh, PA*

ThP 243 **Compounds Screening in Dosed Human Skins by Quantitative Mass Spectrometry Imaging**; David Bonnel[1]; Sylvain Ghilini[2]; Raphael Legouffe[1]; Claude Verrier[2]; Gael Picard-de Muller[1]; Marie-José Cuadrado[2]; Fabien Pamelard[1]; Gregory Hamm[1]; Jonathan Stauber[1]; *[1]ImaBiotech, MS Imaging Dept. Loos, France; [2]Galderma, Sophia-Antipolis, France*

ThP 244 **Imaging of Drugs and Lipids in Living Skin Equivalents by MALDI MS and SIMS**; Josephine Bunch[1]; Rory Steven[1]; Alan Race[1]; *[1]National Physical Laboratory, Teddington, UK*

ThP 245 **Adjustable Hydrophobic GUMBOS Matrices for MALDI Mass Spectral Imaging**; Tia Vargas[1]; Kermit K Murray[1]; Isiah M Warner[1]; *[1]Louisiana State University, Baton Rouge, LA*

ThP 246 **Evaluating DESI Imaging and High Resolution Mass Spectrometry to Improve an Industrial Component Cleaning Process**; Peter Hancock[1]; Jonathan Jones[1];

Eleanor Riches[1]; Vikki Turner[1]; Gordon Jones[1]; Timothy Harford[1]; *[1]Waters, Wilmslow, UK*

ThP 247 **Surface Imaging of Polymers and Polymer Additives with TOF-SIMS Parallel Imaging MS/MS**; John Hammond[1]; Gregory L Fisher[1]; Paul Larson[1]; Scott Bryan[1]; *[1]Physical Electronics, Chanhassen, MN*

INFORMATICS: GENERAL, SRM, AND DIA
248 - 269

ThP 248 **A Glycan Structure MS/MS Search Platform in Python**; Joshua Klein[1]; Kshitij Khatri[2]; Yi Pu[2]; Lin Cheng[2]; Joseph Zaia[2]; *[1]Boston University Program for Bioinformatics, Boston, MA; [2]Boston University, Boston, MA*

ThP 249 **Automatic Quality Assessment of Mass Spectrometry Experiments by Multivariate Quality Control Metrics and the Relation between Low-Quality Experiments and Identifications**; Wout Bittremieux[1]; Pieter Meysman[1]; Lennart Martens[2]; Dirk Valkenborg[3]; Kris Laukens[1]; *[1]University of Antwerp, Antwerp, Belgium; [2]Ghent University, Ghent, Belgium; [3]VITO, Mol, Belgium*

ThP 250 **Spectrum Acquisition for Building the NIST Tandem MS Library**; Yuxue Liang[1]; Pedatsur Neta[2]; Xiaoyu Yang[2]; Stephen Stein[2]; *[1]National Institute of Standards and Technology, Gaithersburg, MD; [2]NIST, Rockville, MD*

ThP 251 **DIAprobe – Implementation of a Statistical Tool for Data Independent Acquisition in Skyline for SWATH Analysis**; Alexandria DSouza[1]; Birgit Schilling[1]; Bradford W Gibson[1]; *[1]Buck Institute for Research on Aging, Novato, CA*

ThP 252 **Automated Design of Optimal SRM &PRM Assays using Empirical Modular Models**; Jerome Renaux[1]; Alexandros Sarafianos; Kurt De Grave; Jan Ramon[2]; *[1]KULeuven, Heverlee, Vlaamse Brabant; [2]KU Leuven, Leuven, Belgium*

ThP 253 **PTM-Annotator: A Python Library for Annotation of Post-Translation Modification from Proteomic Mass Spectrometry Analysis**; Amin Momin[1]; Hailey E Haut[1]; Michela Capello[1]; Juan Chen[1]; Hong Wang[1]; Samir M Hanash[1]; *[1]MD Anderson Cancer Center, Houston, TX*

ThP 254 **Proteomic Sequencing and Resurrection of a Monoclonal Antibody**; Natalie Castellana[1]; Kexin Huang[2]; Hua Tu[2]; *[1]Digital Proteomics, LLC., San Diego, CA; [2]LakePharma, Inc., Belmont, CA*

ThP 255 **MADpipe – An MRM Assay Design PIPEline for Multiplexed Multiple and Parallel Reaction Monitoring (MRM and PRM) Experiments**; Yassene Mohammed[1, 2]; Derek S Smith[1]; Dominik Domanski[1, 3]; Angela M Jackson[1]; Andrew Percy[1]; Andrew G Chambers[1]; Andrea Palmer[4]; Suping Zhang[4]; Christoph H. Borchers[5, 6]; *[1]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [2]Center for Proteomics and Metabolomics, Leiden University Medical Center, Leiden, The Netherlands; [3]Segal Cancer Proteomics Center, Lady Davis Institute, McGill University, Montreal, QC, Canada; [4]MRM Proteomics, Inc., Victoria, BC, Canada; [5]University of Victoria - Genome BC Proteomics Centre, Victoria, BC; [6]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada*

ThP 256 **Scout-MRM: Extended Portability of Large Multiplexed Peptide Assay**; Blandine Rougemont[1]; Romain Carriere[1]; Sophie Ayciriex[1]; Jean Marie Lacroix[2]; David Cox[3]; Yves J C LeBlanc[3]; Jérôme Lemoine[1]; *[1]Institut des Sciences Analytiques, UMR 5280 CNRS, Université de Lyon, Villeurbanne, France; [2]UGSF UMR Lille1/CNRS 8576, Villeneuve D'ascq Cedex, France; [3]SCIEX, Concord, ON*

ThP 257 **EasyCont: Identify Contaminants On-Line for Free on ms.cheminfo.org**; Daniel Ortiz[1]; LAURE MENIN[1]; Luc Patiny[1]; *[1]EPFL, Lausanne, Switzerland*

ThP 258 **BioDocker: An Open Source and Community-Driven Framework for Software Standardization in Proteomics**; Felipe da Veiga Leprevost[1]; Saulo Alves Aflitos[2]; Björn Grüning[3]; Hannes Roest[4]; Harald Barsnes[5]; Rafael Jimenez[6]; Henning Hermjakob[6]; Alexey I. Nesvizhskii[1]; Yasset Perez-Riverol[6]; *[1]University of Michigan, Ann Arbor, MI; [2]Wageningen University, Wageningen, The Netherlands; [3]University of Freiburg, Freiburg, Germany; [4]Stanford University School of Medicine, Palo Alto CA, USA; [5]University of Bergen, Bergen, Norway; [6]EMBL-EBI, Hinxton, UK*

ThP 259 **CRAPome 2.0: A Comprehensive Resource for Affinity Purification Mass Spectrometry Data**; Dattatreya Mellacheruvu[1]; Zachary Wright[1]; Anne-Claude Gingras[2]; Alexey I Nesvizhskii[1]; *[1]University of Michigan, Ann Arbor, MI; [2]Samuel Lunenfeld Research Institute, Mount Sinai H Toronto, ON*

ThP 260 **Without Sacrificing Dwell Time, Achieving 1/N Smaller SWATH Windows (N = Number of MS Samples) to Quantify Low-Abudance Ions**; GAUTAM SAXENA[1]; Vidya Venkatraman[2]; Sarah Parker[2]; Ronald Holewinski[2]; Jennifer E Van Eyk[2]; *[1]Deep Search, Bethesda, MD; [2]Cedars-Sinai Medical Center, Los Angeles, CA - California*

ThP 261 **Analysis of Data Independent Acquisition Mass Spectrometry Data with DIA-Umpire v2**; Chih-Chiang Tsou[1]; Chia-Feng Tsai[2]; Yu-Ju Chen[2]; Guoci Teo[1]; Anne-Claude Gingras[3]; Alexey Nesvizhskii[1]; *[1]University of Michigan, Ann Arbor, MI; [2]Academia Sinica, Taipei, Taiwan; [3]Lunenfeld-Tanenbaum Research Institute, Toronto, Canada*

ThP 262 **Proteomics for Ricin Bioforensics: Protein Content of Castor Seed Extracts and Related Informatics Approaches**; Eric Merkley[1]; Alaine M. Garrett[2]; Kristin H Jarman[3]; Owen P Leiser[1]; Jennifer A Arce[1]; Kristin D Victry[1]; Angela M Melville[1]; David S. Wunschel[1]; Stephen R. Cendrowski[2]; Karen L Wahl[1]; *[1]Chemical and Biological Signature Sciences Group, Pacific Northwest National Laboratory, Richland, WA; [2]National Biodefense Analysis and Countermeasures Center, Fort Detrick, MD; [3]Applied Statistics and Mathematics Group, Pacific Northwest National Laboratory, Richland, WA*

ThP 263 **Simulations Reveal the Pertinent Factors for High Quality Mass Spectrometry Based Microorganism Identification**; Jan Eriksson[1]; David Fenyö[2]; Sabina Koj[3]; Tomasz Niedziela[3]; *[1]Swedish University of Agricultural Sciences, Uppsala; [2]Laboratory of Computational Proteomics, Center for Health Informatics and Bioinformatics, New York University School of Medicine, New York, NY; [3]Institute of Immunology & Experimental Therapy PAN, Wroclaw, Poland*

ThP 264 **Top-down MSMS Data Analysis: Software and Algorithms for Protein Identification and Fragment Ion Assignment**; Christian F. Heckendorf[1]; Roger Theberge[1]; Deborah R. Leon[1]; Kshitij Khatri[1]; Jean L. Spencer[1]; Catherine E. Costello[1]; Mark E. McComb[1]; *[1]Boston University School of Medicine, Boston, MA*

ThP 265 **Process Analytical Technology (PAT) Applications of Mass Spectrometry: Real-time Monitoring of Drying Process**; Heewon Lee; *Boehringer Ingelheim Pharma, Ridgefield, CT*

ThP 266 **New Developments in MSstats: Statistical Process Control, LoD/LoQ, and Relative Protein Quantification with Split Plot Approach**; Meena Choi[1]; Eralp Dogu[2]; Cyril Galitzine[2]; Olga Vitek[2]; *[1]Purdue University, West Lafayette, IN; [2]Northeastern University, Boston, MA*

ThP 267 **Combinatorial Use of Multiple Spectral Libraries Drastically Improves the Number, Breadth, and Confidence of Identified Proteins in a Murine Model**; Mark A. Wingerd[1]; Troy H Patience[1]; Avedis A. Kazanjian[1]; Jessica L. Slack[1]; Vivek S. Ramachandran[1]; Elizabeth H. Yohannes[1]; Andrew S. Thagard[2]; *[1]Department of Clinical Investigation, Madigan Army Medical Center, Tacoma, WA; [2]Maternal Fetal Medicine, Madigan Army Medical Center, Tacoma, WA*

ThP 268 **mzCloud, a First Quantum Chemically Annotated Mass Spectral Database**; Michal Raab[1]; Chongle Pan[2]; Milos Suchy[1]; Martin Mandak[1]; Juraj Lutisan[1]; Robert Mistrik[3]; *[1]HighChem, Bratislava, Slovakia; [2]Oak Ridge National Laboratory, Oak Ridge, TN; [3]HighChem, Bratislava, SK*

ThP 269 **Managing Small Molecule Targeted Mass Spec Assays using Skyline and Panorama**; Josh Eckels[1]; Vagisha Sharma[2]; Brian Pratt[2]; Tom PJ Dunkley[3]; Kristin R Wildsmith[4]; Cory Nathe[5]; Binal Patel[1]; Richard Johnson[2]; Jacob D Jaffe[6]; Michael MacCoss[2]; Brendan MacLean[2]; *[1]LabKey Software, San Diego, CA; [2]University of Washington, Seattle, WA; [3]Hoffmann-La Roche Ltd., Basel, Switzerland; [4]Genentech Inc, San Francisco, CA; [5]LabKey Software, Seattle, WA; [6]The Broad Institute, Cambridge, MA*

INFORMATICS: PROTEIN ID AND QUANTIFICATION 270 - 281

ThP 270 **Evaluation and Improvement of Quantification Accuracy in Isobaric Mass Tag Based Protein Quantification Experiments**; Erik Ahrné[1]; Timo Glatter[1]; Cristina Viganò[1]; Conrad von Schubert[1]; Erich A. Nigg[1]; Alexander Schmidt[1]; *[1]Biozentrum, University of Basel, Basel, Switzerland*

ThP 271 **Analysis Workflow for Quantitative Proteomics, Employing Triplex Dimethyl Labelling and Ion Mobility Assisted Data Independent Acquisition**; Andrew Paul Collins[1, 2]; Antony McCabe[1, 2]; Ian Morns[3]; Chris J Hughes[4]; Johannes PC Vissers[4]; Andrew Robert Jones[1, 2]; *[1]University of Liverpool, Liverpool, UK; [2]Omic Analytics, Liverpool, UK; [3]Nonlinear Dynamics Limited, Newcastle upon Tyne, UK; [4]Waters Corporation, Wilmslow, UK*

ThP 272 ***De novo* Profiling Strategies to Examine Divergent Mutation of Influenza Vaccines**; Ryan D. Leib[1]; Louis Jacob[2]; Allis Chien[1]; Emmanuel Mignot[1]; Christopher M Adams[1]; *[1]Stanford University, Stanford, CA; [2]Descartes University, Paris, France*

ThP 273 **Diffacto: Robust Quantification for Large Sample Size Shotgun Proteomics**; Bo Zhang[1]; Mohammad Pirmoradian[1]; Roman A Zubarev[1]; Lukas Käll[2]; *[1]Karolinska Institutet, Solna, Sweden; [2]KTH Royal Institute of Technology, Stockholm, Sweden*

ThP 274 **Fast and Accurate Protein False Discovery Rates on Human Proteome Study Scale with Percolator 3.0**; Matthew The[1]; Michael J. MacCoss[2]; William S. Noble[2]; Lukas Käll[1]; *[1]KTH - Royal Institute of Technology, Stockholm, Sweden; [2]University of Washington, Seattle, WA*

ThP 275 **New Functionality for the Trans-Proteomic Pipeline: Tools for the Analysis of Proteomics Data**; Luis Mendoza[1]; David Shteynberg[2]; Joseph Slagel[2]; Michael Hoopmann[2]; Jason Winget[2]; Henry Lam[3]; Jimmy K Eng[4]; Eric Deutsch[2]; Robert L Moritz[2]; *[1]Institute For Systems Biology, Seattle, WA; [2]Institute for Systems Biology, Seattle, WA; [3]Hong Kong University of Science and Technology, Hong Kong, China; [4]University of Washington, Seattle, WA*

ThP 276 **Quantification with MultiNotch MS3 across Multiple LC-MS Runs with PEAKS Q**; Lei Xin[1]; Hao Lin[1]; Baozhen Shan[2]; *[1]Bioinformatics Solutions Inc., Waterloo, Canada; [2]Bioinformatics Solutions Inc., Waterloo, ON*

ThP 277 **False Discovery Rate Estimation in Large Scale Proteomic Datasets**; Avinash Shanmugam[1]; Alexey I Nesvizhskii[1]; *[1]University of Michigan, Ann Arbor, MI*

ThP 278 **A Proteogenomic Approach to Identify Sample-Specific Variant Proteins in a Myeloid Cell Line**; Hossein Fazelinia[1]; Kian Huat Lim[1]; Hua Ding[1]; Tina Glisovic-Aplenc[1]; Richard Aplenc[1]; Saar Gill[2]; Sarah Tasian[1]; Steven H. Seeholzer[3]; *[1]Children's Hopsital of Philadelphia, Philadelphia, PA; [2]University of Pennsylvania School of Medicine, Philadelphia, PA; [3]Children's Hospital of Philadelphia, Philadelphia, PA*

ThP 279 **Proteogenomic Approaches to Improve the Identification of Proteins in Non-Human Primate Tissue Samples**; Avinash Jadhav[1]; Michael J Proffitt[1]; Jeremy Glenn[1]; Anthony Cesnik[2]; Michael R Shortreed[2]; Kavanagh Kylie[3]; Laura Cox[1]; Michael Olivier[1]; *[1]Texas Biomedical Research Insttitue, San Antonio, TX; [2]UW-Madison, Madison, U.S.A; [3]Wake Forest University School of Medicine, Winston-Salem, NC*

ThP 280 **A One-Click Graph Visualization R Program for Proteomics Datasets**; Amber K Weiner[1, 2, 3]; Simone Sidoli[3]; Sharon J Diskin[1, 2]; Benjamin A Garcia[1, 3]; *[1]Genomics and Computational Biology, Biomedical Graduate Studies, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA; [2]Division of Oncology, Department of Pediatrics, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA; [3]Epigenetics Program, Department of Biochemistry and Biophysics, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA*

ThP 281 **Elucidation of Molecular Differences Amongst PPARg Selective Modulators**; Vinh Q. Lam[1]; Patrick R. Griffin[2]; *[1]The Scripps Research Institute, Scripps Florida Jupiter, FL; [2]The Scripps Research Institute, Jupiter, FL*

INSTRUMENTATION: NEW DEVELOPMENTS IN IONIZATION AND SAMPLING (IONIZATION) 282 - 308

ThP 282 **Development of a Novel Ion Source for µ-plasma Induced Proton Transfer Reaction Mass Spectrometry**; David Mueller[1]; Yessica Brachthäuser[1]; Nele Hartmann[1]; Robin Hillen[1]; Duygu Erdogdu[1]; Klaus Brockmann[1]; Hendrik Kersten[1]; Thorsten Benter[1]; *[1]University of Wuppertal, Wuppertal, Germany*

ThP 283 **CNT Functionalized Corona Pin Sampling of Benzo(j) fluoranthene**; Keaton Nahan[1]; Anne Vonderheide[2]; Vesselin Shanov[1]; Julio Landero Figueroa[2]; *[1]University of Cincinnati, Cincinnati, OH; [2]University of Cincinnati, Cincinnati, Ohio*

ThP 284 **Formation of Protonated and Metal-Adducted Organic and Biological Compound Ions by High Temperature Plasma/Mass Spectrometry**; Jentaie Shiea [1]; Sy-Chyi Cheng[2]; *[1]National Sun Yat-Sen University, Kaohsiung, Taiwan; [2]National Sun Yat-Sen Univ., Kaohsiung, Taiwan*

ThP 285 **Seconds Per Sample with Echo-DART-MS: Acoustic Loading of a Mass Spectrometer for High-Throughput Label-Free Screening**; Eric Hall[1]; Martin Bachmann[2]; Ian Sinclair[2]; Jonathan Wingfield[3]; Lars Majlof[1]; Musselman Brian[4]; Sammy Datwani[1]; Luke Ghislain[1]; *[1]Labcyte, Sunnyvale, CA; [2]AstraZeneca, Maccelsfield, UK; [3]AstraZeneca, Cambridge, UK; [4]IonSense, Inc. Saugus, MA*

ThP 286 **Utility of an Off-Axis Vapor Sampler with Direct Analysis in Real Time source equipped Mass Spectrometer**; Brian D. Musselman [1]; Joseph Tice[2]; Robert Goguen[2]; Frederick Li[2]; *[1]IonSense, Inc., Saugus , MA; [2]IonSense, Inc. Saugus, MA*

ThP 287 **Molecular Ionization Desorption Analysis Source (MIDAS) for Mass Spectrometry: A Flexible Ambient Platform**; Greg Winter[1]; Joshua Wilhide[1]; William LaCourse[1]; *[1]UMBC Department of Chemistry and Biochemistry, Baltimore, MD*

ThP 288 **Ionization and Tunable Fragmentation of Biopolymers at Atmospheric Pressure with a Direct-Sampling Solution-Cathode Glow Discharge**; Jake Shelley[1]; Andrew J Schwartz[2]; Kelsey L WIlliams[1]; Courtney L Walton[1]; Gary M Hieftje[2]; *[1]Kent State University, Kent, OH; [2]Indiana University, Bloomington, IN*

ThP 289 **Solution-Cathode Glow Discharge: A Versatile Ion Source for Atomic and Molecular Mass Spectrometry**; Andrew Schwartz[1]; Kelsey Williams[2]; Courtney Walton[2]; Gary Hieftje[1]; Jacob Shelley[2]; *[1]Indiana University, Bloomington, IN; [2]Kent State University, Kent, OH*

ThP 290 **An Aerodynamic Perspective on Impactor API Sources**; Steve Bajic; *Waters Corporation, Wilmslow, UK*

ThP 291 **'On-The-Spot' Analysis using Liquid Extraction Probes**; Gary J. Van Berkel[1]; Vilmos Kertesz[2]; *[1]Oak Ridge National Laboratory, Oak Ridge , TN; [2]Oak Ridge National Laboratory, Oak Ridge, TN*

ThP 292 **Monitoring of Chemical Reactions in Real Time by Polarization Induced Electrospray Ionization Mass Spectrometry**; Anil Kumar Meher; *National Chiao Tung University, Hsinchu, Taiwan*

ThP 293 **Paired-Ion Sonic-Spray Ionization Mass Spectrometry (PI-SSI-MS) for the Analysis of Anionic Ions: Progress towards Even Lower Limits of Detection**; Emmanouil Mavrakis[1]; Leonidas Mavroudakis[1]; Spiros Pergantis[1]; *[1]University of Crete, Heraklion, Greece*

ThP 294 **Ultrasonication-spray Ionization Based Micro-reactors for On-line Monitoring of Chemical Reactions and De-salting**; Te-Yu Chen[1]; Yu-Chie Chen[1]; *[1]National Chiao Tung University, Hsinchu, Taiwan*

ThP 295 **CE-nanoESI-MS for Untargeted Proteomic Characterization of Single Embryonic Cells and Small Neuron Populations**; Sam Choi[1]; Marta Zamarbide[2]; M. Chiara Manzini[2]; Sally A Moody[2]; Peter Nemes[2]; *[1]George Washington University, Washington, DC; [2]George Washington University, Washington DC*

ThP 296 **Ion Sampling and Cluster Formation in Nanospray Pulsed-Field Atmospheric-Pressure Ion Mobility MS**; William McMahon[1]; Kaveh Jorabchi[1]; *[1]Georgetown University, Washington, DC*

ThP 297 **Development of a Disposable Cartridge with Integrated Antibody for Protein Detection by Paper Spray Mass Spectrometry**; Chengsen Zhang[1]; Nicholas E Manicke[1]; *[1]IUPUI Department of Chemistry & Chemical Biology, Indianapolis, IN*

ThP 298 **Joule Heating and Thermal Denaturation of Proteins in nano-ESI Theta Tips**; Feifei Zhao[1]; Owen G Rehrauer[1]; Sarah M Matt[1]; Jiexun Bu[1]; Scott A McLuckey[1]; *[1]Purdue University, West Lafayette, IN*

ThP 299 **Next-Generation Multinozzle Emitters for Interfacing Microflow LC and NanoESI-MS**; Pan Mao[1]; Geuncheol Gil[1]; Daojing Wang[1]; *[1]Newomics Inc, Emeryville, CA*

ThP 300 **Development of a Novel Nano-electrospray Ionization Source Coupled with Mass Spectrometer to Achieve Stable and Robust Nano Spray**; Frenny Ruparelia Kaushal[1]; Reza Javahery[1]; Lisa Cousins[1]; *[1]IONICS Mass Spectrometry, Bolton, Canada*

ThP 301 **An Electrospray Ionization Based Approach for Detecting Circulating Tumor Cells (CTCs) using the SIERRA Particle Amplification Method**; Adam Hollerbach[1]; Stephen Ayrton[1]; Zane Baird[1, 2]; Valentina Pirro[1]; Cathleen Hanau[2]; Karen Marfurt[2]; Michael Pugia[2]; Graham Cooks[1]; *[1]Purdue University, West Lafayette, IN; [2]Siemens Healthcare Diagnostics, Elkhart, IN*

ThP 302 **Further Development of an Integrated Acoustic Electrospray Source for High-Throughput Label-Free Mass Spectrometry Biochemical Screening**; Ian Sinclair[1]; Jonathan Wingfield[2]; Bachman Martin[1]; Steven D Pringle[3]; Hall Eric[4]; Lucien Ghislain[5]; Lars Majlof[4]; Stearns Rick[4]; Sammy Datwani[4]; *[1]AstraZeneca, Maccelsfield, UK; [2]AstraZeneca, Cambridge, UK; [3]Waters, Wilmslow, UK; [4]Labcyte, Inc., Sunnyvale, CA - California; [5]Labcyte Inc, Sunnyvale, CA*

ThP 303 **Performance Evaluation of a Pneumatically Assisted Electrospray Ionization Source in the Microflow Regime**; Harikrishnan Sukumar[1]; Eloy R Wouters[1]; Lee Earley[1]; Mark E Hardman[1]; Jean-Jacques Dunyach[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

ThP 304 **On-line Charge State Manipulation using Contained-electrospray Ionization**; Colbert Miller[1]; Jongin Kim[1]; Abraham Badu-Tawiah[1]; *[1]The Ohio State University, Columbus, OH*

ThP 305 **Droplets: IBF Mass Spectroscopy and Analytical Chemistry**; Drew Sauter[1]; Andrew D Sauter[2]; Gary Groenewold[3]; Robert Ross[4]; Patrick A Limbach[4]; *[1]Nanoliter, LLC, Henderson , NV; [2]nanoliter LLC, Henderson, NV; [3]Idaho National Laboratory, Idaho Falls, ID; [4]University of Cincinnati, Cincinnati, OH*

ThP 306 **Thread Spray Mass Spectrometry for Direct Analysis of Capsaicinoids in Evidentiary Garments**; Patricia Capone[1]; Abraham Badu-Tawiah[1]; *[1]The Ohio State University, Columbus, Ohio*

ThP 307 **Exploring the REIMS Interface Using the DSMC Method and Particle Tracing in Realistic Low Pressure Gas Flows**; Athanasios Zacharos[1]; Julia Abda[2]; Alexander Lekkas[1]; Dimitris Papanastasiou[1]; Emmanuel Raptakis[1]; Tamas Karancsi[3]; Zoltan Takats[2]; *[1]Fasmatech, Athens, Greece; [2]Imperial College, London, UK; [3]Waters Research Centre, Budapest, Hungary*

ThP 308 **Optimization of Matrix assisted Rapid Evaporative Ionisation Mass Spectrometry (MAREI-MS) System**; Daniel Simon[1]; Tamas Karancsi[2]; Julia Balog[2]; Emrys A Jones[3]; Steven Pringle[3]; Zoltan Takats[4]; *[1]Waters Research Center Ltd., Budapest, Budapest; [2]Waters Research Center, Budapest, Hungary; [3]Waters, Wilmslow, UK; [4]Imperial College, London, UK*

IONIZATION MECHANISMS
309 - 323

ThP 309 **Impact of Chemical Modifiers on the Cluster Chemistry during Electrospray Ionization**; Marco Thinius[1]; Markus Langner[1]; Thorsten Benter[1]; *[1]University of Wuppertal, Wuppertal, Germany*

ThP 310 **Examination of Droplet Size Dependence of Charge Reduction Methodologies**; Ashley Marie Moon[1]; Bojana Opacic[1]; Peter Ta Reilly[1]; *[1]Washington State University, Pullman, WA*

ThP 311 **Water Phase pH Effects on Electrospray Ionization Efficiency**; Jaanus Liigand[1]; Asko Laaniste[1]; Anneli Kruve[1]; *[1]University of Tartu, Institute of Chemistry, Tartu, Estonia*

ThP 312 **Novel Method for the Detection of Ionization Suppression**; Richard King[1]; Carmen Fernandez-Metzler[2]; *[1]PharmaCadence Analytical Services, LLC, Hatfield, PA; [2]PharmaCadence Analytical Services, LLC Hatfield, PA*

ThP 313 **Incorporating Cations and Anions into Molecular Dynamics Simulations of the Electrospray Process and the Resemblance to a "Salting-Out" Process**; DoYong Kim[1]; Nicole D. Wagner[1]; David H Russell[1]; *[1]Texas A&M, College Station, TX*

ThP 314 **Application of Chemical Supercharging Electrospray Ionization to Small Organic Molecules**; Andrew T. Ball[1]; Anthony W T Bristow[2]; Martin Sims[2]; Mike Morris[3]; Jackie Mosely[1]; *[1]Durham University, Durham, UK; [2]AstraZeneca, Maccelsfield, UK; [3]Waters, Wilmslow, UK*

ThP 315 **Theoretical Investigation of Low Detection Sensitivity of Carbohydrates in ESI and MALDI**; Jien-Liang Chen; *Academia Sinica, Taipei, TAIWAN (R.O.C.)*

ThP 316 **Protonation sites in multifunctional compounds upon positive mode ESI and APCI in a linear quadrupole ion-trap**; Rashmi Kumar[1]; Ravikiran Yerabolu[2]; John Y Kong[2]; Chungang (Chuck) Gu[3]; Hilkka I Kenttamaa[2]; *[1]Purdue University-Department of Chemistry, West Lafaytte, Indiana; [2]Purdue University-Department of Chemistry, West Lafayette, IN; [3]AstraZeneca, Boston, MA*

ThP 317 ***Ab initio* Studies on the Mechanisms of ipso-Substitution Observed in DA-APPI**; Alexander Haack[1]; Clara Markert[1]; Tiina Kauppila[2]; Hendrik Kersten[1]; Thorsten Benter[1]; *[1]University of Wuppertal, Wuppertal, Germany; [2]University of Helsinki, Helsinki, Finland*

ThP 318 **Combined Study of Ionic Processes on Surfaces: Photoelectric and Photocatalytic Effects**; Christine Polaczek[1]; Valerie Derpmann[1]; Hendrik Kersten[1]; Thorsten

Benter[1]; *[1]Bergische Universität Wuppertal, Wuppertal, Germany*

ThP 319 **Production of NH3 in N2-Corona Discharges and 63Ni Sources: Unequivocal Identification and Quantification**; Nele Hartmann[1]; Sonja Klee[1]; Marco Thinius[1]; Sarah Peters[1]; Joerg Kleffmann[1]; Thorsten Benter[1]; *[1]University of Wuppertal, Wuppertal, Germany*

ThP 320 **Importance of Solvent Clusters in the Mechanism of Atmospheric Pressure Photo Ionization Evidenced by Theoretical Calculation and Experimental Results**; Sunghwan Kim[1]; Arif Ahmed[2]; *[1]Chemistry Department, Kyungpook National Universit, Daegu, Asia; [2]Kyungpook National University, Daegu, Republic of Korea*

ThP 321 **Interaction of keV Fullerene Ions with Molecules Supported on Free Standing Graphene: Mechanism of Molecule Ejection and ionization**; Stanislav Verkhoturov[1]; Mikolaj Golunski[2]; Sheng Geng[1]; Dmitriy S Verkhoturov[1]; Michael J Eller[1]; Zbigniew Postawa[2]; Emile A Schweikert[1]; *[1]Texas A&M University, College Station, TX; [2]Department of Physics of Nanostructures and Nanotechnology, Institute of Physics, Jagiellonian University, Krakow, Poland*

ThP 322 **Effects of Nanoelectrospray Emitter Size on Protein Desalting in Native Mass Spectrometry**; Anna Susa[1]; Zijie Xia[1]; Evan R Williams[1]; *[1]UC Berkeley, Berkeley, CA*

ThP 323 **Flow Rate Measurements on a nano-ESI Source by Digital Image Analysis**; Alejandro Cohen[1]; Axel J Soto[1]; Jim P Fawcett[1]; *[1]Dalhousie University, Halifax, NS*

LC-MS: SAMPLE PREPARATION (PART 2)
324 - 345

ThP 324 **iST: Sample Preparation for High Throughput Clinical Proteomics**; Garwin Pichler[1]; Nils A. Kulak[1]; *[1]PreOmics GmbH, Gauting, Germany*

ThP 325 **Automated Desorption, SPE Extraction, and LC/MS/MS Analysis of Dried Blood Spots**; Fredrick Foster[1]; John Stuff[1]; Edward Pfannkoch[1]; *[1]Gerstel, Inc. Linthicum, MD*

ThP 326 **Fast Quantitation of Target Compounds Present in Small Volume of Complex Matrices by Miniaturized Solid Phase Microextraction Device**; Hamed Piri-Moghadam[1]; Fardin Ahmadi[1]; German Augusto Gomez-Rios[1]; Barbara Bojko[1]; Janusz Pawliszyn[1]; *[1]University of Waterloo, Waterloo ON, Canada*

ThP 327 **Developing Methods for Analyzing Proteins from Sperm Cells**; Cheylene Tanimoto[1]; Mark Flory[2]; Parag Mallick[2]; Kevin Wang[2]; Sharon J Pitteri[2]; *[1]Stanford University, Stanford, CA; [2]Stanford University School of Medicine, Palo Alto CA*

ThP 328 **A Rapid Clean-up with Cleanert HFMF-X for The Analysis of 25-OH-Vitamin-D in Human Plasma by LC-MS/MS**; Wan Wang[1]; Ruyi Wang[1]; *[1]Bonna-Agela Technologies, Tianjin, China*

ThP 329 **Electrospray Ionization Analysis of Dextran and Carboxymethylated Dextran**; Jesus Tapia[1]; Karolien Denef[1]; Claudia M Boot[1]; Melissa M Reynolds[1]; *[1]Colorado State University, Fort Collins, CO*

ThP 330 **All Roads Lead to Robots: Automation of Customized, Effective Trypsin Digestion**; Qin Fu[1]; Michael P Kowalski[2]; Christie L Hunter[3]; Mitra Mastali[4]; Tara R Jones-Roe[2]; Jennifer E Van Eyk[4, 5]; *[1]Cedars Sinai Medical Center, Los Angeles, CA; [2]Beckman Coulter Life Sciences, Indianapolis, IN, USA, Indianapolis, IN; [3]SCIEX, Redwood City, CA; [4]Cedars Sinai Medical Center, Los Angeles , CA; [5]Advanced Clinical Biosystems Research Institute, Los Angeles, CA*

ThP 331 **A Scalable Automated Proteomics Pipeline (ASAP2) for Cerebrospinal Fluid Analysis in Large Clinical Studies**; Antonio Nunez Galindo[1]; Martin Kussmann[1]; Loïc Dayon[1]; *[1]Nestle Institute of Health Sciences, Lausanne, Switzerland*

ThP 332 **High pH Reversed-Phase Sample Fractionation for Phosphoproteomic and Glycoproteomic Workflows**; Sergei I Snovida[1]; Jae Choi[1]; Ryan Bomgarden[1]; Julian A Saba[2]; Rosa I Viner[2]; John C Rogers[1]; *[1]Thermo Fisher Scientific, Rockford, IL; [2]Thermo Fisher Scientific, San Jose, CA*

ThP 333 **Design and Evaluation of Peptide Affinity Capture Formats for Selective Extraction of Antibiotics using Liquid Chromatography – Mass Spectrometry**; Yu-Sheng Sung[1]; Veronica B. Waybright[1]; Dananjaya Kalu Appulage[1]; Abu Afzal Mohammed Shaker[1]; Frank W. Foss[1]; Kevin A Schug[1]; *[1]University of Texas at Arlington, Arlington, TX*

ThP 334 **A Comprehensive Evaluation of the Peptide Characteristics of Fast Digestion Methods in Discovery and Targeted Proteomic Analysis**; Zhengguang Guo[1]; Jie Cheng[1]; Wei Sun[1]; *[1]School of Basic Medicine Chinese Academy of Medical Sciences, Beijing, China*

ThP 335 **Determination of Oleanolic acid and Ursolic Acid in Loquat Leaf Extract by Liquid Chromatography-Tandem Mass Spectrometry**; Dan Luo[1]; Yu-Qi Feng[2]; Youbao Sun[1]; Jinting Yao[1]; Taohong Huang[1]; Yuki Hashi[1]; *[1]Shimadzu, Shanghai, China; [2]Wuhan University, Wuhan, CN*

ThP 336 **Rapid Online Desalting Using a Supermacroporous Reversed Phase Cartridge for Intact Monoclonal Antibody Characterization using Mass Spectrometry**; Shane Bechler[1]; Martin Samonig[2]; Kelly Flook[1]; Remco Swart[2]; *[1]Thermo Fisher Scientific, Sunnyvale, CA; [2]Thermo Fisher Scientific, Germering, Germany*

ThP 337 **LC-MS/MS Method for the Determination of Bile Acid in Serum Sample using Cleanert MAS-MAW**; Warren Chen[1]; Suzi Qin[1]; Wan Wang[1]; *[1]Bonna-Agela Technologies, Tianjin, China*

ThP 338 **Investigation of Protein Recovery from Restricted Access Media (RAM) for Development of a LC-MS Method to Analyze Biological Fluids**; Dananjaya Kalu Appulage[1]; Evelyn H Wang[1]; Kevin A Schug[1]; *[1]University of Texas at Arlington, Arlington, TX*

ThP 339 **A 10-Point Time Course Pharmacokinetic Study Collected from a Single Mouse by use of the Mitra Microsampling Devices**; Derek Wachtel[1]; Jenny Tobin[1]; Bobby Virasingh[2]; Adrian Sheldon[3]; Susan Dearborn[3]; Yibo Guo[2]; Peter Germano[1]; Sanjeev Forsyth[1]; Maria Ribadeneira[1]; *[1]Ironwood Pharmaceuticals, Cambridge, MA; [2]Neoteryx, Torrance, CA; [3]Agilux Laboratories, Worcester, MA*

ThP 340 **MegaFASP- Up-scaled FASP Protocol for High Yield Peptide Digest**; Alon Savidor[1]; Alexandra Gabashvili[1]; Dalia Elinger[1]; Meital Kupervaser Cohen[1]; Yishai Levin[1]; *[1]Weizmann Institute of Science, Rehovot, Israel*

ThP 341 **Overcoming Challenges of Captisol Interference in Reversed-Phase based Analytical Characterization**; Hai Yue[1]; Barrier Teresa[2]; Hong Robert[2]; Izydor Apostol[2]; Xin Zhang[3]; *[1]Amgen Inc., Thousand Oaks, CA; [2]Amgen, Inc., Thousand Oaks, CA; [3]Amgen, Inc. Thousand Oaks, CA*

ThP 342 **Efficient Extraction of Residual Pesticides in Agricultural Products and Soils for GC/MS and LC/MS Analysis using Supercritical Fluid Extraction**; Takanari Hattori[1]; Sakai Takero[1]; Hayakawa Yoshihiro[1]; *[1]Shimadzu Corporation, Kyoto, Japan*

ThP 343 **Automation Utility for Method Validation of Nicotine and Metabolites in Urine by HPLC-MS/MS**; Dan Menasco[1]; Matthew Feldhammer[2]; James Ritchie[2]; Willa Zhang[2]; *[1]Biotage, Charlotte, NC; [2]Emory University School of Medicine, Atlanta, GA*

ThP 344 **Advantages of Rapid Automated On-Column Trypsin Digestion on Proteomics Data Quality**; Raghothama Chaerkady[1]; Wen Yu[1]; Kristen Lekstrom[1]; Deniz BaycinHizal[1]; Michael Bowen[1]; *[1]Medimmune, Gaithersburg, MD*

ThP 345 **Optimized Protocol for In-Depth Analysis of Cell Culture Secretomes**; Elke Hammer[1]; Daniela Suhr[2]; Beatrice Engelmann[2]; Eric Witt[2]; Vishnu Mukund Dhople[2]; Uwe Völker[2]; *[1]University Medicine Greifswald, Greifswald,*

Mecklenburg-Vorpommern; [2]University Medicine Greifswald, Greifswald, Germany

LIPIDS: QUANTITATIVE ANALYSIS
346 - 375

ThP 346 **Measuring Biochemical Effects of Pulmonary Rehabilitation and OMT on COPD Patients through LC-MS-MS Analysis of Plasma Metabolites**; Chen Zhang[1]; Sherman Gorbis[1]; John Wang[1]; A. Daniel Jones[1]; *[1]Michigan State University, East Lansing, MI*

ThP 347 **Identification and Comprehensive Structural Characterization of Serum Lipid Biomarkers to Type 1 Diabetes**; Ngoc Vu[1]; Monica Narvaez- Rivas[2]; Qibin Zhang[1, 2]; *[1]Department of Chemistry and Biochemistry, University of North Carolina at Greensboro, Greensboro, NC; [2]Center for Translational Biomedical Research, University of North Carolina at Greensboro, Kannapolis, NC*

ThP 348 **Comprehensive Lipidomics Approach for Platelet Analysis**; Bing Peng[1]; Patrick Münzer[2]; Cristina Coman[1]; Oliver Borst[2]; Robert Ahrends[1]; *[1]Leibniz-Institut für Analyt. Wissensch. - ISAS -, Dortmund, Germany; [2]Medizinische Klinik III, Kardiologie und Kreislauferkrankungen, Universitätsklinikum Tübingen, Tübingen, Germany*

ThP 349 **Shotgun Lipidomics Analysis of Fatty Acid Esters of Hydroxy Fatty Acids Species in Biological Samples**; Miao Wang[1]; Xianlin Han[1]; *[1]Sanford Burnham Prebys Medical Discovery Institute, Orlando, FL*

ThP 350 **Liquid Chromatography Tandem Mass Spectrometric Analysis of Oxidized Products of Polyunsaturated Fatty Acids and Bioactive Eicosanoids in Biological Samples**; Jaeman Byun[1]; Lixia Zeng[1]; Subramaniam Pennathur[1]; *[1]University of Michigan, Ann Arbor, MI*

ThP 351 **Research into Lysosomal Storage Metabolism using Plasma Lipid Characterization by LC-MS/MS**; Sibylle Heidelberger[1]; Daniel Blake[1]; Rachel Webster[2]; Karen Smith[2]; Martin Roch[2]; *[1]SCIEX, Phoenix House Lakeside Drive Warrington Cheshire UK; [2]Queen Elizabeth Hospital Birmingham, Birmingham, UK*

ThP 352 **Robust Automated Lipid Extraction from Human Plasma**; Dain Brademan; *, Madison, WI*

ThP 353 **Differential Complex Lipid Plasma Profiles Reveal Perturbations in Preeclampsia**; Baljit Ubhi[1]; Katherine Williams[2]; Susan Fischer[2]; *[1]AB SCIEX, Redwood City, CA; [2]UCSF, San Francisco, CA*

ThP 354 **Comprehensive Analysis of Polyphosphoinositide Molecular Species by Shotgun Lipidomics**; Chunyan Wang[1]; Juan Pablo Palavicini[1]; Xianlin Han[1]; *[1]Sanford Burnham Prebys Medical Discovery Institute, Orlando, FL*

ThP 355 **LC-ESI-MS/MS Analysis of Oxygenated Lipid Droplets in Dendritic Cells Treated with Tumor Explant Supernatants**; Vladimir Tyurin[1]; Filippo Veglia[2]; Andrew Amoscato[1]; Roberto Angelini[1]; Maureen Murphy[2]; Alexandr Kapralov[1]; Dariush Mohammadyani[1]; Dmitry I. Gabrilovich[2]; Valerian E, Kagan[1]; *[1]University of Pittsburgh, Pittsburgh, PA; [2]The Wistar Institute, Philadelphia, PA*

ThP 356 **Identification and Quantification of Oxygenated arachidonoyl- and adrenoyl-phosphatidylethanolamines as Ferroptotic Death Signals using Oxidative Phospholipidomics**; Yulia Tyurina[1]; Andrew Amoscato[1]; Vladimir Tyurin[1]; Feng Qu[1]; Gaowei Mao[1]; Hulia Bayir[1]; Valerian Kagan[1]; *[1]University of Pittsburgh, Pittsburgh, PA*

ThP 357 **Analysis of Trans-Fatty Acids in Human Plasma using Isotope Dilution-Gas Chromatography-Negative Chemical Ionization-Mass Spectrometry** ; Heather Kuiper[1]; Na Wei[1]; Samantha L McGunigale[1]; Lin Zhang[1]; Hubert W Vesper[1]; *[1]CDC, Atlanta, GA*

ThP 358 **Photochemical Tagging for Rapid Quantitation of Unsaturated Fatty Acids by Mass Spectrometry**; Xiaoxiao Ma[1]; Xu Zhao[1]; Junjie Li[1]; Ji-Xin Cheng[1]; Zheng Ouyang[1]; Yu Xia[1]; *[1]Purdue University, West Lafayette, IN*

ThP 359 **Identification of Pseudomonas aeruginosa Phospholipids Involved in Surface Attachment**; Sébastien Vilain[1]; Caroline Le Senechal[1]; Marc Crouzet[1]; Marc Bonneu[1]; Jean-Marie Schmitter[1]; Corinne Bure[1]; *[1]CNRS/CBMN, Bordeaux, France*

ThP 360 **LC-MRM for Quantitative Analysis of Endotoxins**; Jianjun Li[1]; Jacek Stupak[1]; Kenneth Chan[1]; *[1]National Research Council Canada, Ottawa, Canada*

ThP 361 **Development of a Wide-Targeted Quantitative Lipidomics Methodology by Supercritical Fluid Chromatography Coupled with Fast-Scanning Triple Quadrupole Mass Spectrometry**; Hiroaki Takeda[1]; Yoshihiro Izumi[1]; Thanai Paxton[2]; Noriko Kato[2]; Shinnosuke Horie[2]; Katsutoshi Nagase[2]; Takeshi Bamba[1]; *[1]Medical Institute of Bioregulation, Kyushu Univ. Fukuoka, Japan; [2]Nihon Waters K.K., Tokyo, Japan*

ThP 362 **An Ultrasensitive Assay for Quantification of a Cationic Lipid 1,2-Dioleoyl-3-trimethylammonium Propane in Mouse Plasma by HPLC-MS/MS**; Aihua Liu[1]; Bryce Ashby[2]; Uri Hong[2]; Sherry Liu[2]; Scott Reuschel[2]; Min Meng[2]; *[1]Covance, Salt Lake City, UT; [2]Covance, Salt Lake City, UT*

ThP 363 **Quantitative LC-MS/MS Method Development and Preliminary Analysis of Plasma Endocannabinoid Concentrations in Humans**; Karolina M. Krasinska[1]; Debra S. Karhson[2]; Karen J. Parker[2]; Allis S. Chien[1]; *[1]Stanford University Mass Spectrometry, Stanford, CA; [2]Department of Psychiatry and Behavioral Sciences, Stanford University, School of Medicine, Stanford, CA*

ThP 364 **Resolution of Unexpected Reference Standard Components of (5R,S)-isoprostane F2α Type VI (iPF2α-VI) using a Shallow UHPLC-MS/MS Gradient**; Alan Dzerk[1]; Miller S Patrick[2]; Kirk E Newland[2]; Chris J Kafonek[2]; *[1]Celerion, Inc, Lincoln, NE; [2]Celerion, Inc., Lincoln, NE*

ThP 365 **High-Throughput Approach to Separating and Quantitatively Measuring Hydroxycholesterols in Biological Matrices**; Laura Dubois[1]; Will J Thompson[1]; Eric Benner[1]; Kimberly Cocce[1]; Wen Liu[1]; Donald P McDonnell[1]; Arthur Moseley[1]; *[1]Duke University School of Medicine, Durham, NC*

ThP 366 **Simultaneous Measurement of 25-Hydroxyvitamin-D2, 25-Hydroxyvitamin-D3 and 27-Hydroxycholesterol Levels in Human Serum by LC-MS/MS**; Ludmila Alexandrova[1]; Ken Lau[2]; Allis C Chien[1]; David Feldman[3]; Sharon J Pitteri[2]; *[1]Stanford University Mass Spectrometry, Stanford, CA; [2]Department of Radiology, Canary Center at Stanford for Cancer Early Detection, Stanford, CA; [3]Department of Medicine, Stanford University, Stanford, CA*

ThP 367 **Untargeted Lipidomics with Stable Isotope Labeling (H218O) used to Study Abnormal Development in Vitamin E Deficient Zebrafish Embryos**; Melissa Q McDougall[1, 2]; Jaewoo Choi[3]; Jan. F Stevens[1, 4, 5]; Lisa Truong[5, 6, 7]; Robert L Tanguay[5, 6, 7]; Maret G. Traber[1, 2, 5]; *[1]Linus Pauling Institute, Oregon State University Corvallis, OR; [2]College of Public Health and Human Sciences, Oregon State University, Corvallis, OR; [3]Oregon State University, Corvallis, OR; [4]College of Pharmacy, Oregon State University, Corvallis, OR; [5]Environmental Health Sciences Center, Oregon State University, Corvallis, OR; [6]Sinnhuber Aquatic Research Laboratory, Oregon State University, Corvallis, OR; [7]Environmental and Molecular Toxicology, Oregon State.edu, Corvallis, OR*

ThP 368 **Methylation and Stable Isotopic Labeling-based Novel Method for Quantitative Phospholipidomics**; Tanxi Cai[1]; Shu Qingbo[1]; Liu Peibin[1]; Niu Lili[1]; Guo Xiaojing[1]; Ding Xiang[1]; Xue Peng[1]; Xie Zhensheng[1]; Wang Jifeng[1]; Zhu Nali[1]; Wu Peng[1]; Niu Lili[1]; Yang Fuquan[1]; *[1]Institute of Biophysics, CAS beijing, China*

ThP 369 **Differentially Expressed Nonpolar Lipids in Meibum of Dry Eye: Post-menopausal Women vs Contact Lens-Wearers**; Jianzhong Chen[1]; Kari B Green[2]; Kelly K Nichols[1];

[1]University of Alabama at Birmingham, Birmingham, AL; [2]University of Florida, Gainesville, FL

ThP 370 **Software: Nexus Point of a Targeted Lipid Analyzer**; Pauline J. Vollmerhaus[1]; Baljit K. Ubhi[2]; Sarada Tanikella[3]; Peter Zhu[3]; Corey D. DeHaven[3]; *[1]SCIEX, Concord ON, Canada; [2]SCIEX, Redwood City, CA; [3]Metabolon, Durham, NC*

ThP 371 **Localization and Identification of Biomarkers during Cell Differentiation**; Kendra Adams[1]; Cesar E. Ramirez[1]; Richard H. Gomer[2]; Francisco Fernandez-Lima[1]; Daniel DeBord[1]; *[1]Florida International University, Miami, FL; [2]Texas A&M, College Station, TX*

ThP 372 **Method Development and Validation for the Quantification of D-erythro-Sphingosine-1-phosphate (S1P) in Human Plasma Using LC-MS/MS**; Guodong Gu[1]; Michelle Black[1]; Meng Fang[1]; Deping Cheng[1]; Yinghe Li[1]; Yifan Shi[1]; Maines Lynn[2]; *[1]Alliance Pharma, Inc Malvern, PA; [2]Apogee Biotechnology Corporation, Hummelstown, PA*

ThP 373 **Targeted Sphingolipidomics Using a Novel Single Solvent Extraction and Analysis Platform**; Weilien Chuang[1]; Joshua Pacheco[1]; Samantha Cooper[1]; Jim Dodge[1]; Kate Zhang[1]; *[1]Genzyme, Framingham, MA*

ThP 374 **SIMPLEX: A Combinatorial Multimolecular Omics Approach for Systems Biology**; Cristina Coman[1]; Fiorela Solari[1]; Andreas Hentschel[1]; Albert Sickmann[1]; Rene P Zahedi[1]; Robert Ahrends[1]; *[1]ISAS, Dortmund, Germany*

ThP 375 **Development of a Quantification Method for Monitoring Endogenous Epoxyeicosatrienoic Acids using a Triple Quadrupole Mass Spectrometer**; Masaki Yamada[1, 2]; Hiraki Sakuta[3]; Yoshihiro Kita[4]; Suzumi M. Tokuoka[1]; Takao Shimizu[1]; Masaharu Noda[3]; *[1]The University of Tokyo, Tokyo, Tokyo; [2]Shimadzu Corporation, Kyoto, Japan; [3]National Institute for Basic Biology, Okazaki, Japan; [4]The University of Tokyo, Tokyo, Japan*

MALDI: SAMPLE PREPARATION
376 - 401

ThP 376 **Enabling HT Automated Sample Preparation Workflows with Application to MS Protein Analysis**; Stoyan Stoychev[1]; Busisiwe Twala[2]; Previn Naicker[3]; Justin Jordaan[4]; *[1]CSIR Biosciences, Pretoria, Gauteng; [2]CSIR, Pretoria, SA; [3]CSIR, Pretoria, ZA; [4]Rhodes University, Grahamstown, ZA*

ThP 377 **Analysis of Protein Profile by MALDI-TOFMS using Lyophilized Microalgae Samples Resuspended in Different TFA Content**; Lidiane Andrade[1]; Maria Anita Mendes[1]; Claudio Augusto Oller do Nascimento[1]; *[1]University of São Paulo, São Paulo, SP*

ThP 378 **A New Embedding Method For Mouse Brain Tissue In Preparation For Matrix Assisted Laser Desorption Ionization Mass Spectrometry Imaging (MALDI-MSI)**; Emily L Gill[1]; Richard A Yost[1]; Timothy J Garrett[1]; Vinata Vedam-Mai[1]; *[1]University of Florida, Gainesville, FL*

ThP 379 **Improving Ion Abundances of Oligosaccharides by Decreasing Substrate Temperature During Droplet-Drying Processes in MALDI Mass Spectrometry**; Yu-Meng Ou[1, 2]; Yin-Hung Lai[1]; Hsun Lee[1]; Chien-Wei Tsao[1]; Yi-Sheng Wang[1]; *[1]Academia Sinica, Genomics Research Center Taipei, Taiwan; [2]National Taiwan University, Taipei, Taiwan*

ThP 380 **Structure-Property Relationship and Strategic Synthesis of MALDI Matrix for Low-Molecular-Weight Metabolites Analysis**; Daisuke Miura[1]; Takanori Ishii[2]; Yoshinori Fujimura[2]; Daichi Yukihira[2]; Eisuke Hayakawa[2]; Hiroyuki Wariishi[2]; Mitsuru Shindo[2]; *[1]Kyushu University, Fukuoka, Kyushu; [2]Kyushu University, Fukuoka, Japan*

ThP 381 **A Rapid MALDI-MS Method for the Characterization of Cardiovascular Drugs and Related Impurities**; Wenjing Ning[1]; Jinlan Dong[1]; Jamie D. Dunn[1]; *[1]US Food and Drug Administration, Center for Drug Evaluation and Research (CDER), Division of Pharmaceutical Analysis (DPA), St. Louis, MO*

ThP 382 **Gold Nanoparticles Bridging Infra-Red Spectroscopy and Laser Desorption/Ionization Mass Spectrometry for Rapid Pharmaceutical Products Screening**; Siu-Leung Chau[1]; Ho-Wai Tang[1]; Kwan-Ming Ng[1]; *[1]University of Hong Kong, Hong Kong*

ThP 383 **A Trial of TLC-MALDI for Analysis of Industrial Materials**; Toshiji Kudo[1]; Yoshihiko Morishita[1]; Noriyuki Iwasaki[1]; Takashi Nirasawa[1]; *[1]Bruker Daltonics K.K., Yokohama, Japan*

ThP 384 **Fluorene Derivatives as MALDI Matrices for Electron Transfer Ionization**; Juan Ramirez-Pradilla[1]; Laura Maria Cristancho-González[2]; Cristian Blanco-Tirado[2]; Marianny Y Combariza[2]; *[1]Universidad Industrial de Santander, Floridablanca, Santander; [2]Universidad Industrial de Santander, Bucaramanga, Santander, Colombia*

ThP 385 **Tryptamine as a Derivatization Matrix for Analysis of Carbonyl Compounds by MALDI Mass Spectrometry**; Roman Borisov[1]; Mariya S. Slyundina[2]; Nikolai Yu. Polovkov[2]; Vladimir G Zaikin[2]; *[1]Topchiev Institute of Petrochemical synthesis, Moscow; [2]Topchiev Institute of Petrochemical Synthesis, Moscow, Russia*

ThP 386 **Electrowetting-controlled Sample Preparation Method for MALDI Mass Spectrometry**; Olena Kudina[1]; Eral Burak[2]; Frieder Mugele[1]; *[1]University of Twente, Enschede, Netherlands; [2]eMALDI BV, Enschede, The Netherlands*

ThP 387 **Re-evaluation and Optimisation of Common MALDI Mass Spectrometry Experimental Parameters for a Range of MALDI Matrix Compounds and Analyte Classes**; Kenneth Neil Robinson[1, 2]; Rory T Steven[1]; Josephine Bunch[1, 2]; *[1]National Physical Laboratory, Teddington, UK; [2]University of Nottingham, Nottingham, UK*

ThP 388 **Investigating the Effect of Electrospray Deposition Parameters on the Morphology of Samples and its Implications to MALDI MS Signal Intensity**; Christina Emeigh[1]; Kevin Owens[1]; *[1]Drexel University, Philadelphia, PA*

ThP 389 **Optimized Multiply Charged Ion Production by Liquid MALDI – From High Molecular Protein Ions to Bottom-Up Proteomics using LC-MALDI MS/MS**; Pavel Ryumin[1]; Jeffrey Brown[1, 2]; Michael Morris[2]; Rainer Cramer[1]; *[1]University of Reading, Reading, UK; [2]Waters Corporation, Wilmslow, UK*

ThP 390 **e-MALDI: An Electrowetting-Based Sample Preparation Method for MALDI Mass Spectrometry**; Frieder Mugele[1]; Burak Eral[2]; Olena Kudina[1]; *[1]University of Twente, Enschede, Netherlands; [2]TU Delft, Delft, NL*

ThP 391 **Black Phosphorus-Assisted Laser Desorption Ionization Mass Spectrometry Combined with Stable Isotope Labeling for Quantification of Small Molecules**; He Xiao-Mei[1]; Jun Ding[1]; Yu Lei[1]; Hussain Dilshad[1]; Feng Yu-Qi[1]; *[1]Wuhan University, Wuhan, CN*

ThP 392 **Investigating Complexes from Native-Like Environments: New Developments from LILBID-MS**; Nina Morgner[1]; Tobias Lieblein[2]; Oliver Peetz[2]; Jan Hoffmann[2]; Nils Hellwig[2]; *[1]Goethe University Frankfurt, Frankfurt, Germany; [2]Goethe University, Frankfurt, Germany*

ThP 393 **Using Single Cell MALDI-MS to Guide Follow-Up CE-MS Assays**; Troy Comi[1]; Monika A Makurath[2]; Elizabeth K Neumann[2]; Stanislav S Rubakhin[2]; Jonathan V Sweedler[2]; *[1]University of Illinois at Urbana-Champaign, Urbana, IL; [2]University of Illinois at Urbana-Champaign, Urbana-Champaign, IL*

ThP 394 **A Comparison of Performance Characteristics of Atmospheric Pressure and Low-Pressure Matrix Assisted Laser Desorption Ionization Sources**; Vladimir M Doroshenko[1]; Victor Laiko[1]; Eugene Moskovets[1]; *[1]MassTech, Inc Columbia, MD*

ThP 395 **Matrix-Coated Surface Assisting Ionization, a Sensitive and Efficient Ionization Method for Mass Spectrometry**; Che-I Liao[1]; Kuo-Lung Ku[2]; *[1]Department of Applied Chemistry,National Chiayi University, Chiayi City, Taiwan; [2]National Chiayi University, Chiayi City, Chiayi*

ThP 396 **Performance and Bioanalytical Applicability of MALDI-compatible Protein Chips Prepared by Ambient Ion Soft Landing**; Petr Pompach[1, 2]; Oldřich Benada[1]; Jiří Hausner[1, 2]; Viktor Růžička[3]; Michael Volný[4]; Petr Novák[1]; *[1]Institute of Microbiology, Prague, Czech Republic; [2]Faculty of Science, Charles University in Prague, Prague, Czech Republic; [3]Biovendor, a.s., Brno, Czech Republic; [4]AffiPro, s.r.o., Mratin, Czech Republic*

ThP 397 **Nanopost and Elevated Bowtie Antenna Arrays for Laser Desorption Ionization and Fragmentation of Biomolecules**; Xavier Holmes[1]; Sylwia Stopka[1]; Andrew Korte[1]; Scott Retterer[2]; Akos Vertes[1]; *[1]George Washington University, Washington DC; [2]Oak Ridge National Laboratory, CNMS Oak Ridge, TN*

ThP 398 **Matrix-free Laser-Induced Acoustic Desorption for Large Biomolecule Detection using Charge Monitoring Mass Spectrometer**; Yung-Kun Chuang[1]; Jung-Lee Lin[2]; Szu-Hsueh Lai[2]; Chung-Hsuan Chen[2]; *[1]Academia Sinica, Taipei, Taiwan; [2]Academia Sinica, Genomics Research Center Taipei, Taiwan*

ThP 399 **Development of a Reduced Pressure Infrared Laser Ionization Source as a Novel Interface for Online LC/MS**; Yasunari Iguchi[1]; Hisanao Hazama[1]; Kunio Awazu[1]; *[1]Graduate School of Engineering, Osaka University, Suita, Osaka, Japan*

ThP 400 **New User Friendly and High Sensitivity Approaches to Matrix-Assisted Ionization Directly from Vacuum**; Milan Pophristic[1]; I-Chung Lu[2]; Khoa Hoang[1]; Casey Foley[2]; Sarah Trimpin[2]; Charles N. Mcewen[3]; *[1]University of the Sciences, Philadelphia, PA; [2]Wayne State University, Detroit, MI; [3]Univ. of the Sciences, Philadelphia, PA*

ThP 401 **High Sensitivity MS Analyses by Eliminating the 'Ion Source': Vacuum-Assisted Ionization**; Charles N. McEwen; *Univ. of the Sciences, Philadelphia, PA*

METABOLOMICS: IDENTIFICATION OF UNKNOWN METABOLITES
402 - 425

ThP 402 **The Application of Untargeted Data Acquisition for Identifying Metabolites of 'Designer Drug' 25I-NBOMe in Clinical Samples**; Michael Dunn[1]; Margaret Knight[1]; Clair Roper[1]; Simon Thomas[1]; Peter Blain[1]; *[1]Medical Toxicology Centre, Newcastle University, Newcastle upon Tyne, UK*

ThP 403 **Metabolic Profiling of Type 1 Diabetes From Primary and Established T Cells Using Isotopic Ratio Outlier Analysis by LC-MS**; Candice Ulmer[1]; Elizabeth Urankar Ransom[1]; Christopher Beecher[2]; Timothy Garrett[1]; Jing Chen[1]; Clayton Matthews[1]; Richard A Yost[1]; *[1]University of Florida, Gainesville, Florida; [2]IROA Technologies, Ann Arbor, MI*

ThP 404 **A Critical Comparison of Collision Induced Dissociation and Surface Induced Dissociation for Metabolomics**; Rachel Harris[1]; Ewa Jurneczko[1]; Sophie Harvey[2]; Vicki H Wysocki[2]; John A McLean[1]; *[1]Vanderbilt University, Nashville, TN; [2]The Ohio State University, Columbus, OH*

ThP 405 **The Use of High Resolution Mass Spec and Automated Fraction Collection for High Throughput Metabolite Identification**; Jason Lamar; *PTRL West (a division of EAG, Inc.), Hercules, CA*

ThP 406 **Creation of Libraries of Recurring Mass Spectra: Triple Column Workflow for Improved Characterisation and Mapping of Unknowns across Multiple Samples**; John M. Halket[1]; Anna Caldwell[1]; Gary Mallard[2]; Yuri Mirokhin[2]; Stephen Stein[2]; *[1]King's College London, London, UK; [2]National Institute of Standards and Technology, Gaithersburg, MD*

ThP 407 **Automation in the Creation of Recurrent Unidentified Spectra (RUS) Libraries**; N. Rabe Andriamaharavo[1]; W. Gary Mallard[1]; Yuri A. Mirokhin[1]; Stephen E. Stein[1]; *[1]National Institute of Standards and Technology, Gaithersburg, MD*

ThP 408 **iTreeLib: Development of the MS^n Mass Spectral Tree Library of Plant Natural Products**; Arpana Vaniya[1]; Sajjan Singh Mehta[2]; Oliver Fiehn[2]; *[1]UC Davis, Davis, CA; [2]University of California Davis, West Coast Metabolomics Center, Genome Center, Davis, CA*

ThP 409 **Enabling High-Confidence Human Endogenous Metabolite Identification via High-Resolution MS/MS Retention-Time Library**; Nan Wang[1]; Xian Luo[1]; Shuang Zhao[1]; Yiman Wu[1]; Zhendong Li[1]; Wei Han[1]; Jaspaul Tatlay[1]; Yunong Li[1]; Kevin Hooton[1]; Dorothea Mung[1]; Adriana Zardini Buzatto[1]; Xiaohang Wang[1]; Aiko Barsch[2]; Ulrike Schweiger-Hufnagel[2]; Liang Li[1]; *[1]Department of Chemistry, University of Alberta, Edmonton, Canada; [2]Bruker Daltonic GmbH, Bremen, Germany*

ThP 410 **Identification of a Branched Amino Acid Metabolite Driving Fatty Acid Transport and Insulin Resistance**; Sungwhan F Oh[1]; Cholsoon Jang[2, 3]; Zoltan Arany[2]; Dennis L Kasper[1]; *[1]Harvard Medical School, Boston, MA; [2]University of Pennsylvania, Philadelphia, PA; [3]Beth Israel Deaconess Medical Center, Boston, MA*

ThP 411 **Bioactive Compounds from Bees: Identification of Characteristic Metabolites in Propolis Extracts via UHPLC-MS and –MS/MS Based Metabolite Profiling**; Sven Meyer[1]; Oliver Raether[1]; *[1]Bruker Daltonics Ltd, Bremen, Germany*

ThP 412 **Identification of Metabolites Using Isotopic Fine Structure with UPLC-FTMS**; Jeremy Wolff[1]; Christopher J Thompson[2]; *[1]Bruker Daltonics, Billerica, MA; [2]Bruker Daltonic, Billerica, MA*

ThP 413 **Carbonic Anhydrase Inhibitory Potential of Lagenaria siceraria Stand and Identification of Its Bioactive Compounds - An LC-MS/MS Approach**; Joydeb Chanda[1]; Pulok K Mukherjee[1]; Rajarshi Biswas[1]; Dipankar Malakar[2]; Manoj Pillai[2]; *[1]School of Natural Product Studies, Department of Pharmaceutical Technology, Jadavpur University, Kolkata, India; [2]SCIEX, 121 Udyog Vihar Phase IV Gurgaon, India*

ThP 414 **Annotation of Novel Metabolites in a Pregnancy Study using Accurate Mass GC/QTOF MS and Validated Fragmentation Rules**; Zijuan Lai[1]; Oliver Fiehn[1]; *[1]UC Davis, Davis, CA - California*

ThP 415 **Identifying Pregnancy Biomarkers of Dairy Cows using MALDI-MS**; Tatiane Melina Guerreiro[1]; Mônica Ferreira[1]; Rodrigo Ramos Catharino[1]; *[1]Innovare Biomarkers Laboratory - UNICAMP, Campinas, SP*

ThP 416 **Blood Serum Metabolomics Using Comprehensive Two-Dimensional Gas Chromatography High Resolution Time-of-Flight Mass Spectrometry**; David Alonso[1]; Joe Binkley[2]; Lorne Fell[2]; Christina Kelly[2]; *[1]LECO Corporation, St. Joseph, MI; [2]LECO Corporation, Saint Joseph, MI*

ThP 417 **Comprehensive Profiling of Bile Acids in Human and Mouse Using UPLC-MS/MS-based Metabolomics**; Jun Han[1]; Georgia Mitsa[1]; David Hamelin[1]; Karen Lin[1]; Christoph H. Borchers[1, 2]; *[1]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [2]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada*

ThP 418 **Elucidating Novel Cholesterol Metabolites in Mycobacterium tuberculosis using Mass Spectrometry**; Israel Casabon[1]; Adam Crowe[1]; Kirsten Brown[1]; Jie Liu[1]; jason rogalski[1]; Leonard Foster[1]; Lindsay Eltis[1]; *[1]The University of British Columbia, Vancouver, BC*

ThP 419 **Metabolic Profiling: Linking the IROA Metabolite Library to a Suite of Data Processing Software**; Jeffrey T. Morre[1]; Claudia S Maier[1]; Michael A Stevenson[1]; Jan F Stevens[2]; *[1]Oregon State University, Department of Chemistry Corvallis, OR; [2]Oregon State University, Dept. of Pharmacy, Corvallis, OR*

ThP 420 **The Rise of Ion Mobility in Untargeted Metabolomics - Raising the Isobar in Annotation**; Nicholas Rattray[1]; Cunyu Yan[1]; Perdita Barran[1]; *[1]University of Manchester, Manchester, UK*

ThP 421 **A Software Tool to Automatically Evaluate Scan-by-Scan Spectral Accuracy of Ultra High Resolution LC/MS Data for Unique Elemental Composition Determination**; Yongdong Wang[1]; Ming Gu[1]; Jeff S. Andrews[1]; *[1]Cerno Bioscience, Norwalk, CT*

ThP 422 **Compound Annotation Including Sulfate and Glucuronide Conjugates for Non-Target Analysis**; Tairo Ogura[1]; Takeshi Bamba[2]; Akihiro Tai[3]; Eiichiro Fukusaki[4]; *[1]Shimadzu Scientific Instruments, Columbia, MD; [2]Kyushu University, Fukuoka, Japan; [3]Prefectural University of Hiroshima, Hiroshima, Japan; [4]Osaka University, Osaka, Japan*

ThP 423 **Uncovering Cryptic Secondary Metabolites from Aspergillus nidulans with HDAC Inhibition.**; Matthew Henke[1]; Alexandra A Soukup[2]; Ryan A McClure[1]; Anthony Goering[1]; Regan J Thomson[1]; Nancy P Keller[2]; Neil L Kelleher[1]; *[1]Northwestern University, Evanston, IL; [2]University of Wisconsin Madison, Madison, WI*

ThP 424 **Bar Coding Tandem Mass Spectra for Metabolomic Identifications**; Jonathan Spalding[1]; Kevin Cho[1]; Nathaniel G Mahieu[1]; Stephen L Johnson[2]; Gary J Patti[1, 2]; *[1]Washington University in St. Louis, St. Louis, MO; [2]Washington University School of Medicine, Saint Louis, MO*

ThP 425 **Urinary Exposure Marker Discovery for Toxicants using UPLC-LTQ-Orbitrap and Three Untargeted Metabolomics Approaches**; Jen-Yi Hsu[1]; Jing-Fang Hsu[1]; Yi-Sheng Hsu[1]; Tsai Shu-Han[1]; Pao-Chi Liao[1]; *[1]Department of Environmental and Occupational Health College of Medicine, National Cheng Kung University, Tainan, Taiwan*

METABOLOMICS: QUANTITATIVE ANALYSIS
426 - 446

ThP 426 **Methods for Enhancing Sensitivity and Throughput in LC-MS Analysis of BTEX Metabolites in Biological Fluid**; Yehia Z. Baghdady[1]; C. Phillip Shelor[1]; Purnendu K. Dasgupta[1]; Kevin A. Schug[1]; *[1]Department of Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, TX*

ThP 427 **Development and Evaluation of a Rapid LC-MS/MS Method for Accurate Quantitation of Malondialdehyde in Human and Mouse Plasma**; Constance Sobsey[1]; Jun Han[1]; Karen Lin[1]; Walter Swardfager[2]; Anthony Levitt[3]; Christoph H. Borchers[1, 4]; *[1]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [2]Sunnybrook Health Sciences Centre, Pharmacology and Toxicology Department, Toronto, ON, Canada; [3]Sunnybrook Health Sciences Centre, Department of Psychiatry, Toronto, ON, Canada; [4]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada*

ThP 428 **Development of a New UPLC/MRM-MS Method for Quantitation of Bile Acids in Dried Blood Spots**; Jun Han[1]; Georgia Mitsa[1]; David Hamlin[1]; Karen Lin[1]; Juncong Yang[1]; Christoph H. Borchers[2, 3]; *[1]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [2]University of Victoria - Genome BC Proteomics Centre, Victoria, BC; [3]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada*

ThP 429 **Quantification of Metabolites in Plasma and Blood using a Dual Column-Switching Dual Liquid Chromatography with Tandem Mass Spectrometry Detection**; Kyoko Watanabe[1, 2]; Yoshihiro Hayakawa[2]; Masami Tomita[2]; Gérard Hopfgartner[1]; *[1]Life Sciences Mass Spectrometry, University of Geneva, Geneva, Switzerland; [2]Shimadzu Corporation, Kyoto, Japan*

ThP 430 **Rapid Porphyrin Quantification and Porphyria Differentiation in Urine by LC-MS/MS**; Brian C Netzel[1]; Kimiyo Raymond[1]; Silvia Tortorelli[1]; *[1]Mayo Clinic / DLMP, Rochester, MN*

ThP 431 **Detecting and Quantifying Gastrointestinal Neurotransmitters and Their Metabolites in Mice Feces**; Nitesh Sule[1]; Arul Jayaraman[1]; Lawrence J Dangott[1]; *[1]Texas A&M University, College Station, TX*

ThP 432 **Simultaneous Quantitation of 2-Hydroxy-4-Methoxybenzophenone, a Sunscreen Ingredient, and Its Metabolites in Harlan Sprague Dawley Rat Plasma by LC-MS/MS**; Esra Mutlu[1]; Jessica Pierfelice[2]; Barry S McIntyre[1]; Brian Burback[2]; Suramya Waidyanatha[1]; *[1]Division of the National Toxicology Program, National Institute of Environmental Health Sciences, Research Triangle Park, NC; [2]Battelle Memorial Institute, Columbus, OH*

ThP 433 **Analysis of Polycyclic Aromatic Hydrocarbons using LC/MS/MS: Identification of Carcinogenic Polycyclic Aromatic Hydrocarbons in Bladder Cancer**; Preeti Purwaha[1]; Salil Kumar Bhowmik[1]; Rashmi Krishnapuram[1]; Franklin Gu[1]; Feng Jin[1]; Vadiraja B Bhat[2]; *[1]Baylor College of Medicine, Houston, TX; [2]Agilent Technologies, Wilmington, DE*

ThP 434 **Removing Metabolomics Data Variation from LC-High Resolution Mass Spectrometry with Smart Selection of Internal Standards**; Xiaojing Liu[1]; Jason Locasale[1]; *[1]Duke University, Durham, NC*

ThP 435 **Targeted Metabolomics Analysis on Aromatic Amino Acid on Yeast Strains Treated with Glyphosate**; Gul M Mustafa[1]; Gregory Boyce[1]; Mark A Szewc[1]; *[1]Protea Biosciences, Inc. Morgantown, WV*

ThP 436 **Comparison of Metabolite Quantitation by a Triple Quadrupole vs. an Orbitrap-class Mass Spectrometer**; Thomas D. Horvath[1]; Lin Tan[1]; Michael A Pontikos[1]; Di Du[1]; Yulun Chiu[1]; John N Weinstein[1]; David H Hawke[1]; Phil Lorenzi[1]; *[1]The University of Texas MD Anderson Cancer Center, Houston, TX*

ThP 437 **Metabolomics Analysis of Malonic Acid, Methylmalonic Acid and Ethylmalonic Acid in Urine of Mice with malonyl-CoA Decarboxylase Deficiency**; Chandra Shekar R Ambati[1]; Furong Yuan[1]; Lutfi A Abu-Elheiga[1]; Vivekananda Shetty[1]; *[1]Baylor College of Medicine, Houston, TX*

ThP 438 **A HILIC Method for the Absolute Quantitation of Polar Metabolites in Embryo Growth Media**; Sarah Marie Lyons[1]; Rebecca L. Krisher[2]; Jason Herrick[2]; Jay S. Kirkwood[1]; Corey D Broeckling[1]; Jessica Prenni[1]; *[1]Colorado State University, Fort Collins, CO; [2]Colorado Center for Reproductive Medicine, Lone Tree, CO*

ThP 439 **LC-MRMHR QTOF MS Based Measurement of Metabolite Exchange between Pancreatic Cancer Associated Fibroblasts and Cancer Cells**; Li Zhang[1]; Christopher Halbrook[2]; Daniel Kremer[2]; Shaokun Pang[3]; Jeff Miller[4]; Maureen Kachman[1]; Charles Burant[1]; Costas Lyssiotis[2]; *[1]Michigan Regional Comprehensive Metabolomics Resource Center; University of Michigan, Ann Arbor, MI; [2]Department of Molecular and Integrative Physiology, Internal Medicine, Medical of School, University of Michigan, Ann Arbor, MI; [3]SCIEX, Redwood City, CA; [4]SCIEX, Concord ON, Canada*

ThP 440 **Quantitation of Nucleotides and Nucleosides without Derivatization Using Transient Isotachophoresis-Capillary Electrophoresis Coupled to Tandem Mass Spectrometry**; Jose Luis Gallegos Perez; *SCIEX, Framingham, MA*

ThP 441 **Profiling of Polar Organic Acids in Mouse Muscle Using Ion Chromatography/Mass Spectrometry**; Chris Petucci[1,2]; Andrew Zelenin[1,2]; Jeffrey A. Culver[1,2]; Meghan Gabriel[1]; Ken Kirkbride[3]; Terri T. Christison[3]; Stephen J. Gardell[1,2]; *[1]Sanford Burnham Prebys Medical Discovery Institute, Orlando, FL; [2]Southeast Center for Integrated Metabolomics, Gainesville, FL; [3]Thermo Fisher Scientific, Sunnyvale, CA*

ThP 442 **Data Normalization in MALDI-MSI and UHPLC-TQ-MS: A Cross-Platform Quantitative Analysis**; Lin Wang[1]; Qian Wu[1]; Stanislav Rubakhin[1]; Jonathan Sweedler[1]; *[1]University of Illinois at Urbana-Champaign, Urbana, IL*

ThP 443 **LCMS Analysis of 15 Urine Steroid Hormones in Women's Urine Samples Across a Menstrual Cycle**; Cesar A Masitas[1]; Emily Chester[2]; Virginia Vitzthum[3]; Nicola Pohl[1]; Jonathan C Trinidad[1]; *[1]Indiana University Dept. Chemistry, Bloomington, IN; [2]Indiana University, Bloomington, IN; [3]Indiana University Department of Anthropology, Bloomington, IN*

ThP 444 **Predicting Concentrations of Small Molecules without Standard Substances in LC/ESI/MS via Ionization Efficiency Scales**; Anneli Kruve[1]; Jaanus Liigand[2]; Piia Liigand[2]; Mari Sild[2]; Karl Kaupmees[2]; *[1]University of Tartu, Tartu; [2]University of Tartu, Tart, Estonia*

ThP 445 **Metabolomic Profiling of Beer Types by Widely-Targeted LC/MS Measurement**; Mitsuhiro Kanazawa[1]; Daichi Yukihira[1]; Tsuyoshi Nakanishi[2]; *[1]Reifycs Inc., Tokyo, Japan; [2]Shimadzu Corporation, Kyoto, Japan*

ThP 446 **Analysis of Platelet Metabolism and Function during Storage**; Freyr Jóhannsson; *University of Iceland,Reykjavík, Iceland*

NATURAL AND NANOMATERIALS 447 - 455

ThP 447 **Analysis of Coco Amphoteric Surfactants Used in Personal Care Products by Liquid Chromatography Mass Spectrometry (LCMS)**; Noelle Elliott[1]; Dale Willcox[1]; Jenan Elias[1]; *[1]Intertek, Allentown, PA*

ThP 448 **Chemical Characterization of Environments Containing Ultra-Small Inclusions via Nanoprojectile Impacts**; Aaron Clubb[1]; Michael J Eller[1]; Rachel M Anderson[2]; Richard M Crooks[2]; Stanislav V Verkhoturov[1]; Emile A Schweikert[1]; *[1]Texas A&M, College Station, TX; [2]University of Texas at Austin, Austin, TX*

ThP 449 **In source-CID of CuAu144 Cluster: Evidence of Internally Bound Copper**; Snigdha Boppidi[1]; David M. Black[2]; Stephen Bach[2]; Robert L Whetten[2]; *[1]University of Texas at San Antonio, San Antonio, Texas; [2]University of Texas at San Antonio, San Antonio, TX*

ThP 450 **Vacuum Ultraviolet Ion Mobility Mass Spectrometry of Complex Carbon Nanomaterials**; Ernest K. Lewis[1]; Bruce Brinson[2]; Carter Kittrell[2]; Jerome Moore[3]; Wade Adams[2]; Amina S. Woods[4]; Robert H. Hauge[2]; J. Albert Schultz[5]; *[1]Ionwerks, Inc., Houston , TX; [2]Rice University, Houston, TX; [3]Robot Nose, Lemont, IL; [4]NIH/NIDA-IRP, Baltimore, MD; [5]Ionwerks Inc, Houston, TX*

ThP 451 **Efficient Detection and Identification of Bacteria By Fluorescent Nanodiamond Labeling and Matrix-Assisted Laser Desorption Ionization Time-of-Flight Mass Spectrometry**; Chih-Che Wu; *Department of Applied Chemistry, National Chi Nan University, Puli, Taiwan*

ThP 452 **Enhanced MALDI-MS Detection of Biomolecules Using Gold Nanoparticles and the Synergy between the Gold Core and Matrix**; Alyssa L M Marsico[1]; Bradley Duncan[1]; Ryan Landis[1]; Vincent M Rotello[1]; Richard W Vachet[1]; *[1]University of Massachusetts Amherst, Amherst, MA*

ThP 453 **Silver Nanoparticles Assisted MALDI Mass Spectrometry for Analysis of Personal Care Products in Environmental Water**; Jing-Chang Wang[1]; Maw-Rong Lee[2]; *[1]Department of Chemistry, National Chung-Hsing University, Taichung, Taiwan; [2]National Chung-Hsing University, Taichung, Taichung*

ThP 454 **Reproducibility of MILDI MS Imaging is Rationalized by Physical and Optical Characterization of AgNP Implanted Surface Layers of Brain Tissue**; Samir M Shubeita[1]; Ludovic Muller[2]; Viacheslav Manichev[1]; Damon Barbacci[3]; Shelley N Jackson[2]; Albert J Schultz[4]; Laura Fabris[1]; Carey Balaban[5]; Torgny Gustafsson[1]; Leonard Feldman[1]; Amina S Woods[2]; *[1]Rutgers University, Piscataway, NJ; [2]NIH/NIDA-IRP, Baltimore, MD; [3]Ionwerks, Gaithersburg, MD; [4]Ionwerks Inc, Houston, TX; [5]University of Pittsburgh, Pittsburgh, PA*

ThP 455 **Application of Magnetic Microbead Affinity Selection Screening (MagMASS) towards Discovery of Retinoid X Receptor-α Ligands**; Ruth Muchiri; *University of Illinois at Chicago, Chicago, IL*

PEPTIDES: FRAGMENTATION MECHANISMS 456 - 470

ThP 456 **A Tandem Mass Spectrometry Study of the Transnitrosylation Products of the Dipeptide Cysteinyl-tryptophan**; Matias Butler[1,2]; Michael K W Siu[2,3]; Alan C Hopkinson[2]; *[1]Universidad de Buenos Aires, Ciudad de Buenos Aires, Argentina; [2]York University, Toronto, Canada; [3]University of Windsor, Windsor, Canada*

ThP 457 **Oxidative Coupling of Cysteine Residue in Small Peptides**; Ekram Hossain[1]; Jianhua Ren[2]; *[1]University of Pacific, Stockton, CA; [2]University of the Pacific, Stockton, CA*

ThP 458 **A Comparison of Negative Electron Transfer Dissociation and Negative Ion Collision-Induced Dissociation of Acidic Peptides**; Chelsea L McMillen[1]; Carolyn J Cassady[1]; *[1]The University of Alabama, Tuscaloosa, AL*

ThP 459 **Negative Electron Transfer Dissociation Reagent Cation Discovery**; Matthew J P Rush[1]; Nicholas M Riley[1]; Michael S Westphall[1]; Joshua J Coon[1]; *[1]University of Wisconsin-Madison, Madison, WI*

ThP 460 **Nucleophilic Attack by Amide Nitrogen Atoms on the Aromatic Rings of [zn − H]•+ ions**; Xiaoyan Mu[1]; Kai-Chi Justin Lau[2,3]; Michael K W Siu[2,3]; Alan C Hopkinson[2]; Ivan K. Chu[4]; *[1], Hong Kong, Hong Kong; [2]York University, Toronto, Canada; [3]University of Windsor, Windsor, Canada; [4]The University of Hong Kong, Hong Kong SAR, Hong Kong SAR*

ThP 461 **Singly Protonated Tryptic Peptides with Penultimate Proline: Isomerization is the Gateway to Fragmentation**; Shanshan Guan[1]; Maha T Abutokaikah[1]; Benjamin J Bythell[1]; *[1]University of Missouri-St.Louis, St. Louis, MO*

ThP 462 **A Systematic Investigation of Proline vs. Pipecolic Acid-containing Peptide Fragmentation Chemistry**; Maha Abutokaikah[1]; Shanshan Guan[1]; Benjamin J Bythell[1]; *[1]Univeristy of Missouri- St. Louis, St. Louis, MO*

ThP 463 **Development of a GC-MS Method for Identification of Dipeptides**; Nino G Todua[1]; Stephen E Stein[1]; Anzor Mikaia[1]; *[1]National Institute of Standards and Technology, Gaithersburg, MD*

ThP 464 **An Experimental and Computational Investigation of the Fragmentation of Dipeptide Acids, Esters and Amides**; Michael J. Van Stipdonk[1]; Rebecca McLaughlin[2]; Stephen Koehler[1]; Anil Vishnuvajjhala[1]; *[1]Duquesne University, Pittsburgh, PA; [2]Grove City College, Grove City, PA*

ThP 465 **Investigation of Gas Phase Fragmentation Reaction Mechanism of Doubly-Protonated bn (n=7-9) Ions by Mass Spectrometry**; Ozge Gorgun[1]; Ahmet Emin Atik[1]; Talat Yalcin[2]; *[1]IYTE, Urla-Izmir, Turkey; [2]IYTE, Urla-Izmir*

ThP 466 **Thermal Dissociation of the TIK(H+)2 Tripeptide. Mechanisms, Kinetic Parameters, and Comparison with CID**; Zahra Homayoon[1]; Pratihar Subha[1]; William L Hase[1]; Veronica Macaluso[2]; Ana Martin-Somer[2]; Riccardo Spezia[2]; *[1]Texas Tech University, Lubbock, TX; [2]CNRS, Paris, France*

ThP 467 **Collision Induced Dissociation Products and Mechanisms of di-protonated T-L-K-(H+)2Peptide by Chemical Dynamics Simulations.**; Veronica Macaluso[1]; Ana Martin-Somer[1]; Zahra Homayoon[2]; Subha Pratihar[2]; William L. Hase[2]; Riccardo Spezia[1]; *[1]CNRS, Paris, France; [2]Texas Tech University, Lubbock, TX*

ThP 468 **Dissociation Energetics of Short Doubly Protonated Tryptic Peptides with Polar Side Chains**; O. I. Obolensky[1]; Yi-Kuo Yu[1]; *[1]National Center for Biotechnology Information, NLM, NIH, Bethesda, MD*

ThP 469 **Coupling Tandem Mass Spectrometry with QM+MM Molecular Dynamic Simulations: Understanding Fragmentation Mechanisms of Protonated Uracil in the Gas Phase**; Estefania Rossich Molina[1]; Jean-Yves Salpin[2, 3]; Riccardo Spezia[2, 3]; *[1]CNRS UMR 8587, Evry, Ile de France; [2]CNRS UMR 8587, Evry, France; [3]Université d'Evry Val d'Essonne, Laboratoire Analyse et Modélisation pour la Biologie et l'Environnement., Evry, France*

ThP 470 **Theoretical Mass Spectrometry of Peptides: Statistical vs Non-Statistical Fragmentation**; Riccardo Spezia[1]; Ana Martin-Somer[1]; Veronica Macaluso[1]; Zahra Homayoon[2]; Subha Pratihar[2]; William L. Hase[2]; *[1]CNRS, UMR 8587, Evry, France; [2]Texas Tech University, Lubbock, TX*

PEPTIDES: QUANTITATIVE ANALYSIS 471 - 504

ThP 471 **Selenium Labeling Combined with LC-ICP-MS, a New Methodology in Pharmacology to Measure Protein-Ligand Interactions**; Emmanuelle Cordeau[1]; Carine Arnaudguilhem[2]; Brice Bouyssiere[2]; Agnès Hagège[3]; Jean Martinez[1]; Gilles Subra[1]; Sonia Cantel[1]; Christine Enjalbal[1]; *[1]Institut des Biomolécules Max Mousseron (IBMM), UMR 5247, Université de Montpellier, CNRS, ENSCM, Place Eugène Bataillon, 34095 Montpellier cedex 5, France., Montpellier, France; [2]Laboratoire de Chimie Analytique Bio-inorganique et Environnement LCABIE-IPREM, UMR 5254, Hélioparc, 64053 Pau, France, Pau, France; [3]Université de Lyon, Institut des Sciences Analytiques, UMR 5280, CNRS, Université Lyon 1, ENS Lyon,Villeurbanne, France, Lyon, France*

ThP 472 **Development of a Robust GLP Bioanalytical Method for a Short-lived Therapeutic Peptide**; Christopher Barringer[1]; Daniel J Ricca[2]; Mary Katofiasc[2]; Lesley Marson[2]; *[1]Covance, Durham, NC; [2]Dignify Therapeutics, Research Triangle Park, NC*

ThP 473 **An Alternative and More Sensitive Approach for the Analysis of Neuropeptides in Biological Samples**; Stephen J. Lock[1]; Edna Betgovargez[2]; *[1]SCIEX, Warrington, Cheshire; [2]SCIEX, Concord ON, Canada*

ThP 474 **Development of a MicroFlow LC-MS/MS Method for Quantitation of Peptides**; Kerry Hassell[1]; Joshua J Nicklay[1]; Tara Schroeder[1]; *[1]ThermoFisher Scientific, Somerset, NJ*

ThP 475 **A Simplified Approach to Fast and Accurate, High Throughput Targeted MS2 Quantitation using Internal Standards**; Shannon Eliuk[1]; Romain Huguet[1]; Michael Blank[1]; Vlad Zabrouskov[1]; Graeme C McAlister[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

ThP 476 **Validation and Correlation Strategies for Data Generated by Ligand Binding Assays and LC-MS to Support Product Development and Regulatory Assessment**; Ryan Hill[1]; Trent J. Oman[1]; *[1]Dow AgroSciences, Indianapolis, IN*

ThP 477 **Novel Application of SCIEX 6600 TripleTOF Mass Spectrometer for Quantitative Assessment of Glucagon-Like Peptide-1 (GLP1) Analog Pharmacokinetic Studies**; Yue Huang[1]; Sarah Will[2]; Anish Konkar[2]; Jefferson Revell[3]; Marcella Petrone[3]; Inna Vainshtein[1]; Meina Liang[1]; Raffaella Faggioni[1]; Anton Rosenbaum[1]; *[1]MedImmune, Mountain View, CA; [2]MedImmune, Gaithersburg, MD; [3]MedImmune, Cambridge, UK*

ThP 478 **Effect of Dimethyl Sulfoxide on Sensitivity Improvement of Therapeutic Peptides by LC/MS/MS**; Eric Ma[1]; Moucun Yuan[1]; William Mylott[1]; Bruce Hidy[1]; Rand Jenkins[1]; *[1]PPD, Richmond, VA*

ThP 479 **Improvements in Sensitivity for Biotherapeutics using a Prototype Tandem Quadrupole Mass Spectrometer**; Nikunj Tanna[1]; Kerri Smith[1]; Mark Wrona[1]; Leonard Dillon[2]; Mark Roberts[2]; *[1]Waters Corporation, Milford, MA; [2]Waters Corporation, Wilmslow, UK*

ThP 480 **Peakjuggler – A Proteome Discoverer Node for Label-free MS1 Quantification**; Johannes Doblmann[1]; Karl Mechtler[1, 2]; *[1]Research Institute of Molecular Pathology (IMP), Vienna, Austria; [2]Institute of Molecular Biotechnology (IMBA), Vienna, Austria*

ThP 481 **Evaluation of the Parameters Affecting Interference Levels in Isobaric Tagging Studies**; Matthew Lim[1]; Joao Paulo[1]; Steven P Gygi[1]; *[1]Harvard Medical School, Boston, MA*

ThP 482 **Relative Quantification of Sites of Peptide and Protein Modification using Size Exclusion Chromatography coupled with Electron Transfer Dissociation**; Boer Xie[1]; Joshua Sharp[2]; *[1]The University of Georgia, Athens, GA; [2]The University of Mississippi, Oxford, MS*

ThP 483 **Quantification of Total Hepatocyte-Targeted Membrane-Lytic-Peptide (MLP-NAG) in Rat Plasma by LC-MS/MS using Solid Phase Extraction**; Qingguo Tian[1]; Min Meng[2]; Rogness Juan[3]; Zhen Li[4]; *[1]Arrowhead Research Corporation, Madison, WI; [2]Covance, Salt Lake City, UT; [3]Covance, Salt Lake City, UT; [4]Arrowhead Research Corporation, Madison, WI*

ThP 484 **MALDI Mass Spectrometry and HCCA Labeling as a Powerful Tool for Peptide Quantitation in Biology**; Christine Enjalbal[1]; Maxime Rossato[2]; Sonia Cantel[2]; Gilles Subra[2]; Muriel Amblard[2]; Jean Martinez[2]; *[1]University Montpellier 2, Montpellier, cedex 05; [2]University of Montpellier, IBMM UMR5247, Montpellier, France*

ThP 485 **Extending Targeted Proteomics to Study Molecular Signaling Events**; Thierry Schmidlin[1, 2]; Luc Garrigues[1, 2]; Violette Gautier[1, 2]; Arjen J. Boender[1]; Erik L de Graaf[1, 2]; Roger A H Adan[1]; Albert J R Heck[1, 2]; Maarten A F Altelaar[1,2]; *[1]Utrecht University, Utrecht, The Netherlands; [2]Netherlands Proteomics Center, Utrecht, The Netherlands*

ThP 486 **Isobaric TMT 10-plex Labeled MultiNotch MS3 Analysis of Human Uterine Smooth Muscle in Disparate States of Pregnancy**; Christian Copley Salem[1]; Criag Ulrich[1]; David Quilici[2]; Rebekah Woosley[2]; Iain Buxton[1]; Heather Burkin[1]; *[1]University of Nevada, Reno School of Medicine, Reno, NV; [2]Mick Hitchcock Nevada Proteomics Center, Reno, NV*

ThP 487 **Quantification of Synthetic Peptides by Multiple Reaction Monitoring-Liquid Chromatography-Mass Spectrometry (MRM-LC-MS)**; Praveena Nukareddy[1]; Bruce O'Rourke[1]; Dwight E. Matthews[1]; *[1]University of Vermont, Burlington, VT*

ThP 488 **Precise and High-Throughput Quantitation of Plasma Biomarker Peptides for Alzheimer Disease at Attomole Level by SRM**; Takeshi Tomonaga[1]; Ritsuko Maki[1]; Kanta Yanagida[2]; Shigeru Yamada[3]; Shinji Tagami[2]; Masayasu

Okochi[2]; [1]*Laboratory of Proteome Research, National Institutes of Biomedical Innovation, Health and Nutrition, Osaka, Japan;* [2]*Psychiatry, Department of Integrated Medicine, Division of Internal Medicine, Osaka University Graduate School of Medicine, Osaka, Japan;* [3]*Thermo Fisher Scientific Japan, Yokohama, Japan*

ThP 489 **A High-Throughput Method for Reproducible Global Quantification of the Yeast Proteome using Data Independent Acquisition Mass Spectrometry**; Lindsay Pino[1]; Gennifer E Merrihew[1]; William S Noble[1]; Michael J MacCoss[1]; [1]*University of Washington, Seattle, WA*

ThP 490 **Fast and Sensitive LC-MS Workflow for Determination of Endogenous Secretory Peptides in Biological Fluids**; Liangqiao Bian[1]; Maciej Kukula[2]; [1]*SCAAC, UT Arlington, Arlington, TX;* [2]*SCAAC, University of Texas at Arlington arlington, tx*

ThP 491 **Quantitative Analyses of Microcystins by LC-MS/MS using an Orbitrap Fusion Tribrid Mass Spectrometer**; Raymond West[1]; Dilrukshika S.W. Palagama[1]; Dragan Isailovic[1]; [1]*University of Toledo, Toledo, OH*

ThP 492 **Label-free Quantitation of Opioid Induced Hyperalgesia Related-Peptides in Mice Hypothalamus using Skyline MS1 Filtering Approach**; Ning Yang[1]; Krishna D Anapindi[1]; Stanislav S Rubakhin[1]; Elena V Romanova[1]; Amynah Pradhan[2]; Jonathan v Sweedler[1]; [1]*University of Illinois at Urbana-Champaign, Urbana-Champaign, IL;* [2]*University of Illinois at Chicago, Chicago, IL*

ThP 493 **Characterization of Endoproteolytic Processing of Tachykinins and Substance P using Mouse Spinal Cord Cellular Fractions and High-Resolution Mass Spectrometry**; Mouna Saidi[1]; Francis Beaudry[1]; [1]*Université de Montréal, St-Hyacinthe, QC*

ThP 494 **Selective and Sensitive Quantification of Glucagon and Glucagon-Related Peptide Hormones in Human Plasma using Conventional LC/MS/MS**; Norihide Yokoi[1]; Ritsuko Hoshikawa[1]; Toshiya Matsubara[1, 2]; Ichiro Hirano[2]; Susumu Seino[1]; [1]*Kobe University Graduate School of Medicine, Kobe, Japan;* [2]*Shimadzu Corporation, Kyoto, Japan*

ThP 495 **Quantification of Blood-Brain Barrier Permeation of Glycosylated Peptides using Microdialysis Coupled to Mass Spectrometric Detection**; Catherine Kramer[1]; Evan M. Jones[1]; Meredith Hay[1]; Robin Polt[1]; Michael L Heien[1]; [1]*University of Arizona, Tucson, AZ*

ThP 496 **Ultra Performance Liquid Chromatography−Tandem Quadrupole Mass Spectrometry for High-Sensitivity Profile Analysis of Blood Pressure Modulators Angiotensin Peptides**; Meng Qi[1]; Hui Wang[2]; Jie Wang[1]; Li Yang[1]; Zhengtao Wang[1]; [1]*Shanghai University of Traditional Chinese Medicine, Shanghai, Shanghai;* [2]*Waters Corporation, Shanghai, China*

ThP 497 **Detection of Insulin Analogues and Large Peptides in Urine for Anti-doping**; Holly Cox[1]; Brittney Weber[1]; Daniel Eichner[1]; [1]*Sports Medicine Research and Testing Laboratory, Salt Lake City, UT*

ThP 498 **Validation of Vancomycin Assay in Rat Plasma by Liquid Chromatography /Tandem Mass Spectrometry**; Xiaodong Shen[1]; Chantal Picard[1]; Rwaida Al-Eryani[1]; John Lord[2]; Gary Johnson[1]; [1]*ITR, Baie d'Urfe, Canada;* [2]*Savara Inc., Austin, USA*

ThP 499 **Screening of Glyphosate-Resistant Transgenic Engineering Soy Bean and Maize by Ultra-high Performance Liquid Chromatography Coupled with Tandem Mass Spectrometry**; Wenjuan Zang[1]; Meiling Lu[2]; Shan Zhou[3]; Xiangmin Zhang[1]; [1]*Fudan University, Shanghai, China;* [2]*2Agilent Technologies (China) Limited, Beijing;* [3]*Agilent Technologies (China) Limited, Beijing, China*

ThP 500 **Systematic Comparison of TMT10-plex Quantification Accuracy and Precision in MS2 and SPS-MS3 Mode**; Lauren Clarissa Tang[1]; Jana W Qiao[1]; Rushdy Ahmad[1]; Karl R Clauser[1]; Namrata D Udeshi[1]; Hasmik Keshishian[1]; Caitlin Feeney[1]; Jenn Abelin[1]; Jacob J Jaffe[1]; Philipp Mertins[1]; Steven A Carr[1]; [1]*The Broad Institute, Cambridge, MA*

ThP 501 **One and Done - HRAM MS Protein Quantitation and the Rewards of Retrospective Data Analysis in an Ever-changing Regulatory Landscape**; Trent J Oman[1]; Ryan C Hill[1]; Jeffrey R Gilbert[1]; [1]*Dow AgroSciences, Indianapolis, IN*

ThP 502 **PTM Quantitative Analysis on Monoclonal Antibodies using LC-MS and PEAKS Software**; Baozhen Shan[1]; Xin Lei[2]; [1]*Bioinformatics Solutions Inc., Waterloo, ON;* [2]*Bioinformatics Solutions Inc., Waterloo, Canada*

ThP 503 **The Myocardial Degradome following Ischemia/ Reperfusion Injury**; Melanie Yvonne White[1]; Nina Hartcher[1]; Kiersten A Liddy[1]; Joel A Cain[1]; Stuart J Cordwell[1]; [1]*The University of Sydney, Sydney, Australia*

ThP 504 **Charge Variant Identification and Quantification of Recombinant Antibody, Trastuzmab Using Automated Software**; Jung-Keun Suh[1]; Kui Hyun Kang[2]; John St Skilton[3]; Eric Carlson[4]; Chris Becker[4]; [1]*Korean German Institute of Technology, Seoul, Gangseo-gu;* [2]*BIOnSYSTEMS Inc., Seoul, Korea;* [3]*Protein Metrics Inc., San Carlos, CA;* [4]*Protein Metrics, San Carlos, CA*

PEPTIDES: SEQUENCE ANALYSIS
505 - 518

ThP 505 **LC-MS/MS – Peptide Mapping with Electron Transfer Dissociation (ETD) Reveals Enzyme-Mediated Intramolecular Bond in Transglutaminase**; Thomas W Powers[1]; Andrew W Dawdy[1]; Jason C Rouse[2]; Olga V Friese[1]; [1]*Pfizer, Inc. Chesterfield, MO;* [2]*Pfizer, Inc. Andover, MA*

ThP 506 **Heavyweight Champion: Iodine's Large Mass-Defect Weighs in on the Enhancement of the Sequence Coverage of Tryptic Peptides via ETD**; Emilie Aude Viglino[1]; Christopher Shaffer[1]; František Tureček[1]; [1]*University of Washington, Seattle, WA*

ThP 507 **Electron Transfer Dissociation of Trivalent Metal Cationized Acidic Phosphorylated Peptides**; Juliette Joan Commodore[1]; Carolyn J. Cassady[1]; [1]*The University of Alabama, Tuscaloosa, AL*

ThP 508 **Comparative Study of The Skin peptidomes of Rana ridibunda from Russian and Slovenian Populations**; Tatiana Yu Samgina[1]; Konstantin A Artemenko[2]; Jonas Bergquist[3]; Polonca Trebse[4]; Gregor Torkar[4]; Maria Tolpina[1]; Albert T. Lebedev[5]; [1]*Moscow State University, Moscow, Russia;* [2]*Uppsala University, Uppsala, SE;* [3]*Uppsala University, Uppsala, Sweden;* [4]*Ljubljana University, Ljubljana, Slovenia;* [5]*Moscow State University, Moscow, Moscow*

ThP 509 **Sensitive and Rapid LC/MS Method to Identify Potential T-cell Epitopes of Antibody Drugs**; Nobuo Sekiguchi[1]; Chiyomi Kubo[1]; Ayako Takahashi[1]; Kumiko Muraoka[1]; Akira Takeiri[1]; Mariko Yano[1]; Shotaro Takata[1]; Naoaki Murao[1]; Masaki Ishigai[1]; [1]*Chugai Pharmaceutical Co., Ltd., Gotemba, Shizuoka*

ThP 510 **Complete Sequence Coverage via ECD in a Q-ToF versus ETD/CID/HCD in an Orbitrap of 6+ and 7+ Protonated Ubiquitin**; Yury V Vasil'ev[1]; Nathan I Lopez[1]; Valery G Voinov[1]; Douglas F Barofsky[2]; Joseph S Beckman[1]; [1]*Linus Pauling Institute, Oregon State University Corvallis, OR;* [2]*Oregon State University, Department of Chemistry Corvallis, OR*

ThP 511 **Highly Specific Peptide-Bond Dissociation of Some Peptide Model Molecules**; Chen-Lin Liu; *NSRRC, Hsinchu, Hsinchu*

ThP 512 ***De novo* Sequencing of Novel Antimicrobial Peptides from the Venom of the Scorpion *Isometrus maculatus* using ASDF-incorporated Curved Field Reflectron.**; Yuzo Yamazaki[1]; Atsushi Kitanaka[2]; Mao Yakio[2]; Masahiro Miyashita[3]; Hisashi Miyagawa[3]; [1]*Shimadzu Corporation, Kyoto, Japan;* [2]*Graduate School of Agriculture, Kyoto*

University Kyoto, Japan; [3]Graduate School of Agriculture, Kyoto University, Kyoto, Japan

ThP 513 **Compact Mass Spectrometry (CMS) for Reaction Optimization and Quality Control of Modern Solid Phase Synthesis (SPPS) of Biologically Active Peptides**; Simon J Prosser[1]; Daniel Eikel[1]; James P Cain[2]; Elizabeth Restituyo-Rosario[2]; *[1]Advion, Inc. Ithaca, NY; [2]Protein Technologies Inc., Tucson, AZ*

ThP 514 **3-Hydroxy-4-nitrobenzoic Acid (3H4NBA) as a MALDI Matrix for In-Source Decay**; Yuko Fukuyama[1]; Shunsuke Izumi[2]; Koichi Tanaka[3]; *[1]Shimadzu Corporation, Kyoto; [2]Hiroshima University, Higashi-Hiroshima, Japan; [3]Shimadzu Corporation, Kyoto, Japan*

ThP 515 **Application of Hydrogen Attachment/Abstraction Dissociation (HAD) for Peptide Analysis**; Sadanori Sekiya[1]; Hidenori Takahashi[1]; Takashi Nishikaze[1]; Shosei Yamauchi[1]; Shinichi Iwamoto[1]; Koichi Tanaka[1]; *[1]Shimadzu Corporation, Kyoto, Japan*

ThP 516 **Selective Derivatization of Peptide Carboxyl Groups with Fluorophores for LDI-MS Analyses**; Dilrukshika S. W. Palagama[1]; Raymond E West III[1]; Dragan Isailovic[1]; *[1]The University of Toledo, Toledo, OH*

ThP 517 **Elucidating the Mechanism of Photo-Induced Peptide Cleavage by Uranyl using Mass Spectrometry**; Rasmus Elnegaard[1]; Niels Erik Møllegaard[2]; Thomas J D Jørgensen[1]; Frank Kjeldsen[1]; *[1]Department of Biochemistry and Molecular Biology, University of Sourthern Denmark, Odense, Denmark; [2]Department of Cellular and Molecular Medicine, University of Copenhagen, Copenhagen, Denmark*

ThP 518 **Fragmentation of Model Deprotonated Phosphorylated Peptides by Collision-Induced Dissociation**; Chelsea E Plummer[1]; Suma Kavati[1]; Junjie Gao[1]; Carolyn J Cassady[1]; *[1]The University of Alabama, Tuscaloosa, AL*

PEPTIDOMICS
519 - 530

ThP 519 **Comparing Mass Spectrometric Platforms for Neuropeptide and Neuroproteome Discovery from Well-Defined Neuronal Tissue**; Krishna D.B Anapindi[1]; Elena V Romanova[2, 3]; Bruce R Southey[2]; Jonathan V Sweedler[2]; *[1]University of Illinois-Urbana Champaign, Urbana, IL; [2]University of Illinois at Urbana-Champaign, Urbana-Champaign, IL; [3]Beckman Institute, UIUC Urbana, IL*

ThP 520 **Correlating Differential Peptidomics and Transcriptomics Data for Assessing Seasonal Changes in the Camel Brain**; Elena Romanova[1]; Bruce R Southey[1]; Michael Greenwood[2]; Charles Hindmarch[3]; Yea-Ling Tay[4]; Ahmad Yamin bin Abdul Rahman[4]; Kok-Gan Chan[5]; Mark Rogers[2]; Colin Campbell[2]; F. Zahra Djazouli Alim[6]; David Murphy[2]; Jonathan V. Sweedler[1]; *[1]University of Illinois at Urbana-Champaign, Urbana-Champaign, IL; [2]University of Bristol, Bristol, UK; [3]Queen's University, Kingston, Canada; [4]BioEasy Sdn Bhd, Shah Alam, Selangor Darul Ehsan, Malaysia; [5]University of Malaya, Kuala Lumpur, Malaysia; [6]Université Saad Dahlab de Blida, Blida, Algeria*

ThP 521 **Multifaceted Mass Spectrometric Investigation of Neuropeptide Changes in Blue Crab, Callinectes sapidus, in Response to Ocean Acidification**; Yang Liu[1]; Amanda Buchberger[1]; Lingjun Li[1, 2]; *[1]Department of Chemistry, University of Wisconsin, Madison, WI; [2]School of Pharmacy, University of Wisconsin, Madison, WI*

ThP 522 **Mass Spectrometric Quantification and Imaging of Changes in Crustacean Neuropeptide Expression Levels Resulting from Hypoxia Stress**; Kellen DeLaney[1]; Amanda Buchberger[1]; Yang Liu[1]; Lingjun Li[1]; *[1]UW Madison, Madison, WI*

ThP 523 **A Puzzle Approach on Single Cell Level**; Susanne Neupert; *Biocenter Cologne, University of Cologne 50674 Cologne, Germany*

ThP 524 **Large Scale Discovery and *de novo*-Assisted Sequencing of Native Cationic Antimicrobial Peptides (CAMPs) from the Komodo Dragon (*Varanus komodoensis*).**; Paul Russo[1]; Melanie Juba[2]; Megan Devine[2]; Stephanie Barksdale[2]; Kajal Gupta[2]; Shaylyn Scott[2]; Kent Vliet[3]; Joel Schnur[2]; Monique vanHoek[2]; Barney Bishop[2]; *[1]George Mason University, Manassas, VA; [2]George Mason Universtiy, Manassas, VA; [3]University of Florida, Gainesville, FL*

ThP 525 **Immunogenic HLA-DR-presented-peptides Identified from Clinical Samples of Synovial Tissue/Fluid and Peripheral Blood from Patients with Rheumatoid Arthritis or Lyme Arthritis**; Qi Wang[1]; Elise E Drouin[2]; Chunxiang Yao[1]; Jiyang Zhang[1]; Yu Huang[1]; Deborah R Leon[1]; Allen C Steere[2]; Catherine E Costello[1]; *[1]Boston University School of Medicine, Boston, MA; [2]Massachusetts General Hospital and Harvard Medical School, Boston, MA*

ThP 526 **Proto-Peptidomics: A UPLC-Ion Mobility-MS/MS Proteomics Workflow for Studying Early Peptide Evolution on the Prebiotic Earth**; Jay G. Forsythe[1, 2]; Anton S. Petrov[1, 2]; Sheng-Sheng Yu[1, 2]; W. Calvin Millar[1, 2]; Martha A. Grover[1, 2]; Ramanarayanan Krishnamurthy[2, 3]; Nicholas V. Hud[1, 2]; Facundo M. Fernandez[1, 2]; *[1]Georgia Tech, Atlanta, GA; [2]NSF/NASA Center for Chemical Evolution, Atlanta, GA; [3]The Scripps Research Institute, La Jolla, CA*

ThP 527 **LC-MS-MS identification of Small Cyclic Amphipathic Peptides (SCAmpPs) in citrus phloem**; Leslie Harden[1]; William H. Vensel[2]; Kent F. McCue[2]; William R. Belknap[2]; *[1]USDA/WRRC, Albany, CA; [2]U.S. Dept. of Agriculture, Albany, CA*

ThP 528 **Azoniaspiro[4.4]nonyl Scaffold for Quantitative Peptide Analysis by LC-ESI-MS(/MS)**; Bartosz Setner[1]; Monika Kijewska[1]; Alicja Kluczyk[1]; Piotr Stefanowicz[1]; Zbigniew Szewczuk[1]; *[1]Faculty of Chemistry, University of Wrocław, Wrocław, Poland*

ThP 529 **Electroanalysis and Electrospray Ionization Mass Spectrometry of Intact and Oxidized Hormone Glucagon**; Wendell P. Griffith[1]; Sushma Karra[1]; Robert Kennedy[2]; Waldemar Gorski[1]; *[1]University of Texas at San Antonio, San Antonio, TX; [2]University of Michigan, Ann Arbor, MI*

ThP 530 **Proteomic Landscapes ofPachycondila Villosa Ant Venom by Nano-Scale Chromatography and High Resolution Mass Spectrometry**; Camila Takeno Cologna[1]; Loic Quinton[1]; Edwin De Pauw[1]; Michel Degueldre[1]; *[1]University of Liege, GIGA-Proteomics Liege, Belgium*

PROTEIN THERAPEUTICS: STRUCTURAL CHARACTERIZATION
531 - 566

ThP 531 **Profiling Released High Mannose and Complex N-Glycan Structures from Monoclonal Antibodies Using Optimized Hydr**; Scott McCall[1]; Matthew Lauber[1]; Stephan Koza[1]; Erin Chambers[1]; *[1]Waters, Milford, MA*

ThP 532 **Comprehensively Characterizing the N and O-Linked Glycosylation of a Recombinant Human EPO using HILIC-MS**; Matthew Lauber[1]; Stephan Koza[1]; Erin Chambers[1]; *[1]Waters Corporation, Milford, MA*

ThP 533 **Mass Spectrometry Friendly Method for N-glycan Quantification**; Wei Wu[1]; Jiping Zhou[1]; Subbarao Mantha[1]; Zhichao Fang[1]; Michelle Wang[1]; Li Tao[1]; Tapan Das[2]; Reb Russell[2]; *[1]Bristol-Myers Squibb Company, Bloomsbury, NJ; [2]Bristol-Myers Squibb, Hopewell, NJ*

ThP 534 **Site-specific Characterization of N-/O- Glycosylation on Therapeutic Human Chorionic Gonadotropins using Online LC/MS and Tandem Mass Tags**; Hongbin Zhu[1]; Ashley C Ruth[1]; David A Keire[1]; Hongping Ye[1]; *[1]FDA, St. Louis, MO*

ThP 535 **Substrate- and Substrate-mimetic Chaperone Binding Sites in Human Alpha-Galactosidase Revealed by Affinity- Mass Spectrometry**; Michael Przybylski[1]; Stefan Maeser[2]; Adrian Moise[2]; Frederike Eggers[2]; Mary Murphy[3]; Jeff Bornheim[3]; *[1]Steinbeis Centre Biopolymer Analysis and Biomedical Mass Spectrometry, Ruesselsheim am Main, Germany; [2]Steinbeis Centre Biopolymer Analysis and Biomedical Mass Spectrometry, Rüsselsheim am Main, Germany; [3]Reichert-Ametek Technologies, Buffalo, NY*

ThP 536 **Hydrogen Exchange Mass Spectrometry can Reliably Detect Small Fractions of Destabilized Protein in Comparability Studies**; Tyler Hageman[1]; David D Weis[1]; Jayant Arora[1]; *[1]University of Kansas, Lawrence, KS*

ThP 537 **Characterization of Bispecific Heteromab using LC-MS Based Methods**; Yuping Zhou[1]; Jason Tang[1]; *[1]Eli Lilly and Company, Indianapolis, IN*

ThP 538 **Disulfide Bond Mapping-A Case Study through Partial Reduction**; Song Klapoetke; *KBI, Durham, NC*

ThP 539 **Innovator and Biosimilar Infliximab: Comparability Assessment of the Host Cell Proteins and Protein Higher Order Structure**; Jing Fang[1]; Catalin E Doneanu[1]; William R Alley[1]; Ying-Qing Yu[1]; Asish Chakraborty[1]; Alain Beck[2]; Weibin Chen[1]; *[1]Waters, Milford, MA; [2]Centre d'Immunologie Pierre Fabre, Saint-Julien-en-Genevois, France*

ThP 540 **Protein Conformational Analysis of Native and Stressed Monoclonal Antibodies using Ion Mobility and LC/MS/MS Disulfide Bond Mapping**; David L Wong[1]; Staples O Gregory[1]; Jordy Hsiao[1]; Te-Wei Chu[1]; Stephen Madden[1]; Javier Satulovsky[1]; *[1]Agilent Technologies, Santa Clara, CA*

ThP 541 **Mapping of Disulfide Bonds by Reducing Electrochemistry and Mass Spectrometry**; Christian Cramer[1]; Kim F. Haselmann[1]; Jesper V. Olsen[2]; Peter Kresten Nielsen[1]; *[1]Novo Nordisk A/S, Måløv, Denmark; [2]NNF Center for Protein Research, University of Copenhagen, Denmark*

ThP 542 **Protein Dynamics in the TGF-β Superfamily by Hydrogen Deuterium Exchange Mass Spectrometry**; Roxana E. Iacob[1]; Viet Le[2]; Bo Zhao[2]; Yuan Tian[2]; Timothy A. Springer[2]; John R. Engen[3]; *[1]Northeastern University , Boston, MA; [2]Children's Hospital Boston and Department of Biological Chemistry and Molecular Pharmacology, Harvard Medical School, Boston, MA; [3]Northeastern University, Boston, MA*

ThP 543 **Characterizing Deamidation and Oxidation in Adalimumab with Low pH Peptide Mapping and Middle-Up Mass Spec Analysis**; Chris Hosfield[1]; Eric Largy[2]; Anicet Catrain[2]; Fabrice Cantais[2]; Gery Van Vyncht[2]; Michael M Rosenblatt[1]; Sergei Saveliev[1]; Marjeta Urh[1]; Arnaud Delobel[2]; *[1]Promega Corporation, Madison, WI; [2]Quality Assistance, Thuin, Belgium*

ThP 544 **Deciphering Biotherapeutic Protein Disulfide Bonds by Top and Middle-Down Mass Spectrometry**; Jiang Zhang[1]; Pilsoo Kang[1]; Jianmei Kochling[1]; *[1]Sanofi Genzyme, Framingham, MA*

ThP 545 **Investigation of Antibody Aggregates by Hydrogen / Deuterium Exchange Mass Spectrometry and Other Biophysical Tools**; Richard Yu-Cheng Huang[1]; Deqiang Yu[2]; Yuanli Song[2]; Ryan K. Swanson[2]; Zhijun Tan[2]; Elizabeth Schutsky[2]; Angela Lewandowski[2]; Zhengjian Li[2]; Guodong Chen[1]; *[1]Bristol-Myers Squibb, Princeton, NJ; [2]Bristol-Myers Squibb, Devens, MA*

ThP 546 **Disulfide Bond Identification of Biotherapeutic Proteins using Various Fragmentation Techniques Available on an Orbitrap Fusion Tribrid Mass Spectrometer**; Stephane Houel[1]; Jennifer Sutton[1]; Seema Sharma[1]; Terry Zhang[1]; Romain Huguet[1]; Martin Samonig[2]; Vlad Zabrouskov[1]; Jonathan Josephs[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Germering, Germany*

ThP 547 **Rapid Profiling of Stressed PEGylated Protein Pharmaceuticals using Ion-Exchange Chromatography with Online Detection by Native ESI and Top-Down MS/MS**; Khaja Muneeruddin[1]; Cedric E Bobst[1]; Ruth Frenkel[2]; Damian Houde[2]; Iva Turyan[2]; Zoran Sosic[2]; Igor A Kaltashov[1]; *[1]University of Massachusetts, Amherst, MA; [2]Biogen, Cambridge, MA*

ThP 548 **A High-Throughput, Automated Platform Method for Multi-Attribute LC-MS Analysis of Cell Culture Harvest and Antibody Glycosylation**; Jia Dong[1]; Nicole Migliore[1]; Steven J Mehrman[1]; John Cunningham[1]; Michael J Lewis[1]; Ping Hu[1]; *[1]Janssen Research & Development, Malvern, PA*

ThP 549 **Automated Data Analysis Enabling Mass Spectrometry–based Assays for the Developability Assessment of Biotherapeutics**; Maurizio Bronzetti[1]; Cassandra Wigmore[2]; Joe Shambaugh[1]; David Bush[1]; Arnd Brandenburg[2]; Peter Haberl[3]; *[1]Genedata Inc, Lexington, MA; [2]Genedata AG, Basel, Switzerland; [3]Genedata GmbH, Munich, Germany*

ThP 550 **Characterization of Selected Therapeutic Monoclonal Antibodies under Stressed Conditions**; Robert Carney[1]; Zsuzsa Lakos[1]; Elena Dremina[1]; John Snyder[1]; *[1]Eurofins Lancaster Laboratories, Inc., Lancaster, PA*

ThP 551 **Site-specific Glycoform Mapping of Biotherapeutics with Micro-Heterogeneity and Macro-Heterogeneity**; Youngsuk Seo[1, 2]; Myung Jin Oh[1, 2]; David Bradley[3]; Hyun Joo An[1, 2]; *[1]AGRS, Chungnam National University, Daejeon, Korea; [2]GRAST, Chungnam National University, Daejeon, Korea; [3]Agilent Technologies, Santa Clara, CA*

ThP 552 **Biosimilar Insulin Characterization: Top/Middle/Bottoms up Approaches**; Rishikant Gupta[1]; Mithun Bhatt[1]; Annu Uppal[2]; Manoj Pillai[2]; Archana Krishnan[1]; Sanjay Sonar[1]; *[1]Biogenomics, Thane (w), Mumbai, India; [2]SCIEX, 121 Udyog Vihar Phase IV Gurgaon, India*

ThP 553 **Mass Spectrometry Based Comparison of Rituximab Originator and Biosimilar**; Othman Montacir[1]; Murat Eravci[2]; Andreas Springer[3]; Stephan Hinderlich[4]; Maria Kristina Parr[1]; *[1]Institute of Pharmaceutical and Medicinal Chemistry, Department of Biology, Chemistry, Pharmacy, Freie Universität Berlin, Germany., Berlin, Germany; [2]Institut für Chemie und Biochemie, Department of Biology, Chemistry, Pharmacy, Freie Universität Berlin, Germany., Berlin, Germany; [3]Großgerätezentrum BioSupraMol, Department of Biology, Chemistry, Pharmacy, Freie Universität Berlin, Germany., Berlin, Germany; [4]Beuth Hochschule für Technik Berlin - University of Applied Sciences, Department of Life Sciences and Technology, Berlin, Germany., Berlin, Germany*

ThP 554 **Towards the Fast and Increasingly Simplified Analysis of Trisulfide Formation in Biopharmaceutical Antibodies**; Anja Resemann[1]; Rainer Paape[1]; Christoph Nordmann[1]; Waltraud Evers[1]; Lars Vorwerg[1]; Eckhard Belau[1]; Volker Sauerland[1]; Lisa A Marzilli[2]; Jason C Rouse[2]; Jason S Wood[3]; Detlev Suckau[1]; *[1]Bruker Daltonic GmbH, Bremen, Germany; [2]Biotherapeutics Pharm. Sci., Pfizer Inc. Andover, MO; [3]Bruker Daltonic, Billerica, MA*

ThP 555 **Site-Specific Characterization and Quantitation of Protein Pegylation by LC-UV-MS and Standard Addition Approach**; Yanjun Liu[1]; Shiaw-Lin Wu[1, 2]; William Hancock[1]; *[1]Barnett Inst., Northeastern University Boston, MA; [2]BioAnalytix Inc, Cambridge, MA*

ThP 556 **High Resolution Separations for Protein LC/MS**; Barry Boyes[1]; Benjamin Libert[2]; Stephanie E Schuster[2]; Brian E Wagner[2]; William E Miles[2]; Joseph Kirkland[2]; *[1]Advanced Materials Technology Inc, Wilmington, DE; [2]Advanced Materials Technology Inc, Wilmington, DE*

ThP 557 **Complete Characterization of a Cysteine-linked Antibody-Drug Conjugate Performed on a Hybrid Quadrupole-Orbitrap Mass Spectrometer with High Mass Range**; Aaron Oakley Bailey[1]; Eugen Damoc[2]; Kai

Scheffler[2]; Stephane Houel[1]; Jonathan L Josephs[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Bremen, DE*

ThP 558 **Characterization of Therapeutic Protein Charge Heterogeneity by Isoelectric Focusing and Nano-spray LC-MS**; Janet Lau[1]; Chen Li[1]; Shiaw-Lin (Billy) Wu[1]; *[1]BioAnalytix Inc, Cambridge, MA*

ThP 559 **Separation and Characterization of IgG2 Disulfide Isoforms by pH Gradient Cation Exchange Chromatography and Non-Reduced LC/MS - Peptide Mapping**; Kristin J Boggio[1]; Anastasiya P Manuilov[1]; Thomas J Porter[1]; Jason C Rouse[1]; Tanya Q. Shang[1]; Matthew C Thompson[1]; *[1]Pfizer Inc, Andover, MA*

ThP 560 **High Throughput Screening and Characterization of Bispecifics Using Native Ion Mobility Mass Spectrometry**; Caroline S. Chu[1]; Te-Wei Chu[1]; Gregory O Staples[1]; Patrick D Perkins[1]; Andy Gieschen[2]; Christian Klein[1]; Carol H. Ball[3]; Ning Tang[1]; *[1]Agilent Technologies, Santa Clara, CA; [2]Agilent Technologies, La Jolla, CA; [3]Agilent Technologies, Wilmington, DE*

ThP 561 **MS-Based Epitope Mapping of Malaria Antigens: DBP and CelTOS from *Plasmodium vivax* and *Plasmodium falciparum***; Yining Huang[1]; Manolo D Plasencia[1]; Henry W Rohrs[1]; Nicole D Salinas[2]; Edwin Chen[2]; Niraj H Tolia[2]; Michael L Gross[1]; *[1]Washington University in St. Louis, Saint Louis, MO; [2]Washington University School of Medicine, Saint Louis, MO*

ThP 562 **A Workflow to Identify Mutations of Bulk Recombinant Proteins by using N-terminal Labeling Combined with the MELD Method**; Gabriel Mazzucchelli[1]; Denis Morsa[1]; Dominique Baiwir[1]; Nicolas Smargiasso[1]; Edwin De Pauw[1]; *[1]Univeristy of Liege, MS Lab - GIGA, Liege, Belgium*

ThP 563 **Higher Order Structure of Monoclonal Antibodies using Covalent Labeling Techniques and Integrative Biophysics**; Mark Chance[1]; Parminder Kaur[2]; Janna G Kiselar[1]; *[1]Case Western Reserve University, Cleveland, OH; [2]NeoProteomics, Inc. Cleveland, OH*

ThP 564 **On-line Disulfide Cleavage for Structural Characterization**; J.C. Yves Leblanc[1]; Tanya Gamble[2]; *[1]SCIEX, Concord, ON; [2]SCIEX, Concord ON, Canada*

ThP 565 **Biopharmaceutical Erythropoeitin Characterisation: Critical Quality Attribute (CQA) Mapping using LC-ESI-Qtof and Automated Database Searching of Glycopeptide Analytes**; Daniel Ian Richard Spencer[1]; Julia Smith[2]; Richard Andrew Gardner[1]; Anja Resemann[3]; Peter Hufnagel[3]; Daryl Ludger Fernandes[1]; *[1]Ludger Ltd., Oxford, UK; [2]Bruker Ltd. Coventry, Coventry, UK; [3]Bruker Daltonic GmbH, Bremen, Germany*

ThP 566 **An Investigation into Aβ/Metal Binding via MALDI TOF MS**; Andrea Renee Kelley[1]; George Perry[1]; Stephan B.H. Bach[1]; *[1]University of Texas at San Antonio, San Antonio, TX*

PROTEINS: CONFORMATION ANALYSIS AND STRUCTURAL BIOLOGY
567 - 585

ThP 567 **Mapping Interfaces of Protein Complexes by Deep Chemical Crosslinking Mass Spectrometry (XL-MSn)**; Angela Wiggins[1]; Eric Tse[2]; Daniel Southworth[1, 2]; Philip Andrews[1, 3, 4]; *[1]Dept. of Biological Chemistry, University of Michigan, Ann Arbor, MI; [2]Life Science Institute, University of Michigan, Ann Arbor, MI; [3]Dept. of Chemistry, University of Michigan, Ann Arbor, MI; [4]Dept. of Computational Medicine and Bioinformatics, University of Michigan, Ann Arbor, MI*

ThP 568 **Crosslinking-MS Mapping of the MLL1 Histone H3K4 Methyltransferase Complex using the Fixed-Charge, CID-cleavable Crosslinker, DC4**; Lolita Piersimoni[1]; Young-Tae Lee[2]; Chih-Chiang Tsou[2]; Alexey Nesvizhskii[2]; Yali Dou[2]; Philip C Andrews[1, 3, 4]; *[1]Department of Biological Chemistry, University of Michigan, Ann Arbor, MI; [2]Department of Pathology, University of Michigan, Ann Arbor, MI; [3]Department of Chemistry, University of Michigan, Ann Arbor, MI; [4]Department of Computational Medicine and Bioinformatics, University of Michigan, Ann Arbor, MI*

ThP 569 **Probing GPCR Conformation by In-Cell Crosslinking and Mass Spectrometry**; Bill Huang[1]; Ji-Won Lee[1]; Hee-Yong Kim[1]; *[1]NIAAA/NIH, Rockville, MD*

ThP 570 **Optimizing Carbene Footprinting: Br Encoding Identifies Modified Peptides and Fragments**; Bojie Zhang[1]; Michael L Gross[1]; *[1]Washington University in St. Louis, St. Louis, MO*

ThP 571 **Tertiary Structure Influences the Covalent Labeling Based Structural Analysis of Proteins**; Patanachai Limpikirati[1]; Richard W Vachet[1]; *[1]University of Massachusetts Amherst, Amherst, MA*

ThP 572 **Native MS and Reporter-incorporated FPOP Platform in Studying Human SOD1 and its Mutant Variants**; Ben Niu[1]; Brian Mackness[2]; Hao Zhang[1]; Don Rempel[1]; Weidong Cui[1]; Jill Zitzewitz[2]; Robert C Matthews[2]; Michael L Gross[1]; *[1]Washington University in St. Louis, St. Louis, MO; [2]University of Massachusetts Medical School, Worcester, MA*

ThP 573 **Amyloid-β(1-42) Oligomer Models Developed using Combined Solid State NMR and High Resolution Hydroxyl Radical Footprinting**; Janna Kiselar[1]; Cong Guo[2]; Huan-Xiang Zhou[2]; Anant Paravastu[3]; Andrew J. Nix[4]; Terrone L. Rosenberry[4]; Alexandra Klinger[5]; *[1]Case Western Reserve Univ, Cleveland, OH; [2]Florida State University, Tallahassee, FL; [3]FAMU & FSU College of Engineering, Florida State University, FL; [4]Mayo Clinic, Jacksonville, FL; [5]DecipherBio, Wyndmoor, PA*

ThP 574 **Characterization of a Membrane Protein in Living Cells using in-Cell Carboxyl Group Footprinting and Mass Spectrometry**; Ke Sherry Li[1]; Weikai Li[2]; Yihu Yang[2]; Weidong Cui[1]; Michael L Gross[1]; *[1]Washington University, St Louis, MO; [2]Washington University School of Medicine, St. Louis, MO*

ThP 575 **Structural Characterization of a G Protein-GEF Complex Using Top-Down Ultraviolet Photodissociation Mass Spectrometry**; W. Ryan Parker[1]; Matthew Montana Quick[2]; Elisa Novelli[2]; Lauren Webb[2]; Jennifer S Brodbelt[2]; *[1]University of Texas at Austin, Austin, TX; [2]University of Texas, Austin, Austin, TX*

ThP 576 **Structural Characterization of Myokinase-Ligand Complexes Using Top-Down Ultraviolet Photodissociation Mass Spectrometry**; Rachel Mehaffey[1]; Michael Cammarata[1]; Jennifer S Brodbelt[1]; *[1]The University of Texas, Austin, Texas*

ThP 577 **Let's Twist Again: Modulating p53 N-terminal Helicity - An Ion Mobility-Mass Spectrometry Study**; Eleanor Dickinson[1]; Perdita Barran[1]; *[1]The University of Manchester, Manchester, UK*

ThP 578 **Unfolding Pathways of Anthrax Toxin Proteins Investigated with Native Mass Spectrometry and Ion Mobility**; Micah T Donor[1]; Simon A Ewing[1]; Bryan A Krantz[2]; James S Prell[1]; *[1]University of Oregon, Eugene, OR; [2]University of Maryland School of Dentistry, Baltimore, MD*

ThP 579 **Mechanism of Prion Oligomerization as Determined by Structural Proteomics**; Jason J Serpa[1]; Evgeniy V Petrotchenko[1]; Christoph H. Borchers[1, 2]; *[1]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [2]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada*

ThP 580 **Unraveling Compositional Heterogeneity of Protein Complexes with a Modified Q Exactive Plus Orbitrap Instrument**; Gili Ben-Nissan[1]; Mikhail E. Belov[2]; Maria G. Fuzesi-Levi[1]; Alexander A Makarov[2]; Michal Sharon[1]; *[1]Department of Biological Chemistry, Weizmann Institute of Science, Rehovot, Israel; [2]Thermo Fisher Scientific, Bremen, Germany*

ThP 581 **Identification of Hidden Allosteric Sites of β-Lactamase by Dynamic Simulation and Mass Spectrometry**; Supratik Dutta[1]; Sukrit Singh[2]; Gregory R Bowman[3]; Michael L Gross[3]; *[1]Washington University in St. Louis, Chesterfield, Missouri; [2]Washington University in St. Louis, St. Louis, MO; [3]Washington University in St. Louis, Saint Louis, MO*

ThP 582 **Phosphorylation Effects on the Intact Structure of Eukaryotic Translation Initiation Factor 4B (eIF4B) using Ion Mobility Mass Spectrometry**; Katherine Beglinger[1]; Armann Andaya[1]; Youjin Seo[1]; Masaaki Sokabe[1]; Christopher S Fraser[1]; Julie A. Leary[1]; *[1]UC Davis, Davis, CA*

ThP 583 **Collision Induced Unfolding of Partially-Metalated Methallothionein-2A Provides a More Detailed View of the Effects of Metal Binding**; Shiyu Dong[1]; Nicole Wagner[1]; David H Russell[1]; *[1]Texas A&M, College Station, TX*

ThP 584 **Unravelling the Mechanism of a Novel Bacterial Ferritin-Like Iron Storage System using Native Mass Spectrometry and Structural Biology**; Didi He[1]; Alison Mackenzie[1]; Sally Vanden-Hehir[1]; Sophie Harvey[2]; C. Logan Mackay[1]; Jon Marles-Wright[1]; David James Clarke[1]; *[1]University of Edinburgh, Edinburgh, UK; [2]The Ohio State University, Columbus, OH*

ThP 585 **Higher-Throughput Native Mass Spectrometry for Protein-Ligand Screening with Application for Trimethoprim-Resistant Dihydrofolate Reductase**; Michael Cammarata[1]; Ross Thyer[1]; Andrew Ellington[1]; Jennifer S Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX*

PROTEINS: PTMS (PART 2)
586 - 605

ThP 586 **Mapping and Quantifying Protein O-GlcNAcylation in Human Brain for Studies of Alzheimer's Disease**; Sheng Wang[1]; Feng Yang[1]; Vladislav Petyuk[1]; Shukla Anil[1]; Matthew E Monroe[1]; Marina A Gritsenko[1]; Karin D Rodland[1]; Richard D Smith[1]; Wei-jun Qian[1]; Cheng-Xin Gong[2]; Tao Liu[1]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]The Institute for Basic Research in Developmental Disabilities, Staten Island, NY*

ThP 587 **Comparison and Optimization of First and Second Generation Quadrupole Dual Cell Linear Ion Trap Orbitrap Hybrid MS for Glycopeptide Analysis**; Julian Saba[1]; Sergei I Snovida[2]; Christa Feasley[3]; Nina Soltero[4]; Gauri Muradia[5]; Jeremy P Kunkel[6]; Jessie R Lavoie[6]; *[1]Thermo Fisher Scientific, Mississauga ON, Canada; [2]Thermo Fisher Scientific, Rockford IL, USA; [3]Thermo Fisher Scientific, West Palm Beach FL, USA; [4]Thermo Fisher Scientific, San Jose, CA; [5]Health Canada, Ottawa ON, Canada; [6]Health Canada, Ottawa, Canada*

ThP 588 **N-glycoproteome Profiling of the Mouse Testis**; Xuejiang Guo[1]; Fangjuan Liu[1]; Yueshuai Guo[1]; Tao Zhou[1]; Zhou Zuomin[1]; Jiahao Sha[1]; *[1]Nanjing Medical University, Nanjing, CN*

ThP 589 **Sample Displacement Chromatography (SDC) for Differentiating Glycoforms on Human Glycoproteins for Cancer Biomarker Discovery**; Wonryeon Cho[1]; Jihoon Shin[1]; *[1]Wonkwang University, IKSAN, Jeonbuk*

ThP 590 **Lysine β-hydroxybutyrylation is a New Type of Protein Post-Translational Modification Associated with Diverse Pathophysiology**; Di Zhang[1]; He Huang[1]; Zhongyu Xie[1]; Dongjun Chung[2]; Xiaoyong Yang[3]; Yingming Zhao[1]; *[1]The University of Chicago, Chicago, IL; [2]Medical University of South Carolina, Charleston, SC; [3]Yale University, New Haven, CT*

ThP 591 **Comparative Analysis of Histone PTMs using DDA, DIA and PRM Methods on a QExactive HF Orbitrap**; Joby Cole[1]; Eleanor Hanson[2]; David Dockrell[3, 4, 5]; Mark Dickman[2, 5]; *[1]University of Sheffield, Sheffield, South Yorkshire; [2]Department of Chemical and Biological Engineering, University of Sheffield, Sheffield, UK; [3]Department of Infection, Immunity and Cardiovascular Sciences, University of Sheffield Medical School, Sheffield, UK; [4]Sheffield Teaching Hospitals NHS FT, Sheffield, UK; [5]The Florey Institute, University of Sheffield, Sheffield, UK*

ThP 592 **Altered Lysine Acylation of Mitochondrial Proteins in Response to Macronutrient Stresses in the Mouse Liver**; Jesse G. Meyer[1]; Natan Basisty[1]; Samir Softic[2]; Birgit Schilling[1]; Kahn C. Ronald[2]; Bradford W Gibson[1]; *[1]Buck Institute for Research on Aging, Novato, CA; [2]Joslin Diabetes Center and Harvard Medical School, Boston, MA*

ThP 593 **Proteome wide Profiling of Protein Lysine Propionylome in *Escherichia coli***; Mingwei Sun[1]; Linhui Zhai[1]; Yingming Zhao[1, 2]; Minjia Tan[1]; *[1]Shanghai Institute of Materia Medica, Shanghai, P. R. China; [2]The University of Chicago, Chicago, IL*

ThP 594 **A Ubiquitin-Conjugating Enzyme Mediates Global Remodeling of the Proteome during Terminal Differentiation**; Miguel Prado[1]; Anthony Tuan Nguyen[1]; Mingwei Min[1]; Joao A Paulo[1]; Yuan Shi[1]; Mona Kawan[1]; Verena Dederer[1]; Paul Schmidt[2]; Dean Campagna[2]; Mark D Fleming[2]; Steven P Gygi[1]; Daniel Finley[1]; *[1]Harvard Medical School, Boston, MA; [2]Boston Children's Hospital, Harvard Medical School Boston, MA*

ThP 595 **Acetylation Stoichiometry Analysis of Sirt3 Deficient Liver**; Josue Baeza[1]; Michael Smallegan[1]; James Dowell[1]; Jing Fan[1]; John Denu[1]; *[1]University of Wisconsin Madison, Madison, WI*

ThP 596 **Towards Global, Quantitative and Site-Specific Characterization of the ADP-ribosylated Proteome**; Yajie Zhang[1]; Yuanli Zhen[1]; YONGHAO YU[1]; *[1]UT Southwestern Medical Center, Dallas, TX*

ThP 597 **A Quantitative, 10-tissue Atlas of Mouse Ubiquitin Conjugates using 10-plex TMT**; Marta Isasa[1]; Christopher M. Rose[1]; Mark P Jedrychowski[1]; Steven P Gygi[1]; *[1]Harvard Medical School, Boston, MA*

ThP 598 **Differential Protein Ubiquitination Profiles in Primary Human Skeletal Muscle Cells under Hyperinsulinemic Hyperglycemic Conditions Revealed by HPLC-ESI-MS/MS**; Yue Qi[1]; Majed Alharbi[1]; Abdullah Mallisho[2]; Michael Alexander Caruso[1]; Nishit Shah[1]; Divyasri Damacharla[1]; Alice Hu[1]; Danjun ma[1]; Xiangmin Zhang[1]; Berhane Seyoum[2]; Zhengping Yi[1]; *[1]Wayne State University, Detroit, MI; [2]Detroit Medical Center: Detroit Hospital (DMC), Detroit, MI*

ThP 599 **Identification and Characterization of Unexpected Degradation Pathway for Monoclonal Antibody during Process Characterization**; Ratnesh Pandey[1]; Min (Mandy) Xie; Lin Huang; Yanhong Yang; Paula Lei; Allen Bosley; Min Zhu; *[1]MedImmune, Gaithersburg, MD*

ThP 600 **Identification and Characterization of Hydroxylysines in an Immunoglobulin**; Verena Niggeloh[1]; Georg Drabner[1]; *[1]Roche Innovation Center Penzberg, Penzberg, Germany*

ThP 601 **Dynamic Remodeling of Protein Acetylation in *E. coli* in Response to Different Carbon Sources**; Birgit Schilling[1]; David Christensen[2]; Jesse G Meyer[1]; Alexandria K D'Souza[1]; Dylan J Sorensen[1]; Nicholas Shulman[3]; Brendan MacLean[3]; Christopher V Rao[4]; Alan J Wolfe[2]; Bradford W Gibson[1]; *[1]Buck Institute for Research on Aging, Novato, CA; [2]Loyola University Chicago, Maywood, IL; [3]University of Washington, Seattle, WA; [4]University of Illinois at Urbana-Champaign, Urbana, IL*

ThP 602 **Identification of Prenylome by Chemical Oxidation and CID and ETD Tandem Mass Spectrometry**; Ada Shahinuzzaman[1]; Ruchika Bhawal[1]; Saiful Chowdhury[2]; *[1]University of Texas at Arlington, Arlington, TX; [2]Univerisity of Texas at Arlington, Arlington, TX*

ThP 603 **Proteomics Analysis of Toxoplasma gondii Palmitoylated Proteins and its Impact on Rhoptry Localization**; Bin Deng[1]; Marina C Caballero[2]; Andrés M

Alonso[2]; Marcia Attias[3]; Wanderley de Souza[3]; María M Corvi[2]; *[1]University of Vermont, Burlington, VT; [2]2Laboratorio de Parasitología Molecular, Instituto de Investigaciones Biotecnológicas-Instituto Tecnológico de Chascomús (IIB-INTECH), Universidad Nacional de San Martín (UNSAM) - Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET), Chascomús, Argentina; [3]3Laboratório de Ultraestrutura Celular Hertha Meyer, Instituto de Biofísica, Carlos Chagas Filho and Instituto Nacional de Ciência e Tecnologia em Biologia Estrutural e Bioimagens Universidade Federal do Rio de Janeiro, Rio de Janeiro, Brazil*

ThP 604 **Phosphorylation Ratio in Proteins including Protein Kinases can be Measured by Mass Spectrometry**; Lona Zeneyedpour[1]; Lennard Dekker[1]; Noor Abdulhussain[2]; sandor snoeijers[3]; Jos Joore[3]; Sieger Leenstra[1]; Theo Luider[1]; *[1]Erasmus Medical Center, Rotterdam, The Netherlands; [2]University of Amsterdam, Amsterdam, The Netherlands; [3]Pepscope B.V., Utrecht, Netherlands*

ThP 605 **Suspension-Trapping for Rapid (< 1 hr) and Unbiased Milligram-Scale Digestions**; John Wilson[1]; Nikita Saha Turna[2]; Rosamonde Banks[3]; Darryl Pappin[1, 2]; Zougman Alexandre[3]; *[1]Protifi, Huntington, NY; [2]Cold Spring Harbor Laboratory, Cold Spring Harbor, NY; [3]University of Leeds, Leeds, UK*

PROTEOMICS: NEW APPROACHES (OTHER)
606 - 625

ThP 606 **Dodecenyl Succinic Anhydride (DSA)-based Depletion for Complementary Analysis of Protein N-terminal and C-terminal Peptides**; Brian Dill[1]; Henrik Molina[1]; *[1]The Rockefeller University, New York, NY*

ThP 607 **Supporting Alternative Bottom-Up and Middle-Down Proteomics using Neprosin-1 and Tailored Informatics**; Vladimir Sarpe[1]; Christoph Schraeder[1, 2]; David Schriemer[1]; *[1]University of Calgary, Calgary, Canada; [2]Martin-Luther-Universität, Halle-Wittenberg, Germany*

ThP 608 **Analysis of Specific Synaptic Proteomes in Rodent Models of Autism Spectrum Disorder**; Yi-Zhi Wang[1]; Kira A. Cozzolino[1]; Jeffrey N. Savas[1]; *[1]Department of Neurology, Northwestern University, Feinberg School of Medicine, Chicago, IL*

ThP 609 **Chemical Proteomics Approach for the Characterization of Molecular Targets of Fumaric Acid Esters**; Fiona Pachl[1]; Melanie Shackett Brennan[1]; Robert H. Scannevin[1]; Peter Juhasz[1]; *[1]Biogen Inc., Cambridge, MA*

ThP 610 **Evaluation of Aptamer-based Affinity Enrichment of Proteins for Mass Spectrometry**; Eric Kuhn[1]; Debby Ngo[2,3]; Robert E Gerszten[2, 3]; Steven A Carr[1]; *[1]Broad Institute of MIT and Harvard, Cambridge, MA; [2]Massachusetts General Hospital, Boston, MA; [3]Harvard Medical School, Boston, MA*

ThP 611 **Utilizing Mass Spectrometry-Based Profiling System to Identify SH-SY5Y Cell Response Proteins Induced by Hyaluronic Acid Modified Biomaterials**; Ming-Hui Yang[1]; Yu-Chang Tyan [2]; *[1]Graduate Institute of Medicine, KMU, Kaohsiung, Taiwan; [2]Kaohsiung Medical University, Kaohsiung, Taiwan*

ThP 612 **Characterization of Cardiac Myosin Heavy Chain by Middle-Down Mass Spectrometry**; Yutong Jin[1]; Liming Wei[2, 3]; Ying Peng[3, 4]; Wenxuan Cai[4, 5]; Ying Ge[1, 3, 4]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [2]Institutes of Biomedical Sciences, Fudan Universit Shanghai, China; [3]Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI; [4]Human Proteomics Program, University of Wisconsin-Madison, Madison, WI; [5]Molecular and Cellular Pharmacology Training Program, University of Wisconsin-Madison, Madison, WI*

ThP 613 **Integrating Carbamylation and UVPD to Facilitate Middle-Down Proteomics**; James Sanders[1]; Sylvester M Greer[2]; Jennifer S Brodbelt[2]; *[1]University of Texas Austin, Austin, Texas; [2]University of Texas at Austin, Austin, TX*

ThP 614 **Comparative Proteomics Reveal the Mercury Methylation Process in Geobacter sulfurreducens PCA**; Chen Qian[1]; Alexander Johs[2]; Chen Hongmei[2]; Benjamin Mann[2]; Xia Lu[2]; Paul Abraham[3]; Baohua Gu[2]; Robert Hettich[3]; *[1]Graduate School of Genome Science and Technology, University of Tennessee, Knoxville, TN; [2]Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN; [3]Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN*

ThP 615 **Reverse Phased Dispersive Micropipette Tip Extraction with Multiple Fractionation Strategy for Proteomic Profiling of Human Biofluids for Potential Clinical Applications**; Yuzhe Nie[1]; Qian Wang[1]; Mullis Todd[2]; William Brewer[1]; L. Andrew Lee[3]; *[1]University of South Carolina, Columbia, SC; [2]IMCS, LLC, Columbia, SC; [3]IMCS, Columbia, South Carolina*

ThP 616 **Profiling Protein Expression in Limited Amount of Mouse Cortex using CE-ESI-HRMS**; Eric Corcoran[1]; Peter Nemes[2]; Marta Zamarbide[2]; Chiara M. Manzini[2]; *[1]George Washington University, Washington, DC; [2]The George Washington University, Washington, DC*

ThP 617 **Sub-critical Processing of Proteins: Sequence Coverage, Specificity and Post-Translational Modifications**; Thomas Powell[1]; Steve Bowra[2]; Helen J Cooper[1]; *[1]University of Birmingham, Birmingham, UK; [2]Phytatec, Aberystwyth, UK*

ThP 618 **Investigating the Effectiveness of Precursor Mass Exclusion List use for Proteomics on the Orbitrap Fusion**; Tingting Wang[1]; Rose E Stewart[1]; Tony M Harvey[1]; Tanya T Paull[1]; Maria D Person[1]; *[1]University of Texas at Austin, Austin, TX*

ThP 619 **Combination of Cellular Thermal Shift Assay and Quantitative Proteomic Analysis to Identify Palbociclib Targets in MCF-7 Breast Cancer Cells**; Julien Peltier[1]; Teemu Miettinen[2]; Marek Gierliński[3]; Mikael Björklund[2]; Matthias Trost[1]; *[1]MRC PPU, University of Dundee, Dundee, UK; [2]Division of Cell and Developmental Biology, University of Dundee, Dundee, UK; [3]Division of Computational Biology, University of Dundee, Dundee, UK*

ThP 620 **Surface Sampling and Mass Spectrometry Analysis of the Acquired Enamel Pellicle Formation on Hydroxyapatite Discs**; Sabah Pasha[1]; Melissa Grant[1]; *[1]University of Birmingham, Birmingham, UK*

ThP 621 **An Affinity Capture MALDI TOF MS Method for High Density Multiplexed Profiling of Total and PTM Protein Biomarker Panels**; John Cammarata[1]; Ghaith Hamza[2]; Sergey Mamaev[1]; Jeffrey C Silva[2]; Vladislav Bergo[1]; *[1]Adeptrix Corporation, Beverly, MA; [2]Lighthouse Proteomics, Beverly, MA*

ThP 622 **Protease-resistant Streptavidin for Sensitive Interaction-Proteomics**; Jeroen Krijgsveld[1, 2]; Mahmoud-Reza Rafiee[1]; *[1]German Cancer Research Center, Heidelberg, Germany; [2]University of Heidelberg, Heidelberg, Germany*

ThP 623 **Mass Spectrometry-based Analysis of Potential Targets of Phenyl Vinyl Sulfone and Covalent Kinase Inhibitors by Specific Tagging Immunochemical Detection**; Chi-Chi Chou[1]; Yu Cheng-Han[2]; Chang Geen-Dong[3]; Khoo Kay-Hooi[2]; *[1]Academia Sinica, Taipei; [2]Academia Sinica, Taipei, Taiwan; [3]National Taiwan University, Taipei, Taiwan*

ThP 624 **Investigation of the Crosstalk between Phosphorylation and Cysteine Modifications using a Novel Cysteine Tag in Combination with TiO2 Chromatography**; Honggang Huang[1]; Giuseppe Palmisano[2]; Martin R Larsen[3]; *[1]University of Southern Denmark, Odense M, Denmark; [2]Department of Parasitology, ICB, University of São Paulo,*

São Paulo, BRASIL; [3]Department of Biochemistry and Molecular Biology, University of Southern Denmark, Odense M, Denmark

ThP 625 **Methodology to Fish Peptide Ligands of nAChRs from Cone Snail Venoms by MALDI-TOF Mass Spectrometry**; Julien Echterbille[1]; Nicolas Gilles[2]; Romulo Araoz[2]; Edwin De Pauw[1]; Loïc Quinton[1]; *[1]Laboratory of Mass Spectrometry - University of Liege, Liege, Belgium; [2]Commissariat à l'Energie Atomique - DSV/SIMOPRO- Toxins, Receptors and Channels team, Saclay, France*

PROTEOMICS: QUANTITATIVE (PRE-MS AND PLATFORMS/ INFORMATICS/MULTIOMICS/DYNAMICS) 626 - 649

ThP 626 **Improving Speed and Robustness of DIA Quantitation using Longer microLC Columns**; Remco van Soest[1]; Christie Hunter[1]; Fischer Gavin[2]; *[1]SCIEX, Redwood City, CA; [2]SCIEX, Concord ON, Canada*

ThP 627 **Increasing Protein/Peptide Identification and Quantitation Using Extensive Offline Fractionation for TMT Workflows**; Anthony A High[1]; Vishwajeeth R Pagala[1]; Mingming Niu[1]; Xusheng Wang[1]; Hong Wang[1]; Haiyan Tan[1]; Kiran Kodali[1]; Kanisha Kavdia[1]; Yuxin Li[1]; Zhiping Wu[1]; Ashutosh Mishra[1]; Timothy I Shaw[1]; Ji-Hoon Cho[1]; Junmin Peng[1]; *[1]St Jude Children's Research Hospital, Memphis, TN*

ThP 628 **Use of QconCAT Quantitation Data to Resolve 'Hubs' in the Protein Crosslinkome of a Relatively Rigid-Body Protein Complex**; Ji-Suk Kim[1]; Robert Beynon[2]; Paul Gershon[1]; *[1]UC-Irvine, Irvine, CA; [2]University of Liverpool, Liverpool, UK*

ThP 629 **Quantification of Low-abundant GDF-11 and GDF-8 in Human Serum/Plasma Using LC/MS/MS Analysis after Depleting Bio-Complexity by Cation Ion Exchange SPE**; Liming Peng[1]; Srinivasan Krishnan[2]; Shalender Bhasin[3]; *[1]Brigham and Women's Hospital, Boston, MA; [2]AB Sciex, Framingham, MA; [3]Brigham & Women's Hospital, Harvard Boston, MA*

ThP 630 **Pros and Cons of Gradient Optimization in PRM Protein Assays**; Sebastian Malchow[1]; René P Zahedi[1]; Albert Sickmann[1]; Julia M Burkhart[1]; *[1]Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Dortmund, Deutschland*

ThP 631 **Digestion Rates and Stability of Tryptic Peptides Formed from Plasma Proteins**; Adam M Hawkridge[1]; John Brad Mangrum[2]; Erika J Martin[1]; Donald F Brophy[1]; *[1]Virginia Commonwealth University, Richmond, VA; [2]U.S. Food and Drug Administration, College Park, MD*

ThP 632 **A High-Throughput Sample Preparation Workflow for Quantitative Proteomic Studies**; Leanne Jade G Chan[1]; Yan Chen[1]; Huu M Tran[1]; Paul D Adams[1]; Christopher J Petzold[1]; *[1]Lawrence Berkeley National Laboratory, Berkeley, CA*

ThP 633 **Profiling the Cancer Kinome using Quantitative Chemical Proteomics**; Katherine Johnson[1]; Jennifer Brown[1]; Alison Kurimchak[1]; James Duncan[1]; *[1]Fox Chase Cancer Center, Philadelphia, PA*

ThP 634 **Impact of Cystinosin Mutations on Protein Degradations by Differential Dynamic SILAC and on Protein Network by Interactomics**; Chiara Guerrera[1]; Nathalie Nevo[2]; Thomas Lucie[2]; Cerina Chhuon[1]; Anne Bailleaux[2]; Joanna Lipecka[3]; Zuzanna Andrzejewska[2]; Corinne Antignac[2]; *[1]Plateforme Protéomique Paris Descartes Necker, PPN, 3P5-Necker, SFR Necker, US24, Paris, France; [2]French Institute of Health and Medical Research (INSERM) U1163, Laboratory of Hereditary Kidney Diseases, Paris, France; Paris Descartes-Sorbonne Paris Cité University, Imagine Institute, Paris, France; [3]The CPN Proteomics Facility – 3P5, Center of Psychiatry and Neuroscience, UMR INSERM 894, Paris, France*

ThP 635 **Quantitative Analysis of AKT/mTOR Pathway using Multiplex-Immunoprecipitation and Targeted Mass Spectrometry**; Bhavin Patel[1]; Alex Behling[1]; Leigh Foster[1]; Shouling Xu[2]; Ryan Bomgarden[1]; Carrie Clothier[1]; Kay Opperman[1]; Rosa I Viner[2]; Andreas Huhmer[2]; John C Rogers[1]; *[1]Thermo Fisher Scientific, Rockford, IL; [2]Thermo Fisher Scientific, San Jose, CA*

ThP 636 **Application of Stochastic Protein Turnover Model to *in vivo* and *in vitro* Studies**; Mahbubur Rahman[1]; Rovshan Sadygov[1]; *[1]University of Texas Medical Branch at Galveston, Galveston, TX*

ThP 637 **Direct Measurement and Modeling of Protein Synthesis and Degradation Dynamics during Chemotherapeutic Response in Multiple Myeloma**; Tzu-Yu Liu[1, 2]; Hector Han-Li Huang[3]; Diamond D Wheeler[3]; Yun S Song[1, 2]; Arun Paul Wiita[3]; *[1]UC Berkeley, Berkeley, California; [2]University of Pennsylvania, Philadelphia, PA; [3]UCSF, San Francisco, CA*

ThP 638 **Effects of Cigarette Smoke, Cessation and Switching to Two Heat-Not-Burn Tobacco Products on Lung Lipid Metabolism Intwo Mouse Strains**; Thomas Schneider[1]; Bjoern Titz[1]; Stephanie Boue[1]; Blaine Phillips[2]; Terhi Vihervaara[3]; Marja Talikka[1]; Catherine Nury[1]; Ashraf Elamin[1]; Florian Martin[1]; Walter Schlage[1]; Nikolai V. Ivanov[1]; Patrick Vanscheeuwijck[1]; Manuel C. Peitsch[1]; Julia Hoeng[1]; *[1]Philip Morris International, Neuchatel, Switzerland; [2]Philip Morris International Research Laboratories, Singapore, Singapore; [3]Zora Biosciences Oy, Biologinkuja, Finland*

ThP 639 **Differential Protein Expression Analysis by Mass Spectrometry as a Service**; Claudia Fortes[1]; Jonas Grossmann[1]; Paolo Nanni[1]; Witold Wolski[1]; Christian Panse[1]; Laura Kunz[1]; Christian Trachsel[1]; Nathalie Selevsek[1]; Can Türker[1]; Ugur Gürel[1]; Bernd Roschitzki[1]; Ralph Schlapbach[1]; *[1]Functional Genomics Center Zurich, University of Zurich & ETH Zurich, Zurich, Switzerland*

ThP 640 **Targeted Proteomics Coming of Age: SRM, PRM and DIA Performance Evaluated from a Core Facility Perspective**; Paolo Nanni[1]; Tobias Kockmann[1]; Christian Panse[1]; Christian Trachsel[1]; Jonas Grossmann[1]; Witold Wolski[1]; Nathalie Selevsek[1]; Asa Wahlander[1]; Ralph Schlapbach[1]; *[1]FGCZ, Univ Zurich Zurich, Switzerland*

ThP 641 **Quantitative Spatial Proteomics Analysis of the Cellular DNA Damage Response using 10-plex TMT, 4-plex iTRAQ and 8-plex iTRAQ Isobaric Tags**; Sylvie Bourassa[1]; Benjamin Nehmé[1, 2]; Jean-Philippe Gagné[2, 3]; Daniel Defoy[1, 2]; Frédéric Fournier[1, 2]; Guy G. Poirier[2, 3]; Arnaud Droit[1, 2]; *[1]Proteomics, CHU de Quebec Research Center, Quebec, QC; [2]Laval University, Faculty of medicine, Quebec, QC; [3]CHU de Quebec Research Center, Quebec, QC*

ThP 642 **Neutron-encoded Protein Quantification Integrated in the MaxQuant Platform Allows Highly Accurate and Multiplexed Quantification**; Anna E Merrill[1]; Katherine Overmyer[1]; Derek J Bailey[1]; Nicholas W Kwiecien[1]; Alex S Hebert[1]; Michael S Westphall[1]; Stefka Tyanova[2]; Joshua J Coon[1]; Juergen Cox[2]; *[1]University of Wisconsin Madison, Madison, WI; [2]Max-Planck-Institute of Biochemistry, Martinsried, Germany*

ThP 643 **Development of Universal MS Signal Processor for Improved Data Independent Acquisition Performance**; Yet-Ran Chen; *Academia Sinica, Taipei, Nankang*

ThP 644 **Extreme Discordance in Kinase Quantification Using Isobaric Labeling and Parallel Reaction Monitoring with Stable Isotope Dilution Mass Spectrometry**; Robert William Sprung, Jr.[1]; Qiang Zhang[1]; Petra Erdmann-Gilmore[1]; Sherri R Davies[1]; Rose Connors[1]; Yiling Mi[1]; Gary Johnson[2]; Matthew R Meyer[1]; Shunqiang Li[1]; R. Reid Townsend[1]; *[1]Department of Medicine, Washington University School of Medicine, Saint Louis, MO; [2]Department of Pharmacology, University of North Carolina School of Medicine, Chapel Hill, NC*

ThP 645 **Integrating Protease-Specific Micorarrays (CLIP-CHIP) with Proteomics (SILAC) and Terminomics (TAILS) to Profile Macrophage Differentiation**; Nestor Solis[1]; Antoine Dufour[1]; Reinhild Kappelhoff[1]; Anders Kristensen[2]; Leonard Foster[1]; Christopher M Overall[1]; *[1]University of British Columbia, Vancouver, Canada; [2]BC Cancer Agency, Vancouver, Canada*

ThP 646 **2H-metabolic Labeling Approach Reveals Reduced Synthesis of Hepatic Mitochondrial Proteins in a Mouse Model of NASH**; Kwangwon Lee[1]; Abdullah Osme[1]; Ling Li[2]; Zhicheng Jin[1]; Belinda Willard[2]; Rovshan Sadygov[3]; Takhar Kasumov[1]; *[1]Northeast Ohio Medical University, Rootstown, OH; [2]Cleveland Clinic Lerner Research Institute, Cleveland, OH; [3]University of Texas Medical Branch at Galveston, Galveston, TX*

ThP 647 **The Usual Subsets: Interrogating the Immune System for Proteomic Profiles of Cellular Phenotypes**; Jens Hukelmann[1]; Laura Spinelli[1]; Andrew Howden[1]; Alejandro Brenes Murillo[1]; Doreen Cantrell[1]; Angus Lamond[1]; *[1]University of Dundee, Dundee, UK*

ThP 648 **Constructing V2 Vasopressin Receptor Signaling Network using Integrated and Dynamic Interactome and PTM Data**; Hongda Liu[1]; Lei Song[1]; Kunhong Xiao[1]; *[1]University of Pittsburgh, Pittsburgh, PA*

ThP 649 **Physicochemical, Proteome and Metabolome Studies to Determine Water Use Efficiency in Florida Hybrid Bunch Grape**; Ramesh Katam; *Florida A & M University, Tallahassee, FL*

PROTEOMICS: TISSUE
650 - 675

ThP 650 **Laser Capture Microdissection - Selected Reaction Monitoring for Cortical Layer Specific Protein Quantification in Postmortem Human Brain Tissue**; Matthew MacDonald[1]; Dominique Arion[1, 2]; Ying Ding[1]; Daley Favo[1]; Kelly Rogers[1]; David Lewis[1]; Robert Sweet[1]; *[1]University of Pittsburgh, Pittsburgh, PA; [2]UPMC, Pittsburgh, PA*

ThP 651 **Diagnosis of Thymoma Subtypes Using Proteomic Signatures Detected by Mass Spectrometry**; Linan Wang[1]; Owen Branson[1]; Konstantin Shilo[1]; Charles Hitchcock[1]; Michael A. Freitas[1]; *[1]Ohio State University, Columbus, OH*

ThP 652 **Assessment of Formalin-Fixation on Frozen Tissue Samples for Histopathologic and Proteogenomic Analyses**; Brian L Hood[1]; Pamela Palma[2]; Maikarfi Jordan[2]; Tracy Litzi[1]; Julie Oliver[1]; Glenn Gist[1]; David Mitchell[1]; Guisong Wang[1]; Nicholas W Bateman[1]; Christopher Zahn[3]; Chad A Hamilton[1, 4]; George L Maxwell[1, 5, 6]; Thomas P Conrads[1, 2, 6]; *[1]Women's Health Integrated Research Center, GYN-COE, Annandale, VA; [2]Virginia Commonwealth University School of Medicine, Richmond, VA; [3]American College of Obstetricians and Gynecologists, Washington, DC; [4]Department of Obstetrics and Gynecology, Walter Reed National Military Medical Center, Bethesda, MD; [5]Department of Obstetrics & Gynecology, Inova Fairfax Hospital, Falls Church, VA; [6]The Inova Schar Cancer Institute, Falls Church, VA*

ThP 653 **Deep Proteome Analysis of Murine Islets**; Elyse Freiberger[1]; Mark Keller[1]; Alexander S Hebert[1]; Donald S Stapleton[1]; Alan D Attie[1]; Joshua J Coon[1]; *[1]UW-Madison, Madison, WI*

ThP 654 **Rapid Proteomic Profiling of Human Plasma**; Gary M. Wilson[1]; Evgenia Shishkova[1]; Alex S Hebert[1]; Michael S Westphall[1]; Joshua J Coon[1]; *[1]UW-Madison, Madison, WI*

ThP 655 **Protein Turnover Rate in Mice Gastrointestinal Tract is Affected by the Spatial Location and The Microbiota**; Liisa Arike[1]; Andrus Seiman[2]; Sjoerd van der Post[1]; Ana Maria Rodriguez Piñero[1]; Anna Ermund[1]; André Schütte[1]; Malin E. V. Johansson[1]; Fredrik Bäckhed[3]; Gunnar C Hansson[1]; *[1]Department of Medical Biochemistry, University of Gothenburg, Gothenburg, Sweden; [2]Competence Centre of Food and Fermentation Technologies, Tallinn, Estonia; [3]Department of Molecular and Clinical Medicine, Wallenberg Laboratory, University of Gothenburg, Gothenburg, Sweden*

ThP 656 **A Brain Regional Proteomic Atlas in Mouse**; Jong Min Choi[1]; Sung Yun Jung[1]; Maxime William C. Rousseaux[1]; Anna Malovannaya[1]; Jin Jieun Kim[1]; Joachim Kutzera[2]; Yi Wang[1]; Yin Huang[3]; Weimin Zhu[3]; Suman Maity[1]; Huda Yahya Zoghbi[1]; Jun Qin[1]; *[1]Baylor College of Medicine, Houston, TX; [2]University of Amsterdam, Amsterdam, The Netherlands; [3]Beijing Proteome Research Center, Beijing, China*

ThP 657 **Investigating Mechanisms of Preeclampsia by Probing Low Molecular Weight (LMW) Biomolecules in Human Placenta using Liquid Chromatography/Quadrupole-Orthogonal Time-of-Flight MS (cLC/Q-TOF)**; Komal Kedia[1]; Steven W Graves[1]; Stephen Smith[1]; Andrew Hunter Wright[1]; *[1]BYU, Provo, Utah*

ThP 658 **Proteomics and Imaging Mass Spectrometry of High-Grade Serous Ovarian Cancer Reveals Marked Intratumoral Alterations in Neoadjuvant Chemotherapy-Treated Patients**; Emily R Penick[1, 2]; Nicholas W Bateman[2, 3]; Jessica Moore[4]; Brian L Hood[2]; Jeremy L Norris[4]; David Cohn[5]; Laura Havrilesky[6]; Andrew Berchuck[6]; Chad Hamilton[1, 2, 3]; George Maxwell[2, 3, 7]; Richard M Caprioli[4]; Thomas P Conrads[2, 3, 8]; *[1]Walter Reed National Military Medical Center, Department of Obstetrics and Gynecology, Bethesda, MD; [2]Women's Health Integrated Research Center, Annandale, VA; [3]John P. Murtha Cancer Center, Bethesda, MD; [4]Vanderbilt University School of Medicine, Nashville, TN; [5]Ohio State University, Columbus, OH; [6]Duke University Medical Center, Durham, NC; [7]Inova Fairfax Hospital, Department of Obstetrics & Gynecology, Falls Church, VA; [8]Inova Schar Cancer Institute, Falls Church, VA*

ThP 659 **Clinical Tissue Proteomics Identifies U1 snRNP Pathology and RNA Splicing Dysfunction in Alzheimer Disease**; Junmin Peng; *St. Jude Children's Research Hospital, Memphia, TN*

ThP 660 **Quantitative Proteomic Analysis of Human Testis Reveals System-Wide Molecular Pathways Associated with Non-Obstructive Azoospermia**; Mehdi Mirzaei[1]; Mehdi Alikhani[2]; Marjan Sabbaghian[3]; Mohammad Ali Sadighi Gilani[3]; Masoud zabet Moghaddam[4]; Wu Yunqi[1]; Paul A Haynes[1]; Ghasem Hosseini Salekdeh[2]; *[1]Department of Chemistry and Biomolecular Sciences, Macquarie University, Sydney, Australia; [2]Department of Molecular Systems Biology at Cell Science Research Center, Royan Institute for Stem Cell Biology and Technology, ACECR, Tehran, Iran; [3]Department of Andrology at Reproductive Biomedicine Research Center, Royan Institute for Reproductive Biomedicine, ACECR, Tehran, Iran; [4]Center for Biotechnology and Genomics, Texas Tech University, Lubbock, TX*

ThP 661 **A Proteomic Analysis of Fragile Human Bone**; Corinne Thomas[1]; Timothy Cleland[2]; Deepak Vashishth[1]; *[1]Rensselaer Polytechnic University, Troy, NY; [2]University of Texas at Austin, Austin, TX*

ThP 662 **Characterizing ApoE Expression in AD Brain Tissue**; Diana A.T. Nijholt[1]; Christoph Stingl[1]; M. Arfan Ikram[1]; Peter J Koudstaal[1]; Peter A.E. Sillevis Smitt[1]; Theo M. Luider[1]; *[1]Erasmus Medical Center, Rotterdam, The Netherlands*

ThP 663 **The Protein Composition of the Human Colonic Mucus: Reduced Levels of Core Structural Components in Ulcerative Colitis patients**; Sjoerd Van Der Post[1]; Karolina S Jabbar[1, 2]; Noreen Akhtar[1]; Henrik Sjövall[2]; Malin E.V Johansson[1]; Gunnar C Hansson[1]; *[1]Department of Medical Biochemistry, University of Gothenburg, Gothenburg, Sweden; [2]Department of Internal Medicine, University of Gothenburg, Gothenburg, Sweden*

ThP 664 **Label-Free Quantitative Differential Expression Proteomics of Formalin-Fixed Paraffin-Embedded Liver Biopsy Samples from a Longitudinal Study of Hepatitis C Patients**; Sarah Mabbett[1]; Will J Thompson[1]; Joseph Lucas[1]; Keyur Patel[2]; Arthur Moseley[1]; *[1]Duke University Medical Center, Durham, NC; [2]University of Toronto, Toronto ON, Canada*

ThP 665 **Proteomic Mapping of Enamel Matrix in Mice with Different Susceptibilities to Dental Fluorosis by Gel-Based and Gel-Free Approaches**; Aline Leite[1]; Mileni Silva Fernandes[2]; Senda Charone[2]; Gary M Whitford[3]; Eric T Everett[4]; Marília Afonso Rabelo Buzalaf[2]; *[1]University of São Paulo, São Paulo, SP; [2]University of São Paulo, Bauru, SP-Brazil; [3]University of Georgia, Atlanta, GA; [4]University of North Carolina, Chapel Hill, NC*

ThP 666 **Quantitative Cardiovascular Proteomics of Injured Arterial Tissue by Dileu Isobaric Labelling: Toward Novel Therapeutic Targets for Restenosis**; Matthew S. Glover[1]; Qing Yu[1]; Bowen Wang[1]; Xudong Shi[1]; Lian-Wang Guo[1]; K. Craig Kent[1]; Lingjun Li[1]; *[1]University of Wisconsin-Madison, Madison, WI*

ThP 667 **Changes in Protein Expression Levels of Drug-Metabolizing Enzymes and Transporters in Liver and Kidney between Germ-Free and Specific Pathogen-Free Mice**; Takuya Kuno[1]; Mio Hirayama[1]; Shingo Ito[1]; Sumio Ohtsuki[1]; *[1]Kumamoto University, Kumamoto, Japan*

ThP 668 **Quantitative Proteomics of Mouse Skeletal Muscles after 30 Days Of Microgravity on the BION-M1 Biosatellite**; Georg Tascher[1, 2, 3]; Pauline Maes[1]; Alain Van Dorsselaer[1]; Stephane Blanc[2]; Guillemette Gauquelin-Koch[3]; Fabrice Bertile[1]; *[1]LSMBO, DSA IPHC Strasbourg, France; [2]DEPE, IPHC Strasbourg, France; [3]CNES, Paris, France*

ThP 669 **Enhanced Multiplexing to Study the Alzheimer's Disease Proteome across Tissues**; Christina King[1]; Liqing Gu[1]; Renã Robinson[1]; *[1]University of Pittsburgh, Pittsburgh, PA*

ThP 670 **Unravelthe Mechanism of PP2Acα Positively Regulating Liver Regeneration Termination in Mice through a TMT Labeling-Based Phosphoproteomic Approach**; Bin Xue; *Medical Shcool of Nanjing University, Nanjing, Jiangsu*

ThP 671 **Label Free Proteomic Analyses of CEACAM1 Knockout Mouse Liver and Adipose Tissue**; Gabriel Gugiu[1]; Ge Helen[1]; Moore Roger[1]; Deirdre La Placa[1]; Zhifang Zhang[1]; John E. Shively[1]; *[1]City of Hope, Duarte, CA*

ThP 672 **Quantitative, Global Proteomic Analysis of the Damaged Sensory Periphery in Noise-Induced Hearing Loss**; Ann E. Hickox[1]; Ann C. Y. Wong[2, 3, 4]; Kwang Pak[2, 3]; Chelsee Strojny[1]; Allen F. Ryan[2, 3]; Jeffrey N. Savas[1]; *[1]Northwestern Feinberg School of Medicine, Chicago, IL; [2]University of California San Diego, San Diego, CA; [3]Veterans Administration Medical Center, La Jolla, CA; [4]University of New South Wales, Sydney, Australia*

ThP 673 **Nitrite-Induced Preconditioning Elicits Significant Long-Term Alterations to Key Heart Proteins Involved in Redox Stress Protection and Mitochondrial Function**; David H. Perlman[1, 1]; Giuseppe Infusini[1]; Selena Bauer[1]; Bernadette O Fernandez[1]; Mark E McComb[1]; Martin Feelisch[1]; Catherine E Costello[1]; *[1]Boston University School of Medicine, Boston, MA*

ThP 674 **Novel Functional Roles of Acid Sensing Ion Channel Implicated by Proteomics**; Zhihua Yang[1]; Mingli Liu[1]; Zhigang Xiong[1]; An Zhou[1]; *[1]Morehouse School of Medicine, Atlanta, GA*

ThP 675 **Proteomics and Transcriptomics of Therapeutic Ultrasound Treatment on Pancreatic Cells**; S. L. Ng[1]; S. T. Tsai[1]; T. K. Ju[1]; N. G. Chen[2]; Y. P. Kuo[1]; I. L. Tsai[3]; C. H. Chen[1]; *[1]Genomic Research Center, Academia Sinica, Taipei, Taiwan (R.O.C.); [2]Institute of Biomedical Engineering/ Department of Electrical and Computer Engineering, National Chiao Tung University, Hsinchu, Taiwan (R.O.C.); [3]Department of Biochemistry and Molecular Cell Biology, School of Medicine, College of Medicine, Taipei Medical University, Taipei, Taiwan (R.O.C.)*

SMALL MOLECULES: QUANTITATIVE ANALYSIS (PART 2) 676 - 698

ThP 676 **Quantitative Analysis of Thyroid Hormones by Pulsed Glow Discharge Mass Spectrometry**; Xiaqing Xu; *Morgantown, WV*

ThP 677 **Development of a Surrogate Matrix for Cerebral Spinal Fluid for LC/MS Based Analytical Methods**; Shirin Hooshfar[1]; Babak Basiri[1]; Michael G Bartlett[1]; *[1]University of Georgia, Athens, GA*

ThP 678 **Impact of Anticoagulant on the Recovery Efficiency of Minocycline and Doxycycline in Different Matrices by LC-MS/MS**; Richard Lavallée[1]; Vinicio Vasquez[1]; Nikolay I Youhnovski[1]; Milton Furtado[1]; Anahita keyhani[1]; *[1]Algorithme Pharma Inc., Laval, Canada*

ThP 679 **Quantitative Analysis and Protein Binding Determination of fXa Inhibitors in Human Plasma Containing Andexanet Alfa by HPLC-MS/MS**; Chad Christianson[1]; Janet M. Leeds[2]; Sharon DeChenne[1]; Tara Summer[1]; Ryan Collins[1]; *[1]Alturas Analytics, Moscow, ID; [2]Portola Pharmaceuticals, Inc., South San Francisco, CA*

ThP 680 **LC/MS/MS Quantitation of Hydrochlothiazide from Human EDTA Dried Whole Blood Spots**; Rachel Sun[1]; Robert Clegg[1]; Tim Shoaf[1]; Hasantha Jayaratna[1]; *[1]BASi, West Lafayette, IN*

ThP 681 **High-throughput UPLC-ESI-MS/MS Method for the Simultaneous Measurement of Urinary Aliphatic Diamines, Trimethylamine N-oxide, and Beta-methylamino-L-alanine**; Deepak Bhandari[1]; Jonathan P. Rasio[1]; John R. E. Ruhl[1]; David M. Chambers[1]; Benjamin C. Blount[1]; *[1]Centers for Disease Control and Prevention, Atlanta, GA*

ThP 682 **High Throughput Quantitation for Therapeutic Drug Monitoring with Open Access LC/MS/MS System**; Miho Kawashima[1]; Yoshihiro Hayakawa[2]; Taku Tsukamoto[2]; Masafumi Kikuchi[3]; Masaki Tanaka[3]; Shinya Takasaki[3]; Hiroaki Yamaguchi[3]; Nariyasu Mano[3]; *[1]Shimadzu Corporation, Tokyo, Japan; [2]Shimadzu Corporation, Kyoto, Japan; [3]Tohoku University Hospital, Sendai, Japan*

ThP 683 **A Simple and Effective Strategy to Improve Bioanalysis with Capillary Microsampling (CMS): The Use of Internal Standard in Capillary (ISIC)**; Yonghua Ling[1]; Jun Wang[2]; Rand Jenkins[3]; Fumin Li[1]; *[1]PPD, Middleton, WI; [2]Illumina, Inc, Madison, WI; [3]PPD, Richmond, VA*

ThP 684 **Highly Sensitive LC-MS/MS Method for the Quantification of Fluticasone Propionate in Human Plasma, Feasible for Reinjection and Repeat Analysis**; Jeyan Albert[1]; Praveen V Kumar[2]; Manoj Bob[2]; Ravisekhar K[2]; Anoop Kumar[3]; Manoj Pillai[3]; *[1]SCIEX, Gurgaon, Haryana; [2]Lupin Bioresearch Center, Pune, Maharasthra; [3]SCIEX, Gurgaon, Haryana*

ThP 685 **A Highly Sensitive Method for the Quantification of Dexmedetomidine in Human Plasma by Liquid Chromatography-Tandem Mass Spectrometry**; Min Chang Kim[1]; Joo-Youn Cho[1]; Seo Hyun Yoon[1]; *[1]Seoul National University College of Medicine, Seoul, South Korea*

ThP 686 **A Novel Approach to Minimize Matrix Effect in LC-MS/MS Method for Quantitation of Buprenorphine and Norbuprenorphine in HumanUrine**; Dawei Zhou[1]; Pei Li[1]; Shu Zhang[1]; Xuejun Sun[1]; Xinping Fang[1]; *[1]WuXi AppTec Co., Plainsboro, NJ*

ThP 687 **Development and Validation of a Selective Method for Determination of Carboplatin in Human Plasma Using Liquid Chromatography-tandem Mass Spectrometry**; Hyesoo Lee[1]; Seo Hyun Yoon[1]; Joo-Youn Cho[1]; *[1]Seoul National University College of Medicine, Seoul, South Korea*

ThP 688 **Quantification of Lamotrigine and Caffeine in Human Blood using Dried Blood Spot MALDI-MS**; Anne Arnold[1]; Michael Karas[1]; *[1]Goethe University, Frankfurt Am Main, Germany*

ThP 689 **High-Throughput Validated Method for the Quantification of Nicotine and Cotinine in Serum using Ultra Fast SPE-MS/MS**; Matthew Bjergum[1]; Paul J Jannetto[2]; Loralie J Langman[1]; *[1]Mayo Clinic, Rochester, Mn; [2]Mayo Clinic, Rochester, MN*

ThP 690 **High Variation of Internal Standard Response Between Known and Incurred Samples Using LC-MS/MS Method**; Weixing Sun[1]; John Chapdelaine[2]; Zhao Heng Ge[2]; Adrien Musuku[2]; *[1]Pharmascience Inc., Montreal, QC; [2]Pharmascience, Montreal, Canada*

ThP 691 **Plasma 9- and 13-hydroxy-octadecadienoic Acids are Inversely Related to Granulocyte Colony Stimulating Factor and IL-6 in Runners after Heavy Exertion**; David C. Nieman[1]; Mary Pat Meaney[1]; Casey John[1]; Kevin Knagge[2]; Huiyuan Chen[2]; *[1]Appalachian State University, North Carolina Research Campus, Kannapolis, NC; [2]Kannapolis, NC*

ThP 692 **Evaluation of Two Sample Preparation Methods, Precipitation-Derivatization and SPE, for Quantitative LC-MS Analysis of Methylmalonic Acid in Plasma**; Mindy gao; *ThermoFisher Scientific, San Jose, CA*

ThP 693 **Development and Validation of a High Throughput LC-MS/MS Method for Determination of 17-desacetyl Norgestimate in Human Plasma**; Jasper X. Chu[1]; Mary Hillegas[1]; Yuzhu Xue[1]; Yuan-Shek Chen[1]; Ben Hsu[1]; *[1]QPS LLC, Newark, DE*

ThP 694 **A Strategy for Maintaining Chromatographic Peak Shape Due to Incompatible Extract and Mobile Phase by LC-MS/MS**; Mathieu Lahaie[1]; Milton Furtado[1]; Anahita Keyhani[1]; *[1]Algorithme Pharma Inc., Laval, Canada*

ThP 695 **How Low Can We Go? Analysis of Aldosterone using a High Sensitivity Tandem Quadrupole Mass Spectrometer for Clinical Research**; Dominic Foley[1]; Lisa Calton[1]; *[1]Waters, Wilmslow, UK*

ThP 696 **Quantitation of Pegylated Drug Conjugate Interferon Alfa-2b in Human Serum using QTRAP® 6500**; Faraz Rashid[1]; Dipankar Malakar[1]; Anoop Kumar[2]; Manoj Pillai[3]; Praveen Kumar Vittala[4]; Manoj Bob[4]; Ravisekhar K[4]; *[1]SCIEX, 121 Udyog Vihar Phase IV Gurgaon, India; [2]SCIEX, Gurgaon, Haryana; [3]SCIEX, 121 DHR holding Udyog Vihar Phase-4, HR; [4]Lupin bioresearch Center, Pune Maharashtra, MH*

ThP 697 **A Sub-Picogram per Milliliter Method for the Bioanalysis of Fluticasone Propionate Combined with Azelastine in Human Plasma by LC-MS-MS**; Michael Sullivan[1]; Laura Binneboese[1]; Jennifer Bosco[1]; *[1]Worldwide Clinical Trials, Austin, TX*

ThP 698 **Highly Sensitive and Selective Bioanalytical Quantitation Method for Docetaxelin Human Plasma**; santosh kapil kumar Gorti[1]; Aman Sharma[1]; Jeyan Albert[1]; Anoop Kumar[1]; Manoj Pillai[1]; *[1]SCIEX, 121 Udyog Vihar Phase IV Gurgaon, India*

SYSTEMS BIOLOGY (PROTEIN MODIFICATIONS AND CELLS) 699 - 719

ThP 699 **JUMPk Algorithm for Identifying Activated Kinase Modules in a Signaling Network**; Timothy Shaw[1]; Hong Wang[1]; Ji-hoon Cho[1]; Yuxin Li[1]; Xusheng Wang[1]; Suiping Zhou[1]; Alexander Diaz[1]; Chunxu Qu[1]; Yiping Fan[1]; Suzanne J Baker[1]; Jinghui Zhang[1]; Junmin Peng[1]; *[1]St Jude Children's Research Hospital, Memphis, TN*

ThP 700 **Defining the Consequences of Genetic Variation on a Proteome- and Phosphoproteome-Wide Scale**; Joel Chick[1]; Steven C Munger[2]; Petr Simecek[2]; Edward L Huttlin[1]; Kwangbom Choi[2]; Dan Gatti[2]; Narayanan Raghupathy[2]; Karen Svenson[2]; Gary Churchill[2]; Steven P Gygi[1]; *[1]Harvard Medical School, Boston, MA; [2]The Jackson Laboratory, Bar Harbor, ME*

ThP 701 **Selectivity Profiling of Kinase Inhibitors - From Label Free DDA Quantification to Spectral Libraries for Sub-Proteomes**; Susan Klaeger[1, 2, 3]; Stephanie Heinzlmeir[2, 3, 4]; Mathias Wilhelm[1]; Maria Reinecke[1]; Dominic Helm[1]; Huichao Qiao[1]; Guillaume Médard[1]; Bernhard Kuster[1, 5]; *[1]Technical University Munich, Munich; [2]German Cancer Consortium (DKTK), Munich, Germany; [3]German Cancer Research Center, Heidelberg, Germany; [4], Freising; [5]Center for Integrated Protein Science, Munich, Germany*

ThP 702 **Intensity-Based Label-Free Quantification of the Kinome and Total Proteome across 65 Colorectal Cancer Cell Lines: The CRC65 Cell Line Panel**; Martin Heinrich Frejno[1, 2]; Riccardo Zenezini Chiozzi[2, 3]; Mathias Wilhelm[2]; Benjamin Ruprecht[2]; Heiner Koch[2, 4, 5]; Runsheng Zheng[2]; Susan Klaeger[2, 4, 5]; Chen Meng[2]; Anna Jarzab[2]; Stephanie Heinzlmeir[2, 4, 5]; Guillaume Médard[2]; Stephan Michael Feller[6]; Stefan Knapp[1, 7]; Bernhard Kuster[2, 8, 9]; *[1]University of Oxford, Oxford, UK; [2]Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; [3]University of Rome, La Sapienza, Rome, Italy; [4]German Cancer Consortium (DKTK), Muenchen, Germany; [5]German Cancer Research Center (DKFZ), Heidelberg, Germany; [6]Martin-Luther-Universität, Halle-Wittenberg, Germany; [7]Goethe University, Frankfurt Am Main, Germany; [8]Bavarian Biomolecular Mass Spectrometry Center, Freising, Germany; [9]Center for Integrated Protein Science, Muenchen, Germany*

ThP 703 **Proteome Wide Selectivity Profiling of Cyclin-dependent Kinase Inhibitors**; Huichao Qiao[1]; Susan Klaegar[1, 2, 3]; Mathias Wilhelm[1]; Stephanie Heinzlmeir[1, 2, 3]; Dominic Helm[1]; Guillaume Médard[1]; Bernhard Kuster[1, 4]; *[1]Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; [2]German Cancer Consortium (DKTK), Munich, Germany; [3]German Cancer Research Center, Heidelberg, Germany; [4]Center for Integrated Protein Science, Munich, Germany*

ThP 704 **A Comprehensive Study of the Ponatinib-Induced Kinome Changes in Drug-Resistant Leukemia**; Laura Herring[1]; Denis Okumu[1]; Karim Gilbert[1]; Michael East[1]; Lee Graves[1]; *[1]University of North Carolina at Chapel Hill, Chapel Hill, NC*

ThP 705 **MAPKi Inhibitor Induced Signaling Modulation in BRAF-mutated, BRAFi Resistant Colorectal Cancer Cells: A Step Toward Informing Clinical Combination Dose Strategy**; AN CHI; *Merck , Boston, MA*

ThP 706 **Defining Mutant and Wild-Type Colorectal Cancer Signalling Networks with an Integrated Multi-Omics Approach**; Rob Ewing[1]; Zhenghe Wang[2]; Jing Song[2]; *[1]University of Southampton, Southampton, HANTS; [2]Case Western Reserve University, Cleveland, OH*

ThP 707 **Combination of Phosphoproteomics and Machine Learning Approaches Allow Large Scale Identification of Direct Kinase Substrates *in vivo***; Evgeny Kanshin[1]; Sebastien Giguere[2]; Jing Cheng[2]; Mike Tyers[2, 3]; Pierre Thibault[2, 4]; *[1]IRIC, Montreal, QC; [2]IRIC-Université de Montréal, Montréal, QC; [3]Department of Medicine, University of Montréal, Montreal Quebec, Canada; [4]Department of Chemistry, University of Montreal, Montreal Quebec, Canada*

ThP 708 **PKCε and CDKs Regulate Insulin Signaling in Response to a 3-Day High Fat Diet**; Brandon Gassaway[1, 2]; Max Petersen[1, 3]; Hans Rudolf Aerni[1, 2]; Yulia Surovtseva[4]; Karl W Barber[1, 2]; Joshua B Sheetz[1]; Svetlana Rogulina[1]; Janie Merkel[4]; Varman Samuel[1, 5]; Gerald Shulman[1, 3]; Jesse Rinehart[1, 6]; *[1]Yale School of Medicine, New Haven, CT; [2]Systems Biology Institute, West Haven, CT; [3]Howard Hughes Medical Institute, Chevy Chase, MD; [4]Yale Center for Molecular Discovery, West Haven, CT; [5]Veterans Affairs*

Medical Center, West Haven, CT; [6]Systems Biology Institute, Yale University, West Haven, CT

ThP 709 **Profiling Changes in the Phosphoproteome of Hematopoietic Cells in Response to a Novel Class of Anti-Oncogenic Sphingolipid Derived Small Molecules**; Peter Kubiniok[1]; Alison McCracken[2]; Michael Perryman[1]; Stephen Hanessian[1]; Aimee Edinger[2]; Pierre Thibault[1]; *[1]University of Montreal, Montreal Qc, Canada; [2]University of California - Irvine, Irvine, CA*

ThP 710 **Mapping the Ubiquitin Regulatory Networks by Global Proteomic Measurements**; Jeremy O'Connell[1]; Ekaterina Stepanova[1]; Joao Paulo[1]; Steven P Gygi[1]; *[1]Harvard Medical School, Boston, MA*

ThP 711 **Monitoring of the AKT/mTOR Pathway using Internal Standard Triggered-Parallel Reaction Monitoring (IS-PRM)**; Shou Ling Xu[1]; Michael Blank[1]; Sebastien Gallien[2]; Bhavin Patel[3]; Alex Behling[3]; Leigh Foster[3]; John D Rogers[3]; Bruno Domon[2]; Andreas Huhmer[3]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Luxembourg Clinical Proteomics Center, Strassen, Luxembourg; [3]Thermo Fisher Scientific, Rockford, IL*

ThP 712 **Topological Analysis of Perturbed Protein Interaction Networks**; Mihaela Sardiu[1]; Joshua Gilmore[2]; Brad Groppe[3]; Laurence Florens[1]; Michael Washburn[4]; *[1]Stowers Institute for Medical Research, Kansas CIty, MO; [2]Boehringer Ingelheim Vetmedica, St Joseph, MO; [3]Thermo Fisher, San Jose, CA; [4]Stowers Institute for Medical Research, Kansas City, MO*

ThP 713 **Targeted Proteomics-Driven Computational Modeling of Microbial Sensing and Chemotactic Signaling Pathways in Macrophages**; Nathan P Manes[1]; Jessica M Mann[1]; Bastian R Angermann[1]; Marijke Koppenol-Raab[1]; Eunkyung An[1, 2]; Virginie H Sjoelund[1]; Jing Sun[1]; Masaru Ishii[3]; Ronald N Germain[1]; Martin Meier-Schellersheim[1]; Aleksandra Nita-Lazar[4]; *[1]NIH/NIAID, Bethesda, MD; [2]OncoPlex Diagnostics, Rockville, MD; [3]Osaka University, Suita, Japan; [4]NIH/NIAID/LSB, Bethesda, MD*

ThP 714 **To Interact or Not to Interact? The CLASP2 Interactome, a Case Study**; Paul Langlais[1]; Rikke Kruse-Sorensen[2]; James Krantz[1]; Natalie Barker[1]; Richard Coletta[3]; Kristin Ricklefs-Johnson[1]; Moulun Luo[3]; Kurt Hojlund[2]; Lawrence Mandarino[1]; *[1]Mayo Clinic, Scottsdale, AZ; [2]University of Southern Denmark, Odense, Denmark; [3]Arizona State University, Tempe, AZ*

ThP 715 **Deciphering Proteostasis Network by Quantitative Proteomics and Azido-homoalanine Labeling**; Haiping Tang[1]; Qintao Wang[2]; Zhenyu Zhang[2]; Haiteng Deng[3]; *[1]Tsinghua University, Beijing, China; [2]Chaoyang Hospital Affiliated to Capital Medical University, Beijing, China; [3]Tsinghua University, Beijing*

ThP 716 **MSCypher: A High-Throughput Peptide Identification Strategy for Complex Mixtures**; Eugene Kapp[1]; Giuseppe Infusini[1]; Yunshan Zhong[1]; Laura Dagley[1]; Terry Speed[1]; Liam O'Connor[1]; Andrew Webb[1]; *[1]The Walter & Eliza Hall Institute, Parkville, Australia*

ThP 717 **Yeast Proteome Dynamics are Revealed by hyperLOPIT: A High Resolution Spatial Proteomics Approach**; Daniel J.H. Nightingale[1]; Lisa M Breckels[1, 2]; Laurent Gatto[1, 2]; Stephen G Oliver[3]; Kathryn S Lilley[1]; *[1]Cambridge Centre for Proteomics, Department of Biochemistry, University of Cambridge, Cambridge, UK; [2]Computational Proteomics Unit, Department of Biochemistry, University of Cambridge, Cambridge, UK; [3]Cambridge Systems Biology Centre, Department of Biochemistry, University of Cambridge, Cambridge, UK*

ThP 718 **Revealing the Biology between Mass Spectral Molecular Networks with a Novel Dissimilarity Measure**; Ricardo Silva[1]; James T. Morton[2]; Robert Andrew Quinn[1]; Rob Knight[3]; Pieter C. Dorrestein[4]; *[1]Collaborative Mass Spectrometry Innovation Center, Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California, San Diego, La Jolla, CA; [2]Department of Computer Science and Engineering, University of California San Diego, La Jolla, CA; [3]Department of Pediatrics, University of California San Diego, La Jolla, CA; [4]Collaborative Mass Spectrometry Innovation Center, Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California, San Diego, La Jolla, CA*

ThP 719 **Gene Network Analysis Coupled with Bottom-Up Proteomics to Identify Novel Pathways of Aging**; Maneesha Aluru[1]; Tori McKinney[1]; Matthew Torres[2]; *[1]Georgia Institute of Technology, Atlanta, GA; [2]Georgia Institute of Technology, Atlanta, GA*

TOXICOLOGY
720 - 748

ThP 720 **GC-MS/MS Analyses of Skin Tissues in Support of Developmental Toxic Effects on Percutaneous Exposure to VX in Rats**; Jeffrey Michael Mcguire[1]; Lucille Lange[2]; Michael Busch[3]; Linnzi Wright[3]; Paul Demond[4]; *[1]US Army ECBC, Aberdeen Proving Ground, MD; [2]US Army Medical Research Institute of Chemial Defense, Aberdeen Proving Ground, MD; [3]Excet, Inc., Springfield, VA; [4]LEIDOS, Gunpowder, MD*

ThP 721 **GC-MS/MS Analysis of Enantiomers of Ethyl Methlyphosphonofluoridate (VX-G), a Biomarker to Determine Exposure to the Chemical Warfare Agent VX**; Susan Byers[1]; Michael W Busch[1]; Ronald A Evans[2]; Jeffrey M McGuire[2]; Paul S Demond[1]; *[1]Excet Corporation, Aberdeen Proving Ground, MD; [2]US Army ECBC, Aberdeen Proving Ground, MD*

ThP 722 **LC-MS-MS Determination of VX in Contaminated Latex Gloves Following IPA Extraction**; Christopher Byers[1]; Susan Lynn Byers[2]; Ronald A Evans[1]; Terrance G D'Onofrio[1]; *[1]US Army ECBC, Aberdeen Proving Ground, MD; [2]Excet Corporation, Aberdeen Proving Ground, MD*

ThP 723 **Multi-fold Reduction in Drugs of Abuse Detection Limits using Full Scan GCMS with a High Efficiency Source**; Melissa Churley [1]; Luis Cuadra-Rodriguez[2]; Bruce Quimby[3]; *[1]Agilent Technologies, Santa Clara , CA; [2]Agilent Technologies, Santa Clara, CA; [3]Agilent Technologies, Little Falls, DE*

ThP 724 **Unsuspected Exposure to Drugs of Abuse in Young Children Presenting for Emergency Care**; David Colantonio[1]; Gal Neuman[2]; Joshua Ye[3]; *[1]Hospital for Sick Children, Toronto, Canada; [2]Ruth Rappaport Children's Hospital, Haifa, Israel; [3]IONICS Mass Spectrometry, Bolton, ON*

ThP 725 **Definitive Drug and Metabolite Screening in Urine by UPLC-MS/MS using a Novel Calibration Technique**; Thomas G Rosano[1, 2]; Patrice Y Ohouo[2]; John J LeQue[2]; Scott M Freeto[3, 3]; Michelle Wood[4]; *[1]Forensic Toxicology Laboratory, Department of Pathology and Laboratory Medicine, Albany Medical Center Hospital and College, Albany, NY; [2]Clinical and Forensic Toxicology Laboratory, National Toxicology Center, Schuylerville, NY; [3]Waters Corporation, Beverly, MA; [4]Waters, Wilmslow, UK*

ThP 726 **Increasing Sample Throughput for Detecting Drugs of Abuse and Metabolites in Urine by UHPLC-MS/MS for Forensic Toxicology**; Kevin J. McHale[1]; Kerry M Hassell[2]; *[1]Thermo Fisher, Somerset, NJ; [2]Thermo Fisher Scientific, Somerset, NJ*

ThP 727 **The Application of Data Independent Acquisition Techniques for Identifying Established and Emerging Psychoactive Substances in Clinical Samples**; Michael Dunn[1]; Margaret Knight[1]; Clair Roper[1]; Simon Hill[1]; Simon Thomas[1]; Peter Blain[1]; *[1]Medical Toxicology Centre, Newcastle University, Newcastle upon Tyne, UK*

ThP 728 **Meconium Targeted Drug Screening in 9 Seconds per Sample Using Laser Diode Thermal Desorption Mass Spectrometry (LDTD-MS/MS)**; Serge Auger[1]; Stephanie J. Marin[2]; Gwendolyn A McMillin[2, 3]; Alex Birsan[1]; Jean Lacoursière[1]; Pierre Picard[1]; *[1]Phytronix Technologies, Inc. Quebec, Canada; [2]ARUP Institute for Clinical and Experimental Pathology, Salt Lake City, UT; [3]University of Utah, Department of Pathology, Salt Lake City, UT*

ThP 729 **Ultra-Fast Quantification of Antidepressants in Urine at 9 Seconds per Sample using LDTD-MS/MS**; Alex Birsan[1]; Annie-Claude Bolduc[2]; Serge Auger[1]; Jean Lacoursière[1]; Pierre Picard[1]; *[1]Phytronix Technologies, Inc. Quebec, Canada; [2]Université Laval, Québec, Canada*

ThP 730 **A Rapid Quantification of Phenobarbital in Urine by Dilute and Shoot-Flow Injection MS/MS Method**; ravali alagandula; *Cleveland, OH*

ThP 731 **Toxicological General Unknown Screening (GUS) by Triple Quadrupole LCMS/MS with High Sensitivity Product Ion Scan Library Identification**; Alan Barnes[1]; Tiphaine Robin[2]; John Warrander[1]; Neil Loftus[1]; Pierre Marquet[2]; Sylvain Dulaurent[2]; Franck Saint-Marcoux[2]; *[1]Shimadzu, Manchester, UK; [2]CHU Limoges, Limoges, France*

ThP 732 **Characterization of Aerosol Exposure, Metabolism and Pharmacokinetics for Toxicological Assessment using *in vitro* Organotypical Airway Models**; Arno Knorr[1]; Quentin Dutertre[1]; Mounir Rhouma[1]; Elyette Martin[1]; Martin Almstetter[1]; Shoaib Majeed[1]; Carole Mathis[1]; Stefan Frentzel[1]; Mark Bentley[1]; Julia Hoeng[1]; Patrick Vanscheeuwijck[1]; Manuel C. Peitsch[1]; *[1]Philip Morris International Research & Development, Neuchâtel, Switzerland*

ThP 733 **Analysis of Deuterated Phenanthrene Tetraols and Phenanthrene Phenols in Human Urine by Gas Chromatography-Tandem Mass Spectrometry**; Viviana Paiano[1]; Steven Carmella[1]; Jon Hochalter[1]; Stephen Hecht[1]; *[1]University of Minnesota, Minneapolis, MN*

ThP 734 **Data-independent Mass Spectrometry to Assess Secondhand Cigarette Smoke Exposure Biomarkers**; Pretal P Muldoon[1]; Jillian E Stafflinger[1]; Andrew K Ottens[1]; *[1]Dept. Anatomy and Neurobiology, Virginia Commonwealth University, Richmond, VA*

ThP 735 **Dilute-and-Shoot Method for Determination of Tobacco-Specific Nitrosamines (TSNAs) in Tobacco and E-Cigarette Products by UPLC-MS/MS**; Narendra Meruva[1]; Xiaojie Tan[2]; Dimple Shah[1]; ADAM LADAK[1]; Larissa Fenn[1]; *[1]Waters, Milford, MA; [2]Waters Coorporation, Shanghai, China*

ThP 736 **Determination of PON in Tobacco and Tobacco Products using LC/MS/MS**; Huihua Ji[1]; Ying Wu[1]; Lowell Bush[2]; *[1]Center for Tobacco Reference Products, University of Kentucky, Lexington, KY; [2]Department of Plant and Soil Science, University of Kentucky, Lexington, KY*

ThP 737 **A High Resolution/Accurate Mass (HRAM) Data-Dependent MS3 Neutral Loss Screening and Classification Methodology for Aldehydes in Saliva**; Romel P Dator[1]; Peter W Villalta[1]; Andrea Carra'[1]; Silvia Balbo[1]; *[1]Masonic Cancer Center, University of Minnesota, Minneapolis, MN*

ThP 738 **Qualitative Assessment of Cyanotoxin Co-Occurrence using Time-Of-Flight Mass Spectrometry**; I-Shuo Huang[1]; Marwah Ashok[2]; Marwah Padma[3]; Zimba Paul[1, 3]; *[1]Texas A&M University, Corpus Christi, TX; [2]Corpus Christi, TX; [3]Center for Coastal Studies, Corpus Christi, TX*

ThP 739 **Structural Characterization and Mutagenicity of the Aflatoxin B2a-Amino Acid Adduct as a Potential Detoxification Product**; Blake Rushing[1]; Mustafa Selim[1]; *[1]East Carolina University, Greenville, NC*

ThP 740 **Ultrasensitive Measurements of Endogenous and Exogenous Formaldehyde-Induced DNA-Protein Crosslinks using Nano-LC-ESI-MS/MS**; Yongquan Lai[1]; James A Swenberg[1]; *[1]University of North Carolina at Chapel Hill, Chapel Hill, NC*

ThP 741 **Targeting the Endocannabinoid System to Enhance Innate Immunity Using Chemoproteomics**; Jung Hwa Lee; *Mississippi State University, Mississippi State, MS*

ThP 742 **Effect of Iron Supplementation on Lead Exposure in Liver of Rats: A Proteomic Analysis**; Mileni Silva Fernandes[1]; Aline Lima Leite[1, 2]; Lucas Ferreira Almeida[3]; Fernanda Zucki[2]; Camila Peres-Buzalaf[4]; Marília Afonso Rabelo Buzalaf[2]; *[1]Federal University of São Carlos, São Carlos, SP, Brazil, São Carlos, SP-Brazil; [2]Bauru Dental School, Bauru, SP-Brazil; [3]Faculty of Medicine of Ribeirão Preto, Ribeirão Preto, SP-Brazil; [4]Center on Health Sciences, USC, Bauru, SP-Brazil*

ThP 743 **Non-targeted Identification of the Protein Targets of Reactive Drug Metabolites using Stable Isotopic Labeling and High-Resolution Mass Spectrometry**; Michael G. Leeming[1]; William A. Donald[2]; Richard A.J. O'Hair[1]; *[1]The University of Melbourne, Melbourne, Australia; [2]The University of New South Wales, Sydney, Australia*

ThP 744 **Targeted Proteomic Analysis of Abrin**; Alena Myslivcova Fucikova[1]; Jana Klimentova[1]; Miloslava Duracova[1]; Jiri Dresler[2]; Zuzana Krocova[1]; *[1]University of Defence, Hradec Kralove, CZ; [2]Central Military Health Institute, Prague, CZ*

ThP 745 **Arsenite Binds to the PHD-type Zinc Finger Domain of FANCL E3 Ubiquitin Ligase and Inhibits DNA Interstrand Crosslink Repair**; Ji Jiang[1]; Yinsheng Wang[1]; *[1]University of California - Riverside, Riverside, CA*

ThP 746 **High Throughput Pharmacovigilance Screening of Nutraceuticals and Alternative Medicines**; Elly Crighton[1,2]; Joel Gummer[1, 2, 3]; Oliver Jones[4]; Garth Maker[1,2]; Ian Mullaney[1]; Megan Coghlan[5]; Michael Bunce[5]; Claire Hoban[6]; Ian Musgrave[6]; Roger Byard[6]; Robert Trengove[7]; *[1]School of Veterinary and Life Sciences, Murdoch University, WA, Australia, Perth, Australia; [2]Separation Science and Metabolomics Laboratory, Murdoch University, Perth, Australia; [3]Metabolomics Australia, WA Node, Perth, Australia; [4]RMIT University, School of Science, Melbourne, Australia; [5]Curtin University, Perth, Australia; [6]The University of Adelaide, Adelaide, Australia; [7]Murdoch University, Murdoch , WA*

ThP 747 **MALDI Imaging MS in Neurotoxicology:Proteomic Biomarker Discovery in the Rat Brain with Jet Fuel Inhalation Exposures**; Lining Qi[1]; Pavel Shiyanov[1]; Karen Mumy[2]; Camilla Mauzy[1]; *[1]711HPW/RHDJ, US Air Force Research Lab, WPAFB, OH; [2]Naval Medical Research Unit-Dayton, WPAFB, OH*

ThP 748 **Integrated Proteomic Analysis of Human Airway Epithelial Cells after Exposure to Diacetyl Vapor**; Matthew Foster[1]; William Gwinn[2]; Francince kelly[3]; David Brass[3]; Ashlee Valente[3]; Will J Thompson[3]; Daniel Morgan[4]; Arthur Moseley[3]; Scott Palmer[3]; *[1]Duke University, Durham, NC; [2]NIEHS, RTP, NC; [3]Duke University Medical Center, Durham, NC; [4]NIEHS / NIH, RTP, NC*

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INDEX OF AUTHORS

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