



Welcome to the 67th ASMS Conference on Mass Spectrometry and Allied Topics. Conference program activities and exhibit booths are in the Georgia World Congress Center. Corporate Member hospitality suites are located in the Omni CNN Hotel.

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PROGRAM HIGHLIGHTS

REGISTRATION, is open 10:00 am - 8:00 pm on Sunday and 7:30 am - 5:00 pm Monday - Thursday, Building B Main Lobby

ATTENTION UNDERGRADUATE STUDENTS AND FIRST TIME (AT ASMS) GRADUATE STUDENTS

4:00 - 4:45 pm, Sunday, B302-305, Level Three
Plan Your Strategy: What to See and Do at ASMS

TUTORIALS

SUNDAY TUTORIAL SESSION I, 5:00 - 6:30 PM

Murphy Ballroom, Level Five



5:00 - 5:45 pm
Lipidomics
Stephen Blanksby
Queensland Univ. of Technology
& **Gavin Reid**
University of Melbourne



5:45 - 6:30 pm
Targeted Imaging

Enrico Davoli
Mario Negri Institute

SUNDAY TUTORIAL SESSION II, 5:00 - 6:30 PM

B302-305, Level Three



5:00 - 5:45 pm
Native Mass Spectrometry

Michal Sharon
Weizmann Institute



5:45 - 6:30 pm
Data Independent Acquisition

Birgit Schilling
The Buck Institute

PLENARY SESSIONS

SUNDAY CONFERENCE OPENING, 6:45 - 7:45 PM

Murphy Ballroom, Level Five



Welcome

Susan Richardson
University of South Carolina
ASMS Vice President for Programs



Transitioning the World Energy for All Purposes to Stable Electricity Powered by 100% Wind, Water, and Sunlight

Mark Z. Jacobson
Stanford University

SUNDAY WELCOME RECEPTION, 7:45 - 9:00 PM

Poster/Exhibit Hall, Hall B-2 & B-3, Level One.
Conference name badge is required.

MONDAY AWARD LECTURE, 4:45 - 5:30 PM

Murphy Ballroom, Level Five



John B. Fenn Award for a Distinguished Contribution in Mass Spectrometry

John R. Yates
The Scripps Research Institute

TUESDAY AWARD LECTURE, 4:45 - 5:30 PM

Murphy Ballroom, Level Five



Biemann Medal

Sarah Trimpin
Wayne State University

THURSDAY PLENARY SESSION, 4:45 - 5:30 PM

Murphy Ballroom, Level Five



Chemistry of Food and Soft Drinks

Lilly D'Angelo
Global Food & Beverage Technology Associates

THURSDAY CLOSING EVENT AT THE GEORGIA AQUARIUM, 6:30 - 9:30 PM, \$40/PERSON



Tickets must be purchased in advance by Monday 12 noon. Join us for an enchanting evening at the Georgia Aquarium. Dinner buffets close at 8:00 pm, dessert available until close. Ticket includes aquarium entry for our private event, dinner buffet and one drink ticket for soda, beer, or wine. Cash bars available until close



ORAL SESSIONS are 8:30 - 10:30 am and 2:30 - 4:30 pm Monday through Thursday.

Building B – Level Five

Session A (MOA, TOA, WOA, ThOA)..... Murphy Ballroom

Building B – Level Four

Session B (MOB, TOB, WOB, ThOB) B401-402

Session C (MOC, TOC, WOC, ThOC) B405-407

Building B – Level Three

Session D (MOD, TOD, WOD, ThOD) B302-305

Session E (MOE, TOE, WOE, ThOE) B308-309

Session F (MOF, TOF, WOF, ThOF)..... B312-314

Building A – Level Four

Session G (MOG, TOG, WOG, ThOG) Auditorium

Session H (MOH, TOH, WOH, ThOH) A411-412

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 ready room is B301, Building B, Level Three. 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 Welcome Reception 7:45 pm - 9:00 pm

Monday - Wednesday 7:00 am - 8:00 pm

Thursday 7:00 am - 2:30 pm

POSTER SET-UP is 7:00 - 8:00 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.

HISTORY POSTERS are on display all week in Building B, Main Lobby.

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. The following was new in 2018 (and may be new to some presenters for 2019) and allows for a one-hour non-overlapping lunch break. All presenters are now scheduled for 3 hours (authors welcome to attend the full four hours).

Odd-number posters present:

10:30 - 11:30 am PLUS 12:30 - 2:30 pm

Even-number posters present:

10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

Poster Pick-Me-Up Snacks served at 1:30 pm.

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 be removed between 7:00 - 8:00 pm on Monday, Tuesday and Wednesday. Thursday posters should be removed between 2:30 - 3:00 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 on Level Three of Building A.

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 AND INTERNET STATIONS are available 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 slides will be printed to PDF and used as proceedings submission for speakers who fail to submit on their own.**

WEBCASTING includes tutorial lectures, plenary lectures, and oral sessions. Webcasts will be available to conference attendees for four months after the conference. ASMS does not retain rights to material included in webcasts.

CORPORATE HOSPITALITY SUITES may open 8:00 – 11:00 pm, Monday through Wednesday. Suites are located in the **Omni CNN Hotel.**

CAREER CENTER is located in B211-212. 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 booths are available for onsite reservations (one-day advance reservation is recommended.)

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 welcome reception. The badge does not gain entrance to oral sessions or the Poster/Exhibit Hall.

GENDER NEUTRAL RESTROOMS are designated in Building A and B, level three.

MAMAVA/LACTATION PODS AND MOTHER'S LOUNGE

The center is equipped with two Mamava (lactation) pods, one in Building A (outside room A411) and one in Building B (across from B405). These pods are free for attendees to use. Meeting room B201 is also available for mothers to use.



Don't Miss these Resources in the Poster/Exhibit Hall



- Learn from experts – designated times to come, ask questions, and get advice.
- Designated programs and debates to illuminate specific topics and tools.
- Look for schedule details on the hub's wiki (linked to www.asms.org) and entry sign at the conference.



Meet with representatives from various funding agencies. Appointment sign up sheets will be posted on 'office' entry sign. Attendees are encouraged to take advantage of this valuable resource while at the conference.

CONFERENCE REGULATIONS

Please review these policies which are intended to assure the comfort and privacy of all conference participants.

Name badge is required for all conference sessions, including the Poster/Exhibit Hall and Career Center, and off site events such as the hospitality suites and closing event (ticket required).

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 are permitted in the poster hall, and parents/caregivers are asked to keep in mind safety and well-being of children and conference attendees, taking care to avoid crowded spaces. Strollers are prohibited in the 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).

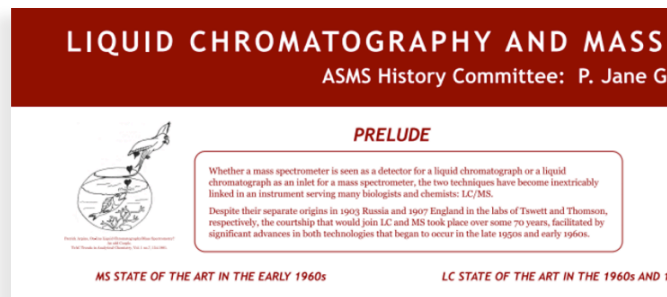
Corporate hospitality suites may be used during the daytime hours of 8:00 am - 8:00 pm for one-on-one and small group meetings (no more than 25 persons per organization) by appointment only (no walk-ins). No music, programs, seminars, or refreshments may be included in these private, business meetings.

Corporate or institutional logos on slides or posters may appear only one time in the presentation.



2019 CONFERENCE HISTORY POSTER DISPLAY

Similar to previous years, the History Committee will again display a selection of posters that describe the historical development of our field and our Society with focus on key figures, pioneering instrument designs, and innovative applications of technology. We'll also continue the Vendor History theme initiated in 2018. This year's display will include vendor-created posters from last year plus two new ones: a second contribution from Waters highlighting the development of their quadrupole mass analyzers through the line of companies VG/Fisons/Micromass/Waters and one from Agilent describing quadrupole instrument development at Hewlett-Packard/Agilent. Finally, we'll celebrate ASMS's 60th birthday by re-displaying the anniversary decade posters for the years 1953-1992 and extending the series with two new additions: the 1993-2002 decade, "Biology Meets Mass Spectrometry," and the succeeding 2003-2012 decade, "The Era of 'Omics." Plan to spend some time with us at the History Poster Display in the main lobby/registration area!



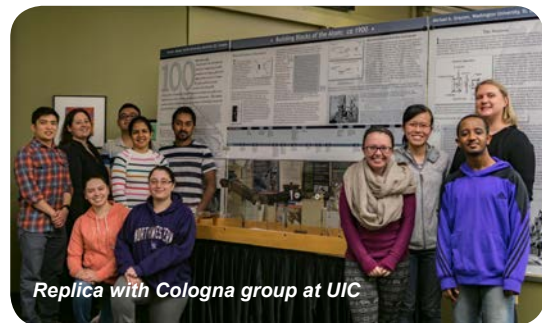
NEW MEMBERS OF THE HISTORY COMMITTEE

The History Committee welcomed two new members in 2018: Phil Price, a long-time ASTM E-14 and ASMS member whose work for the Society actively shaped the history of Standards and Nomenclature, and Glen Jackson, ASMS member since 2001 and a Fellow of the American Academy of Forensic Sciences who has written extensively on the history of Forensics Mass Spectrometry.

New History Committee members Phil Price (left) and Glen Jackson (right)

HISTORIC INSTRUMENT REPLICAS

The Replica Display has a new home! After an 18-month stay at the University of Illinois at Chicago, jointly hosted by Professors Stephanie Cologna and Laura Sanchez, the Replica Display has moved to the University of Texas at Austin under the auspices of Professor Livia Eberlin. Read about the genesis of the Replica project, follow the display's itinerary, and learn how to add your institution to the list of future venues on its newly-created webpage (<https://www.asms.org/about/history/historical-instruments-replica>).



Replica with Cologna group at UIC

IN MEMORIAM

The ASMS website now contains links to JASMS articles that celebrate the lives of deceased ASMS members. Check out <https://www.asms.org/publications/journal-of-the-american-society-for-mass-spectrometry-group/obituaries-from-jasms> for remembrances of scientists whose work was seminal to the development of our field.

SCIENCE HISTORY INSTITUTE

ASMS continues to partner with the Science History Institute (formerly Chemical Heritage Foundation) to preserve the Society's history. As Oral Histories of ASMS members are completed and published, links to the full interviews are added to the History web page. Soon to come at <https://www.asms.org/about/history/oral-history-project>: Ron Macfarlane, David Sparkman and Jack Watson! The Institute also provides archival storage for ASMS ephemera, both for the Society and for its members. If you have documents of historical importance you'd like to donate – like meeting programs, instrument manuals, photographs or other artifacts – please contact ASMS Archivist/Historian Jane Gale (jane.pjgale@gmail.com).





CONFERENCE HOTELS

- 1** AC Hotel by Marriott Downtown Tel. (404) 524-5555
- 2** Aloft Atlanta Downtown Tel. (678) 515-0300
- 3** Atlanta Marriott Marquis Tel. (404) 521-0000
- 4** Embassy Suites Atlanta Tel. (404) 223-2300
- 5** Omni Atlanta Hotel at CNN Center Tel. (404) 659-0000
- 6** Westin Peachtree Plaza Tel. (404) 659-1400





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to these members who were elected to the ASMS Board

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<i>Biotherapeutics</i>	Andrew W. Dawdy Hao Zhang
<i>Career Development</i>	Lucinda Hittle Charles Veltri
<i>Clinical Chemistry</i>	Don Chace Candice Ulmer
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<i>Flavor, Fragrance and Foodstuff</i>	Melanie Downs James Redwine
<i>Forensics & Homeland Security</i>	Brittany Casey Chris Mulligan
<i>FTMS</i>	Melinda McFarland Matthew B. Renfrow
<i>Fundamentals</i>	Christian Bleiholder Alexandre Shvartsburg
<i>H/D Exchange, Covalent Labeling & Cross Linking</i>	Jim Bruce Kasper D. Rand
<i>Imaging MS</i>	Peggi Angel Martina Marchetti-Deschmann
<i>Ion Mobility MS</i>	Brian Clowers Valerie Gabelica
<i>Ion Trap MS</i>	Glen Jackson Desmond Kaplan
<i>LC/MS Related Topics</i>	Eric Soderblom Will Thompson
<i>Lipids & Lipodomics</i>	John A. Bowden Kim Ekroos
<i>Metabolomics</i>	Gary Patti Jon Sobus
<i>Metal Ion Coordination Chemistry</i>	Franklin Leach Nicolas Polfer
<i>Oligonucleotides & Nucleic Acids</i>	Samuel Wainhaus Laixin Wang
<i>Pharmaceuticals</i>	Andrew W. Dawdy Richard Rogers
<i>Photoionization MS</i>	Sven Ehlert Matthias Lorenz Eleanor Riches

<i>Polymeric Materials</i>	Jessica Hoskins Christina Mastromatteo
<i>Regulated Bioanalysis</i>	Fabio Garofolo Jian Wang
<i>Top-Down Proteomics</i>	Frederik Lermyte Nicholas Young
<i>Undergraduate Research in MS</i>	Jay G. Forsythe Christine Hughey
<i>Young Mass Spectrometrists</i>	Veronica Anania Sharon Pitteri

COMMITTEES

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<i>Publications</i>	Amanda B. Hummon, Chair Theodore Alexandrov Peter Nemes Olga Ovchinnikova Candice Ulmer Joseph Loo, <i>ex officio</i>
<i>Sanibel Conference</i>	Melinda McFarland, Chair Leslie Hicks Shi Stone Kevin Bateman (ASMS Board Rep.)



JOHN B. FENN AWARD FOR A DISTINGUISHED CONTRIBUTION IN MASS SPECTROMETRY

2019 RECIPIENT: **JOHN R. YATES III**

AWARD LECTURE: 4:45 PM, MONDAY, MURPHY BALLROOM, BUILDING B, LEVEL 5



The ASMS Award for Distinguished Contribution in Mass Spectrometry honors the memory of John B. Fenn who shared the 2002 Nobel Prize for the development of electrospray ionization. John joined ASMS in 1986 and remained an active member until his passing in 2010. The award is conferred at the ASMS Annual Conference with the presentation of a \$10,000 cash award, a recognition plaque, and the award lecture.

Dr. John R. Yates III is the recipient of the 2019 ASMS John B. Fenn Award for a Distinguished Contribution in Mass Spectrometry, for development of automated, large-scale interpretation of peptide tandem mass spectral data. Dr. Yates' SEQUEST algorithm laid a critical foundation for the field of proteomics and has enhanced the accuracy and effectiveness of mass spectrometry to understand important biological and clinical questions.

Subsequent software developments continue to empower molecular and cellular biology research, including peptide and protein quantitation, identification of posttranslational modifications, and the use of DNA sequences to enable proteogenomic methods. Dr. Yates also enabled large-scale studies to identify the components of protein complexes in single celled organisms and mammalian cells. Proteomics is now practiced by thousands of researchers all over the world to study proteins in almost every organelle in prokaryotic and eukaryotic cells. The comprehensive analysis of cells and tissues is now routinely used to understand differences between normal and disease states.

Dr. Yates is Professor, Department of Molecular Medicine, The Scripps Research Institute.

AL YERGEY MS SCIENTIST AWARD

2019 RECIPIENT: **JEFFERY SHABANOWITZ**

AWARD PRESENTATION: 4:45 PM, MONDAY, MURPHY BALLROOM, BUILDING B, LEVEL 5



The Al Yergey Mass Spectrometry Scientist Award is sponsored by ASMS to recognize dedication and significant contributions to mass spectrometry-based science by "unsung heroes." This award is named in memory of Al Yergey a well-respected scientist who was known as a dedicated mentor.

Dr. Jeffrey Shabanowitz is the inaugural recipient of the Al Yergey MS Scientist Award. For more than forty years Dr. Shabanowitz has worked with Professor Donald Hunt at the University of Virginia, where he co-authored more than 330 peer-reviewed scientific papers and is co-inventor on ten issued patents. He played a major role in development of peptide sequence analysis by tandem mass spectrometry. The methods and instrumentation he helped to develop underpin the field of proteomics, and have led to major breakthroughs, especially in immunology and epigenetics research. He has also been a valued mentor to dozens of graduate students, postdocs, and visiting scientists. Dr. Shabanowitz is Principal Scientist in the Hunt Laboratory at the University of Virginia

BIEMANN MEDAL

2019 RECIPIENT: **SARAH TRIMPIN**

AWARD LECTURE: 4:45 PM, TUESDAY, MURPHY BALLROOM, BUILDING B, LEVEL 5



The Biemann Medal is awarded to an individual early in his or her career to recognize significant achievement in basic or applied mass spectrometry. The Medal is conferred at the ASMS Annual Conference with the presentation of a \$5,000 cash award, a recognition plaque, and the award lecture.

Dr. Sarah Trimpin is the recipient of the 2019 Biemann Medal for discovery and development of novel ionization processes. Dr. Trimpin's unusual observation of highly charged protein ions in an atmospheric pressure MALDI experiment led to her discovery that ionization occurs simply by passing compounds through the inlet of a mass spectrometer. She demonstrated that this simple approach achieves sensitivity comparable with, and frequently better than, electrospray or MALDI.

Through fundamental studies, Dr. Trimpin discovered solid matrices that produce highly charged ions upon laser ablation using MALDI ion sources. Even more astonishing is her discovery of matrix compounds that spontaneously produce multiply charged ions when exposed to vacuum (termed matrix-assisted ionization, MAI). No heat, nebulizing gases, laser, or voltage is required and exceptionally low chemical background is achieved for a variety of compounds, including proteins at least as large as bovine serum albumin (66 kDa). She has now discovered more than forty matrices that spontaneously produce analyte ions. Her work has been recognized by numerous awards and has led to commercialization.

Dr. Trimpin is Professor of Chemistry at Wayne State University.



ASMS AWARDS

2019 RESEARCH AWARDS

AWARD PRESENTATIONS: 4:45 PM, TUESDAY, MURPHY BALLROOM, BUILDING B, LEVEL 5

Research awards promote the research of academic scientists within the first four years of joining the tenure track or research faculty of a North American University at the time the award is conferred. The awards, in the amount of \$35,000 each, are fully supported by Bruker, Thermo Fisher Scientific, and Waters Corporation.

Sponsored by
BRUKER



James F. Davies
University of California, Riverside

Sponsored by
THERMO FISHER SCIENTIFIC



Nicolas L. Young
Baylor College of Medicine

Sponsored by
WATERS CORPORATION



Eleanor Browne
University of Colorado, Boulder

2019 PRIMARILY UNDERGRADUATE INSTITUTION RESEARCH AWARD

AWARD PRESENTATIONS: 4:45 PM, TUESDAY, MURPHY BALLROOM, BUILDING B, LEVEL 5

SPONSORED BY **AGILENT TECHNOLOGIES**

This award promotes academic research in mass spectrometry by faculty members and their students at primarily undergraduate institutions (PUIs). The award of \$20,000 is made to the recipient's institution on behalf of the recipient's research.

Callie Cole
Fort Lewis College



RON HITES AWARD FOR OUTSTANDING RESEARCH PUBLICATION IN JASMS

AWARD PRESENTATIONS: ASMS MEETING, 4:45 PM, WEDNESDAY, B302-305, LEVEL 3



The Ron Hites Award recognizes an outstanding publication of original research based on innovative aspects, technical and presentation quality, and likely stimulation of future research or 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 certificates.

The 2019 Ron Hites Award recognizes Dr. Julia Laskin, Purdue University and her co-authors for their paper **Towards High-Resolution Tissue Imaging Using Nanospray Desorption Electrospray Ionization Mass Spectrometry Coupled to Shear Force Microscopy**; Son N. Nguyen, Ryan L. Sontag, James P. Carson, Richard A. Corley, Charles Ansong, and Julia Laskin; *J. Am. Soc. Mass Spectrom.* (2018) 29:316Y322.



2019 POSTDOCTORAL CAREER DEVELOPMENT AWARDS
AWARD PRESENTATIONS: ASMS MEETING, 4:45 PM, WEDNESDAY, B302-305, LEVEL 3

Up to five awards in the amount of \$5,000 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.



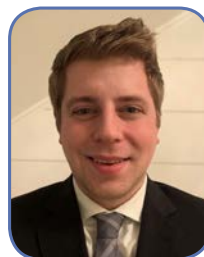
Christopher Ashwood
Medical College of Wisconsin



Josue Baeza
University of Pennsylvania



Gongyu Li
University of Wisconsin-Madison



Jared Kafader
Northwestern University



Nicholas Riley
Stanford University

2019 STUDENT TRAVEL AWARDS
AWARD PRESENTATIONS: ASMS MEETING, 4:45 PM, WEDNESDAY, B302-305, LEVEL 3

ASMS supports up to twenty 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.

GRADUATE STUDENT AWARDS

Molly Blevins, *University of Texas at Austin*
Wanying Cao, *University of Nebraska-Lincoln*
Ming Cheng, *Washington University in St. Louis*
Sean Cleary, *University of Oregon*
Mariel Coradin, *University of Pennsylvania*
Kellen DeLaney, *University of Wisconsin-Madison*
Kristen Fowble, *University at Albany-SUNY*
Naren Gajenthra Kumar, *Virginia Commonwealth University*
Praveen Kumar, *University of Minnesota*
Ting-Hao Kuo, *National Taiwan University*
Chenxi Liu, *University of Arizona*
Elijah McCool, *Michigan State University*
Sibylle Pfammatter, *IRIC-Université de Montréal*
Jaqueline A. Picache, *Vanderbilt University*
Erika Portero, *University of Maryland, College Park*
Marta Sans Escofet, *University of Texas at Austin*
Leah Schaffer, *University of Wisconsin-Madison*
Savannah Snyder, *The University of Akron*
Yang Tang, *Boston University*
Trisha Tucholski, *University of Wisconsin - Madison*

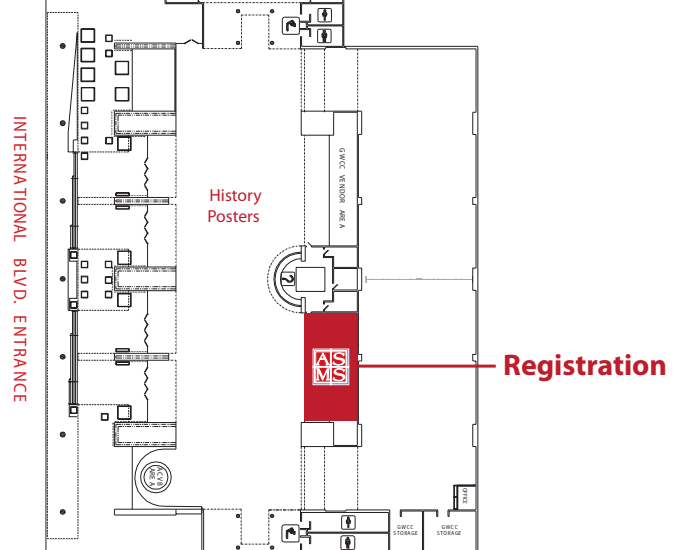
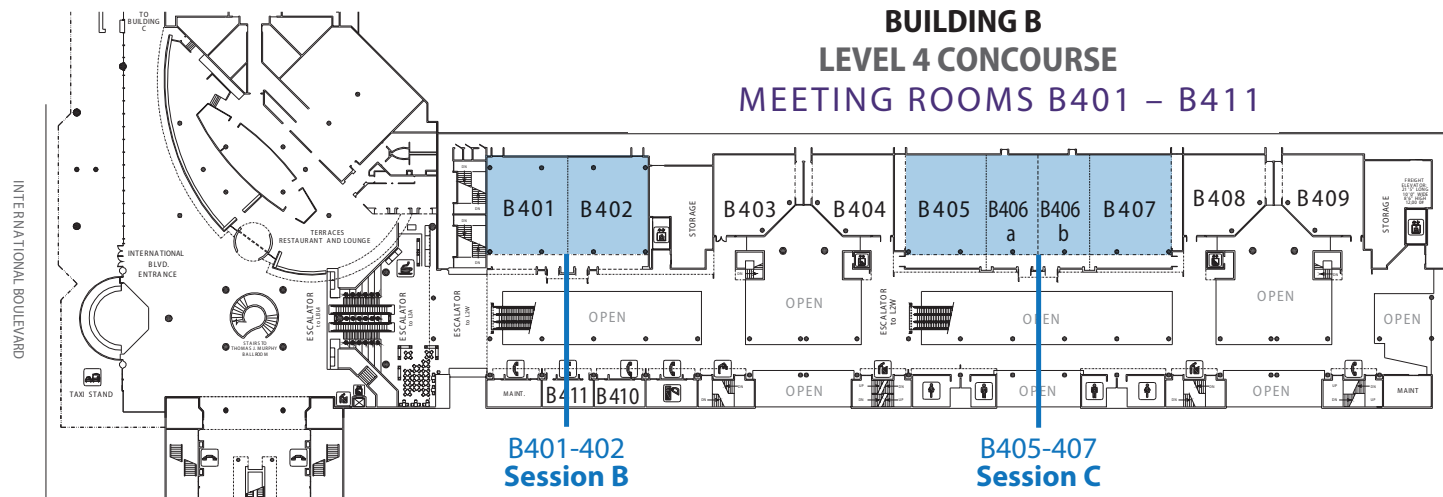
UNDERGRADUATE STUDENT AWARDS

Shelby Beasley, *University of Oklahoma*
Alisha Birk, *Stanford University*
Cameron Davis, *National High Magnetic Field Laboratory*
Richard Dilworth, *University of Florida*
Anna Iacovino, *Duquesne University*
Kaylie Kirkwood, *North Carolina State University*
Abigail Lemmon, *University of Pennsylvania*
Javier Moreno, *Florida International University*
Amanda Wong, *Saint Mary's College of California*
Emily Ziperman, *Baylor University*

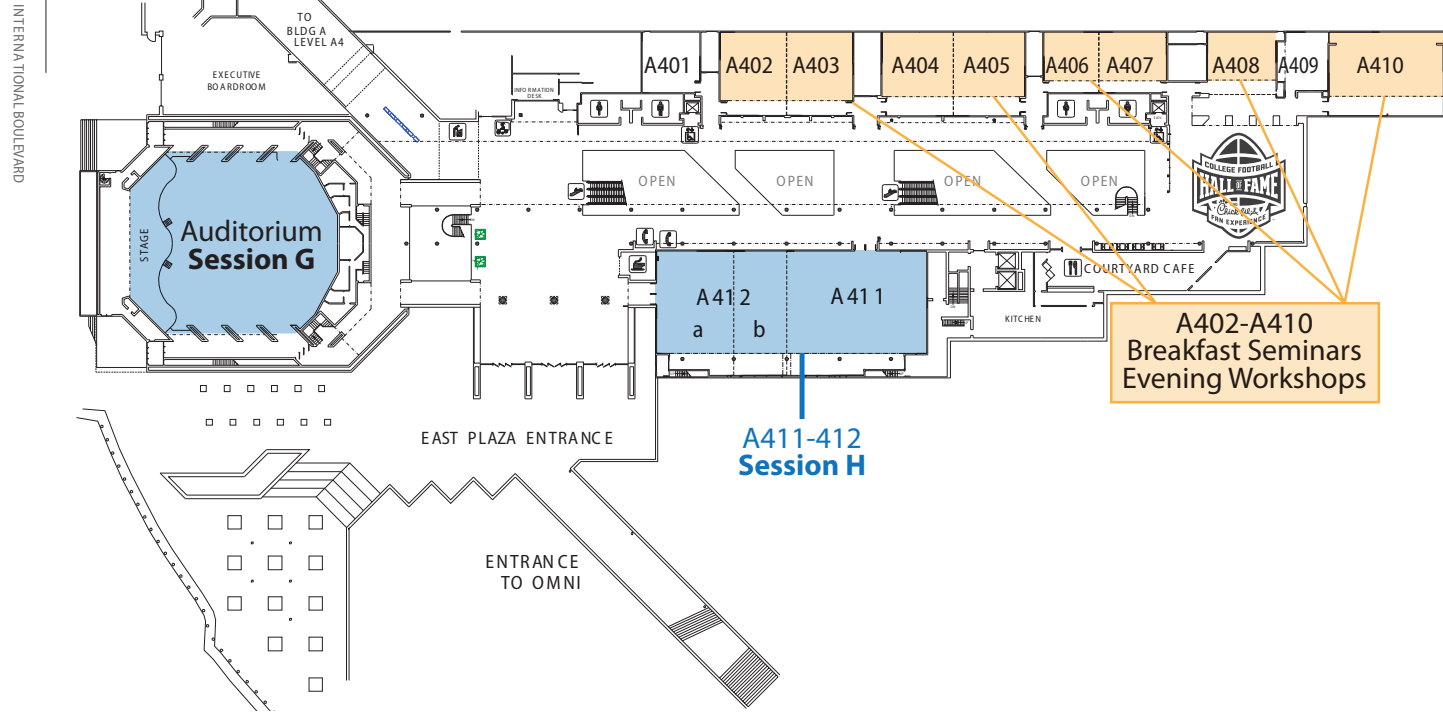


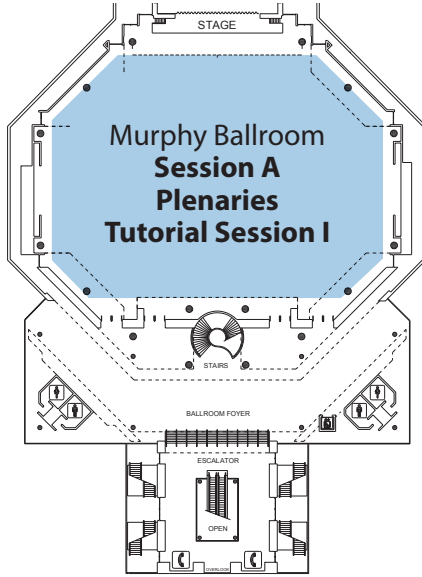
GEORGIA WORLD CONGRESS CENTER

BUILDING B LEVEL 4 CONCOURSE MEETING ROOMS B401 – B411



BUILDING A LEVEL 4 CONCOURSE MEETING ROOMS A402 – A412





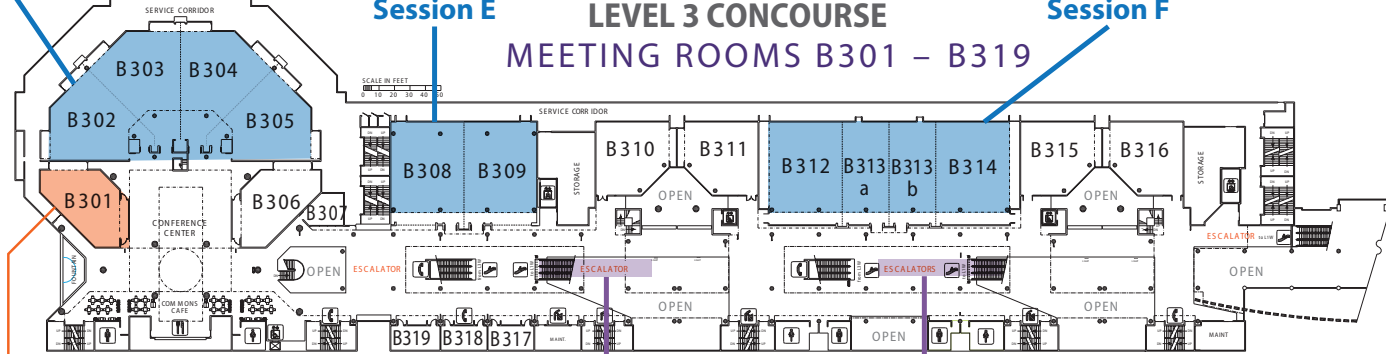
Thomas B. Murphy Ballroom
BUILDING B
Level 5 Concourse

B302-305
Session D
Tutorial Session II
ASMS Meeting

B308-309
Session E

B312-314
Session F

BUILDING B
LEVEL 3 CONCOURSE
MEETING ROOMS B301 – B319

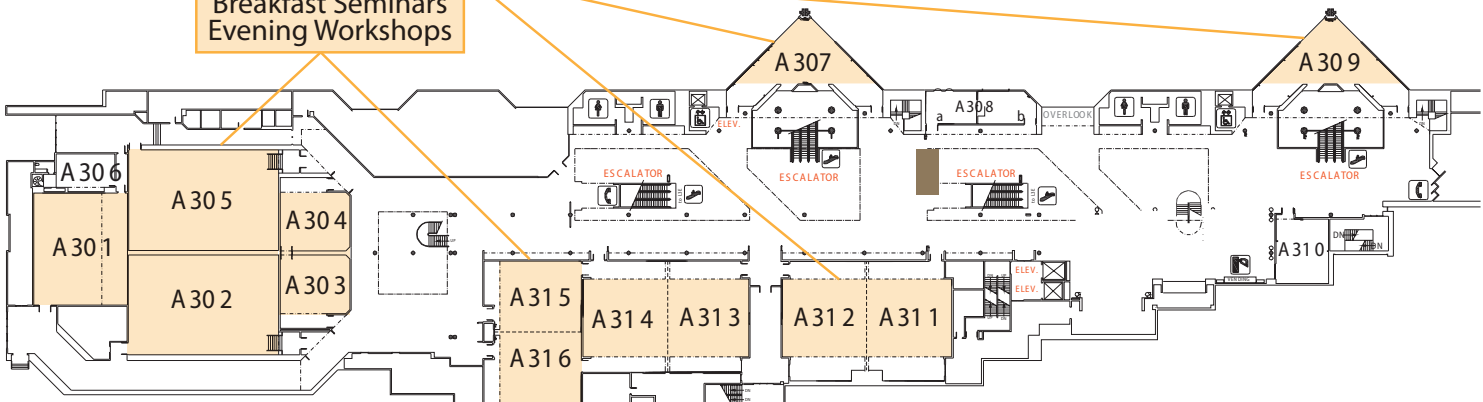


B301
Speaker Ready
Room

Down to:
B200 Meeting Rooms
Career Center
Exhibits / Posters

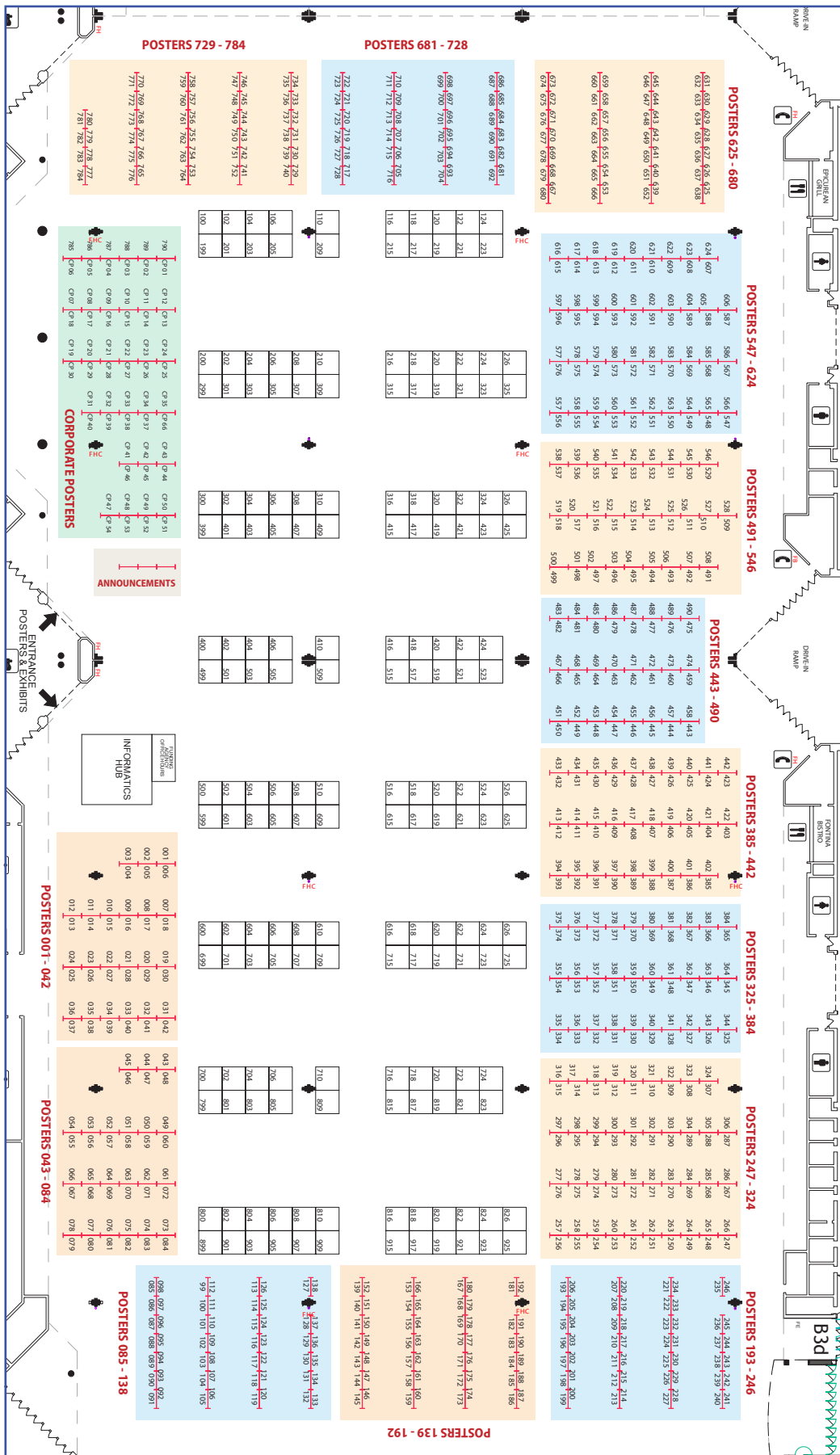
BUILDING A
LEVEL 3 CONCOURSE
MEETING ROOMS A301 – A316

A301-A316
Breakfast Seminars
Evening Workshops



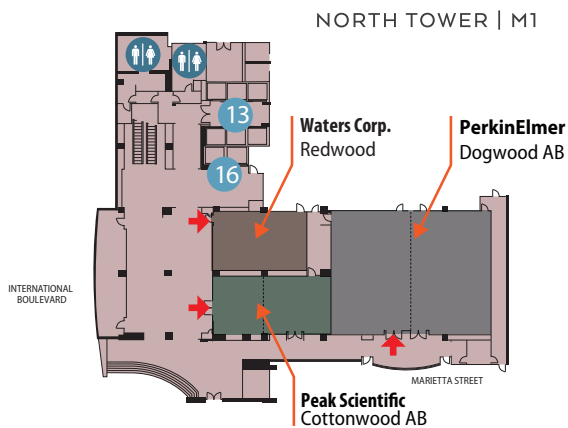
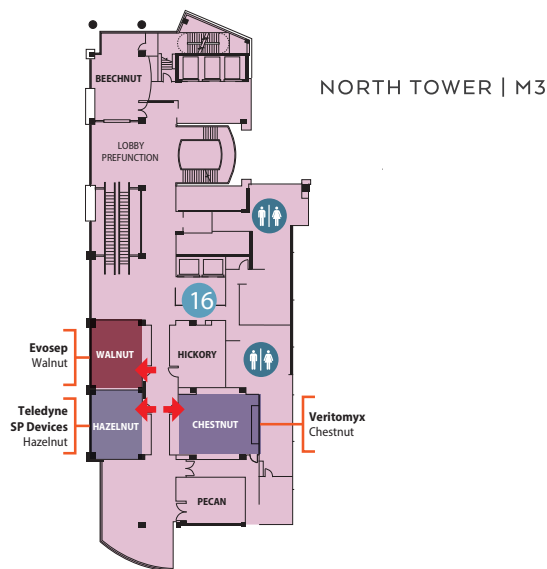
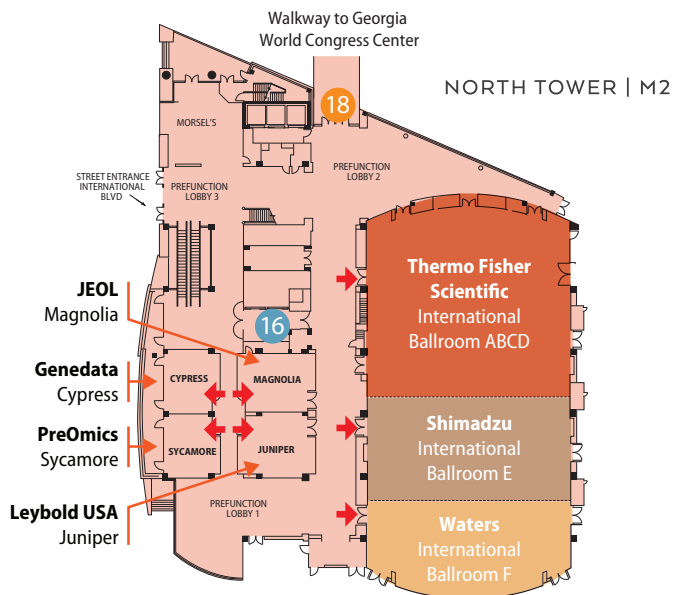
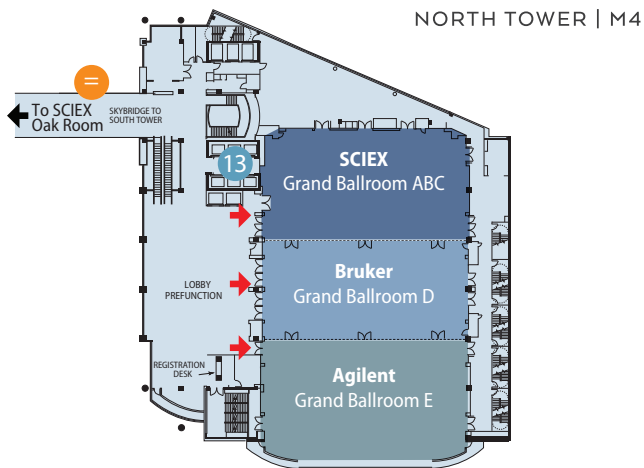


POSTER / EXHIBIT HALL





NORTH TOWER



- ELEVATORS**
- 13 Guest Room Elevators (North Tower M1, M4, N6-28)
 - 16 Meeting Room Elevators (North Tower M1-M4)
- LANDMARKS**
- = Skybridge
 - 18 Walkway to Georgia World Congress Center and College Football Hall of Fame
- RESTROOMS**



CORPORATE MEMBER HIGHLIGHTS

HOSPITALITY SUITES 2019

In Atlanta hospitality suites will continue to embrace the back to basics atmosphere to allow attendees to learn more about the latest and greatest products and services of our Corporate Members while enjoying some fun, food and drink – *and conversation*.

Conference name badges are required for access to all conference activities including hospitality suites.

MEDIA EVENTS (PRESS CONFERENCES)

The following media events are scheduled **Monday, June 3** in the Omni CNN Center Hotel. All press are invited to attend these events.

8:00 - 9:00 am	Shimadzu Scientific Instruments	International Ballroom E
9:30 - 10:30 am	Bruker Daltonics	Grand Ballroom D
11:00 am - 12:00 pm	SCIEX	Grand Ballroom ABC
1:30 - 2:30 pm	Agilent	Grand Ballroom E
3:00 - 4:00 pm	Thermo Fisher Scientific	International Ballroom ABCD
4:30 - 5:30 pm	Waters Corporation	International Ballroom F

BREAKFAST SEMINARS

Breakfast seminars are hosted by Corporate Members at either the Convention Center or the Omni Hotel at CNN Center (inside hospitality suites). Pre-registration (RSVP) is recommended because room set-up and catering are arranged in advance. Please look for Breakfast Seminars page on www.asms.org and in the mobile app to find online registration links.

MONDAY BREAKFASTS	CONVENTION CENTER <i>All breakfast seminars begin at 7:00 am</i>	
	Advanced Chemistry Development (ACD/Labs)	Room A313
	Bruker Daltonics	Room A302
	LECO Corporation	Room A314
	MassTech Inc.	Room A315
	Matrix Science	Room A410
	Pressure BioSciences Inc.	Room A312
	SCIEX (3)	Rooms A404-405, A406-407, A408
	Shimadzu Scientific Instruments	Room A305
	Waters Corporation	Room A402-403
OMNI HOTEL AT CNN CENTER		
Agilent Technologies	Grand Ballroom E	
Thermo Fisher Scientific	International Ballroom ABCD	
Waters Corporation	International Ballroom F	
TUESDAY BREAKFASTS	CONVENTION CENTER <i>All breakfast seminars begin at 7:00 am</i>	
	Biognosys	Room A312
	Biotage	Room A316
	Bruker Daltonics	Room A302
	Evosep	Room A311
	Genedata	Room A315
	LECO Corporation	Room A314
	Matrix Science	Room A410
	New Objective Inc.	Room A313
	SCIEX (3)	Rooms A404-405, A406-407, A408
Shimadzu Scientific Instruments	Room A305	
Waters Corporation	Room A402-403	
OMNI HOTEL AT CNN CENTER		
Agilent Technologies	Grand Ballroom E	
Thermo Fisher Scientific	International Ballroom ABCD	
Waters Corporation	International Ballroom F	

WEDNESDAY BREAKFASTS	CONVENTION CENTER <i>All breakfast seminars begin at 7:00 am</i>	
	Avanti Polar Lipids	Room A410
	Bruker Daltonics	Room A302
	LECO Corporation	Room A314
	MassTech Inc.	Room A315
	New Objective Inc.	Room A313
	SCIEX (3)	Rooms A404-405, A406-407, A408
	Shimadzu Scientific Instruments	Room A305
	OMNI HOTEL AT CNN CENTER	
	Agilent Technologies	Grand Ballroom E
Thermo Fisher Scientific	International Ballroom ABCD	
Waters Corporation	International Ballroom F	
THURSDAY BREAKFASTS	CONVENTION CENTER <i>All breakfast seminars begin at 7:00 am</i>	
	MassTech Inc.	Room A315
	SCIEX (3)	Rooms A404-405, A406-407, A408
	Shimadzu Scientific Instruments	Room A305
	Thermo Fisher Scientific	Room A302



ASMS CORPORATE MEMBERS



Corporate Member	Exhibit Booth	Corporate Poster or Publisher Tabletop	Hospitality Suite at at Omni Hotel at CNN Center	Breakfast Seminar
908 Devices	802	Corporate Poster		
AcroMass Technologies, Inc.	724			
ACS Publications	919			
Adaptas Solutions	216	Corporate Poster		
Advanced Chemistry Development (ACD/Labs)	316	Corporate Poster		Conv Ctr Room A313: Mon 6/3
Advion	718			
Agilent Technologies	400	Corporate Poster	Grand Ballroom E	Omni Grand Ballroom E: Mon-Wed (6/3-6/5);
AIM Research Company	224			
Alliance Pharma	202			
Analytical Sales and Services, Inc.	302	Corporate Poster		
Analytical Scientific Instruments US Inc.	318			
Antec Scientific	505	Corporate Poster		
APEX - Alberta Precision Exchange	222			
Apricot Designs	522	Corporate Poster		
ASTA	617	Corporate Poster		
Avanti Polar Lipids, Inc.	199			Conv Ctr Room A410: Wed 6/5
Baran Bioscience, LLC		Corporate Poster		
BaySpec, Inc.	220			
Beckman Coulter	818			
BGI	703			
Bioanalysis Zone	219			
BioChromato	208	Corporate Poster		
Biocrates Life Sciences AG	706			
Biognosys	517			Conv Ctr Room A312: Tue 6/4
Bioinformatics Solutions Inc.	409	Corporate Poster		
Biotage	526			Conv Ctr Room A316: Tues 6/4
Biotech Support Group	719			
Bruker Daltonics	515	Corporate Poster	Grand Ballroom D	Conv Ctr Room A302: Mon-Wed (6/3-6/5)
Cambridge Isotope Laboratories, Inc.	502			
Cayman Chemical Company	710	Corporate Poster		
Cerno Bioscience	909			
ChemoPower Technology	819			
Coann Technologies	423			
Compare Networks		Publisher's Tabletop		
CovalX	299			
CSS Analytical Co. Inc				
CTC Analytics AG	519			
Ebara Technologies	419	Corporate Poster		
Edwards Vacuum	705			
El-Mul Technologies	301			



ASMS CORPORATE MEMBERS

Corporate Member	Exhibit Booth	Corporate Poster or Publisher Tabletop	Hospitality Suite at at Omni Hotel at CNN Center	Breakfast Seminar
e-MSion, Inc.	424			
Entech Instruments	826			
ESI Source Solutions	116			
Evosep	518		Walnut	Conv Ctr Room A311: Tue 6/4
Extrel CMS	325			
Fasmatech	717			
F-DGSI	803			
Fossil Ion Technology	704	Corporate Poster		
Genedata	510	Corporate Poster	Cypress	Conv Ctr Room A315: Tue 6/4
Genetic Engineering & Biotechnology News		Publisher's Tabletop		
GenNext Technologies, Inc.	816			
Genovis Inc	323	Corporate Poster		
GenTech Scientific, Inc.	317			
GERSTEL, Inc.	716			
GL Sciences	215			
Grenova	509			
Hamamatsu Corporation	110	Corporate Poster		
Hamilton Company	307	Corporate Poster		
Harris Corporation	604	Corporate Poster		
HILICON AB		Corporate Poster		
HTX Technologies, LLC	404			
HVM Technology, Inc.	622			
IDEX Health & Science	402	Corporate Poster		
IMCS	305			
Imtakt USA	406			
Institute for Systems Biology	118			
Intavis, Inc	722			
INTEGRA Biosciences	610			
International Ceramic Engineering	217			
International Equipment Trading Ltd	602			
International Labmate Ltd.		Publisher's Tabletop		
Ion Opticks Pty Ltd	524			
IonBench	226			
IONICON	799	Corporate Poster		
Ionoptika Ltd.	707			
Ionsense Inc.	506	Corporate Poster		
IONTOF GmbH	425			
IP2	801			
IROA Technologies LLC	223			
IsoSciences	421			
JASMS	915			
JEOL USA, Inc.	200		Magnolia	

ASMS CORPORATE MEMBERS



Corporate Member	Exhibit Booth	Corporate Poster or Publisher Tabletop	Hospitality Suite at at Omni Hotel at CNN Center	Breakfast Seminar
JG Finneran Associates, Inc.	310			
Kashiyama USA	804			
Kura Biotech Inc.	620	Corporate Poster		
Lab Tech Support	322			
Larodan AB	221			
LCGC/Spectroscopy	702			
LECO Corporation	401	Corporate Poster		Conv Ctr Room A314: Mon-Wed (6/3-6/5)
Leybold USA	403		Juniper	
Linden CMS GmbH	721			
LNI Swissgas	806	Corporate Poster		
MAC-MOD Analytical	720			
MasCom Technologies	615			
MassTech Inc.	624			Conv Ctr Room A315: Mon 6/3, Wed-Thurs (6/5-6/6)
MathSpec, Inc.		Corporate Poster		
Matrix Science	523			Conv Ctr Room A410: Mon-Tue (6/3-6/4)
Matsusada Precision Inc	815			
McKinley Scientific	605			
MDC Vacuum Products LLC	203			
Merck - DUE				
MetaSci Inc.	817			
Microsaic Systems plc	618	Corporate Poster		
Moeller Medical GmbH	810			
Mott Corporation	405	Corporate Poster		
MPF Products Inc	410			
MRM Proteomics	124			
MS Bioworks	319			
MS Ekspert	306			
MS Noise	626			
MSTM, LLC	601			
Nacalai USA	422	Corporate Poster		
National Institute of Standards and Technology (NIST)	616			
Nest Group, Inc., The		Corporate Poster		
New England Biolabs	901			
New England Peptide Inc.	417			
New Objective Inc.	324			Conv Ctr Room A313: Tue-Wed (6/4-6/5)
Newomics Inc.	606			
Novatia LLC		Corporate Poster		
Omics Informatics LLC	321			
Omni International	415			
OMNI Lab Solutions	418	Corporate Poster		



ASMS CORPORATE MEMBERS

Corporate Member	Exhibit Booth	Corporate Poster or Publisher Tabletop	Hospitality Suite at at Omni Hotel at CNN Center	Breakfast Seminar
Opentrons	905			
Optimize Technologies	700	Corporate Poster		
Parker Hannifin	805			
Peak Scientific	699	Corporate Poster	Cottonwood AB	
PerkinElmer, Inc.	899		Dogwood AB	
Pfeiffer Vacuum	599	Corporate Poster		
Pharmafluidics	303	Corporate Poster		
Phenomenex	508			
Phoenix S&T, Inc.	503			
PHOTONIS	609	Corporate Poster		
Phytronix Technologies	300			
Polymer Factory	520	Corporate Poster		
PreOmics GmbH	407		Sycamore	
Pressure BioSciences Inc.	823			Conv Ctr Room A312: Mon 6/3
Prolab Instruments GmbH	709	Corporate Poster		
Promega Corporation	315			
PROMISE Advanced Proteomics	201	Corporate Poster		
Protein Metrics Inc.	416			
Proteome Software Inc.	725			
PURSPEC Technologies Inc.	218			
Rapid Novor Inc.	723	Corporate Poster		
Ray Biotech	625			
Regeneron Pharmaceuticals	102			
Regis Technologies	808			
Restek Corporation	210			
ReSyn Biosciences	623	Corporate Poster		
SamIn Science Co. Ltd.	309			
Sciencix	106			
SCIEX	500		Grand Ballroom ABC & Oak Room	Conv Ctr Room A404-405: Mon-Thurs (6/3-6/6); Conv Ctr Room A406-407: Mon-Thurs (6/3-6/6); Conv Ctr Room A408: Mon-Thurs (6/3-6/6)
Shimadzu Scientific Instruments, Inc.	499	Corporate Poster	International Ballroom E	Conv Ctr Room A305: Mon-Thurs (6/3-6/6)
Shodex, Showa Denko America	304			
Sierra Analytics, Inc.	206	Corporate Poster		
Silantes GmbH	608			
SoCal Bioinformatics, Inc.	715			
Sound Analytics	701			
Spark Holland	603			
SpectralWorks	504	Corporate Poster		
Spectroswiss	516			
Spellman High Voltage Electronics Corp.	420			



Corporate Member	Exhibit Booth	Corporate Poster or Publisher Tabletop	Hospitality Suite at at Omni Hotel at CNN Center	Breakfast Seminar
SPEX SamplePrep LLC	308			
SunChrom GmbH	209			
Synpeptide Co., Ltd.	607			
Tecan	800			
Teledyne SP Devices		Corporate Poster	Hazelnut	
Teledyne Tekmar	320			
The Analytical Scientist		Publisher's Tabletop		
Thermo Fisher Scientific	600		International Ballroom ABCD	Omni International Ballroom ABCD: Mon-Wed (6/3-6/5); Conv Ctr Room A302: Thurs 6/6
Tosoh Bioscience LLC	326			
Trajan Scientific and Medical	100	Corporate Poster		
Veritomyx	809		Chestnut	
VICI Valco Instruments	204	Corporate Poster		
VRS Recruitment	501			
Waters Corporation	399	Corporate Poster	International Ballroom F & Redwood	Omni International Ballroom F: Mon-Wed (6/3-6/5); Conv Ctr Room A402-403: Mon-Tue (6/3-6/4)
XP Power LLC	205			
Xtreme Power	521			
Zef Scientific, Inc.	621			
Zhejiang Haochuang Biotech Co. Ltd.	619			





PROGRAM ACKNOWLEDGEMENTS

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Susan Richardson
University of South Carolina
Vice President for Programs

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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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Si Wu
Nicolas Young
Hao Zhang

PROGRAM OVERVIEW



SATURDAY

9:00 AM - 4:30 PM	SHORT COURSES
2:00 - 5:00 PM	REGISTRATION , Building B Main Lobby

SUNDAY

9:00 AM - 4:30 PM	SHORT COURSES												
10:00 AM - 8:00 PM	REGISTRATION , Building B Main Lobby												
4:00 - 4:45 PM	ATTENTION! FIRST-TIME GRADUATE STUDENTS AND UNDERGRADUATE STUDENTS Plan your Strategy: What to See and Do at ASMS , B302-305, Level Three												
5:00 - 6:30 PM	<p>TUTORIAL SESSION I, Murphy Ballroom, Bldg. B, Level Five</p> <table border="0"> <tr> <td>5:00 - 5:45 pm Lipidomics</td> <td>5:45 - 6:30 pm Targeted Imaging</td> </tr> <tr> <td>Stephen Blanksby, <i>Queensland U. of Technology</i> & Gavin Reid, <i>University of Melbourne</i></td> <td>Enrico Davoli <i>Mario Negri Institute</i></td> </tr> <tr> <td></td> <td></td> </tr> </table> <p>TUTORIAL SESSION II, B302-305, Level Three</p> <table border="0"> <tr> <td>5:00 - 5:45 pm Native Mass Spectrometry</td> <td>5:45 - 6:30 pm Data Independent Acquisition</td> </tr> <tr> <td>Michal Sharon <i>Weizmann Institute</i></td> <td>Birgit Schilling <i>The Buck Institute</i></td> </tr> <tr> <td></td> <td></td> </tr> </table>	5:00 - 5:45 pm Lipidomics	5:45 - 6:30 pm Targeted Imaging	Stephen Blanksby , <i>Queensland U. of Technology</i> & Gavin Reid , <i>University of Melbourne</i>	Enrico Davoli <i>Mario Negri Institute</i>			5:00 - 5:45 pm Native Mass Spectrometry	5:45 - 6:30 pm Data Independent Acquisition	Michal Sharon <i>Weizmann Institute</i>	Birgit Schilling <i>The Buck Institute</i>		
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5:00 - 5:45 pm Native Mass Spectrometry	5:45 - 6:30 pm Data Independent Acquisition												
Michal Sharon <i>Weizmann Institute</i>	Birgit Schilling <i>The Buck Institute</i>												
													
6:45 - 7:45 PM	<p>CONFERENCE OPENING, Murphy Ballroom, Bldg. B, Level Five</p> <p>Susan Richardson, <i>University of South Carolina</i> ASMS Vice President for Programs</p> <p> 7:00 - 7:45 pm Transitioning the World Energy for All Purposes to Stable Electricity Powered by 100% Wind, Water, and Sunlight</p> <p>Mark Z. Jacobson <i>Stanford University</i></p>												
7:45 - 9:00 PM	WELCOME RECEPTION IN THE POSTER/EXHIBIT HALL Undergraduate Student Poster Competition												



PROGRAM OVERVIEW

MONDAY

7:00 AM	CORPORATE BREAKFAST SEMINARS , Convention Center and Omni CNN Center Hotel
7:30 AM - 5:00 PM	REGISTRATION , Building B Main Lobby
8:30 - 10:30 AM	<p>ORAL SESSIONS</p> <p>MOA am: Cannabis Testing, <i>Murphy Ballroom, Bldg. B, Level Five</i></p> <p>MOB am: Glycopeptides and Glycoproteins, <i>B401-402</i></p> <p>MOC am: Membrane Protein MS, <i>B405-407</i></p> <p>MOD am: Imaging: Instrumentation & Method Development, <i>B302-305</i></p> <p>MOE am: Lipidomics: Targeted and Untargeted, <i>B308-309</i></p> <p>MOF am: Fundamentals: Ion Mobility and MS (In Memory of Al Yergey), <i>B312-314</i></p> <p>MOG am: Instrumentation: Portable and Transportable Mass Spectrometers, <i>Auditorium, Bldg. A</i></p> <p>MOH am: Biomarkers: Qualitative Analysis, <i>A411-412</i></p>
10:30 AM - 2:30 PM	<p>POSTER SESSION AND EXHIBITS, Monday Posters, Poster/Exhibit Hall ground level</p> <p>Odd-number posters present: 10:30 - 11:30 am PLUS 12:30 – 2:30 pm</p> <p>Even-number posters present: 10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm</p> <p>11:30 am - 1:00 pm: Undergraduate students look for reserved tables and free lunch vouchers to Meet the Experts</p>
2:30 - 4:30 PM	<p>ORAL SESSIONS</p> <p>MOA pm: Informatics: Multiomics Integration and Applications, <i>Murphy Ballroom, Bldg. B</i></p> <p>MOB pm: Homeland Security: Chemical/Biological Defense, <i>B401-402</i></p> <p>MOC pm: Food Safety & Chemistry: Foodomics, Allergens, Bacteria, Foods, and Supplements, <i>B405-407</i></p> <p>MOD pm: Therapeutic Proteins, Antibodies, and Antibody/Drug Conjugates, <i>B302-305</i></p> <p>MOE pm: Lipidomics: New MS Technologies and Applications, <i>B308-309</i></p> <p>MOF pm: Biomarkers: Quantitative Analysis, <i>B312-314</i></p> <p>MOG pm: Instrumentation: New Developments in Ionization and Sampling, <i>Auditorium, Bldg. A</i></p> <p>MOH pm: Art, Archaeology, and Paleontology, <i>A411-412</i></p>
4:45 - 5:30 PM	<p>AWARD LECTURE, Murphy Ballroom, Bldg. B, Level Five</p> <p>Award for a Distinguished Contribution in Mass Spectrometry</p> <div style="display: flex; align-items: center;">  <div> <p>John R. Yates III <i>The Scripps Research Institute</i></p> </div> </div>
5:45 - 7:00 PM	<p>WORKSHOPS There are light refreshments in Building A foyers, 5:30 - 5:45 pm.</p> <ol style="list-style-type: none"> 01. High Spatial Resolution 2D and 3D Mass Spectrometry Analysis: Current Trends, <i>A402-403</i> 02. Enhancing MS-Based Glycomics and Glycoproteomics Toolbox: Round-table Discussion, <i>A404-405</i> 03. MassIVE Translation of Public Mass Spectrometry Big Data into Reusable Community Resources, <i>A406-407</i> 04. Mass Spectrometry in the Developing World: Supporting Education and Research, <i>A408</i> 05. Ion Trap Mass Spectrometry: Latest Trends (Ion Trap MS Interest Group), <i>A410</i> 06. FAIMS/DIMS/DMS Technology and its Impact on Current Day MS Analyses, <i>A307</i> 07. Food Safety and Quality Applications: Tools for Putting MS Methods into Practice (Flavor Fragrance & Foodstuff Interest Group), <i>A309</i> 08. Automation for Proteomics Sample Preparation, <i>A311</i> 09. MS Software: Peak Picking - Paramount Practices and Perilous Pitfalls, <i>A312</i> 10. Solid Phase Microextraction Approaches Applied with Mass Spectrometry Techniques, <i>A313</i> 12. LC-MS Jeopardy - I'll Take Increasing Throughput for \$200 (LCMS & Related Topics Interest Group), <i>A315</i> 13. Art and Cultural Heritage: Mass Spec Applications, <i>A316</i> 14. Photoionization (APPI/PI) - Bridging the Gap between Academic and Industrial Research (Photoionization MS Interest Group), <i>A303</i> 15. MS-Based Multi-Attribute Method (MAM): The Future of Biotherapeutic Development Analytics (Biotherapeutics Interest Group), <i>A302</i> 16. MS Career Options: How to Kick Start Your Career (Young Mass Spectrometrists Interest Group), <i>A301</i> 17. Membrane Proteins, Nanodiscs, and Beyond: MS Analysis in Academia and Industry, <i>A305</i> 18. Energy, Petroleum, and Biofuels MS: Targeted Analysis, Fingerprinting and Speciation in Complex Mixtures (Energy Petroleum & Biofuels Interest Group), <i>A304</i>
7:00 - 8:00 PM	DINNER BREAK
AFTER 8:00 PM	CORPORATE HOSPITALITY SUITES , Omni CNN Center Hotel



TUESDAY

7:00 AM	CORPORATE BREAKFAST SEMINARS , Convention Center and Omni CNN Center Hotel
7:30 AM - 5:00 PM	REGISTRATION , Building B Main Lobby
8:30 - 10:30 AM	<p>ORAL SESSIONS</p> <p>TOA am: Informatics: Innovations, <i>Murphy Ballroom, Bldg. B, Level Five</i></p> <p>TOB am: Fundamentals: Photoionization and Photodissociation, <i>B401-402</i></p> <p>TOC am: Native MS in Structural Biology, <i>B405-407</i></p> <p>TOD am: Imaging: Pharmaceuticals, Metabolites, and Lipids, <i>B302-305</i></p> <p>TOE am: Environmental: Emerging Contaminants (In Honor of Ron Hites), <i>B308-309</i></p> <p>TOF am: Protein-Ligand Interactions, <i>B312-314</i></p> <p>TOG am: MS in the QC Lab, <i>Auditorium, Bldg. A</i></p> <p>TOH am: Nucleic Acids and Oligonucleotides, <i>A411-412</i></p>
10:30 AM - 2:30 PM	<p>POSTER SESSION AND EXHIBITS, Tuesday Posters, Poster/Exhibit Hall ground level</p> <p>Odd-number posters present: 10:30 - 11:30 am PLUS 12:30 – 2:30 pm</p> <p>Even-number posters present: 10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm</p>
2:30 - 4:30 PM	<p>ORAL SESSIONS</p> <p>TOA pm: Informatics: Data-Independent Acquisition, <i>Murphy Ballroom, Bldg. B, Level Five</i></p> <p>TOB pm: GC/MS, GCxGC/MS, GC-MS/MS, and GC/HRMS, <i>B401-402</i></p> <p>TOC pm: Top Down Protein Analysis, <i>B405-407</i></p> <p>TOD pm: Drug Target Identification by MS, <i>B302-305</i></p> <p>TOE pm: Food Safety & Chemistry: Innovations, <i>B308-309</i></p> <p>TOF pm: Cancer Research, <i>B312-314</i></p> <p>TOG pm: Instrumentation: Innovative Separations Approaches Coupled to MS, <i>Auditorium, Bldg. A</i></p> <p>TOH pm: Energy, Petroleum, and Biofuels: Instrumentation and Applications, <i>A411-412</i></p>
4:45 - 5:30 PM	<p>AWARD LECTURE, Murphy Ballroom, Bldg. B, Level Five</p> <p>Biemann Medal</p> <p>Sarah Trimpin <i>Wayne State University</i></p> 
5:45 - 7:00 PM	<p>WORKSHOPS There are light refreshments in Building A foyers, 5:30 - 5:45 pm.</p> <ol style="list-style-type: none"> 01. Top Down Proteomics: Advancing Widespread Adoption and Expanding Applications (Top-Down Proteomics Interest Group), <i>A402-403</i> 02. Networking for Scientists: Celebrating Women Mass Spectrometrists (Year 2), <i>A404-405</i> 03. Say No to Drugs: Forensic Applications Outside of Traditional Illicit Drug Analysis (Forensics & Homeland Security Interest Group), <i>A406-407</i> 04. Proteoform Identification and Quantification Using Toppic Suite, <i>A408</i> 05. Protein Biomarkers Method Development & Validation by LCMS, HRMS and Hybrid LBA/LCMS: Recent Advancements (Regulated Bioanalysis Interest Group), <i>A410</i> 06. Improving Scientific Writing Skills, <i>A307</i> 07. Metal Ions and Non-Threshold Ion Activation in Biomolecules (Metal Ion Coordination Chemistry Interest Group), <i>A309</i> 08. Protein Imaging - Are We There? Are All Issues Solved? (Imaging MS Interest Group), <i>A311</i> 09. Metabolomics: Points of Agreement and Disagreement (Metabolomics Interest Group), <i>A312</i> 10. Environmental MS: Detection of Emerging Contaminants (Environmental Applications Interest Group), <i>A313</i> 11. Visualization, Comparison and Accessibility of Large Data Sets (Analytical Lab Managers Interest Group), <i>A314</i> 12. Advances in Polymer Mass Spectrometry - Architecture (Polymeric Materials Interest Group), <i>A315</i> 13. (Emotional) Intelligence Gathering (Career Development Interest Group), <i>A316</i> 14. MS in Extractable and Leachable Analysis, <i>A303</i> 15. HDX, Covalent Labeling & Cross-Linking: Status of Community-Initiatives and New Developments and Applications (HDX Covalent Labeling & Cross Linking Interest Group), <i>A302</i> 16. Lipidomics: Path to Clinical Utility (Lipids & Lipidomics Interest Group), <i>A301</i> 17. Data Independent Acquisition: Expanding the Scope of DIA Strategies for Quantitative Mass Spectrometry (Data Independent Acquisition Interest Group), <i>A305</i> 18. Trans-Proteomic Pipeline: Recent Advances and Future Directions, <i>A304</i>
7:00 - 8:00 PM	DINNER BREAK
AFTER 8:00 PM	CORPORATE HOSPITALITY SUITES , Omni CNN Center Hotel



PROGRAM OVERVIEW

WEDNESDAY

7:00 AM	CORPORATE BREAKFAST SEMINARS , Convention Center and Omni CNN Center Hotel
7:30 AM - 5:00 PM	REGISTRATION , Building B Main Lobby
8:30 - 10:30 AM	<p>ORAL SESSIONS</p> <p>WOA am: Metabolomics: New Technologies and Applications, <i>Murphy Ballroom, Bldg. B, Level Five</i></p> <p>WOB am: Carbohydrates, <i>B401-402</i></p> <p>WOC am: Fundamentals for Everyone: Peptides and Proteins, <i>B405-407</i></p> <p>WOD am: Microdosing and Microsampling: Analytical Challenges, <i>B302-305</i></p> <p>WOE am: Environmental: Innovative Approaches and Instrumentation, <i>B308-309</i></p> <p>WOF am: Ion Mobility: New Developments & Applications, <i>B312-314</i></p> <p>WOG am: Fundamentals for Everyone: Structural elucidation, <i>Auditorium, Bldg. A</i></p> <p>WOH am: Synthetic Polymers, <i>A411-412</i></p>
10:30 AM - 2:30 PM	<p>POSTER SESSION AND EXHIBITS, Wednesday Posters, Poster/Exhibit Hall ground level</p> <p>Odd-number posters present: 10:30 - 11:30 am PLUS 12:30 – 2:30 pm</p> <p>Even-number posters present: 10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm</p>
2:30 - 4:30 PM	<p>ORAL SESSIONS</p> <p>WOA pm: Metabolomics: Untargeted Profiling, <i>Murphy Ballroom, Bldg. B, Level Five</i></p> <p>WOB pm: Hydrogen-Deuterium Exchange MS: Innovations, <i>B401-402</i></p> <p>WOC pm: Forensics: Innovations and Applications, <i>B405-407</i></p> <p>WOD pm: Endogenous Protein Biomarkers in Drug Discovery and Development: Quantitative Analysis, <i>B302-305</i></p> <p>WOE pm: Clinical Analysis: MS in the Operating Room, <i>B308-309</i></p> <p>WOF pm: Ion Mobility: Small Molecules, Pharmaceuticals, and DMPK, <i>B312-314</i></p> <p>WOG pm: Instrumentation: Ambient Ionization & Applications, <i>Auditorium, Bldg. A</i></p> <p>WOH pm: Fundamentals: DDA and DIA LC-MS, <i>A411-412</i></p>
4:45 - 5:30 PM	ASMS MEETING , B302-305, Level Three: Awards, board reports, wine, beer, soft drinks - and more!
5:45 - 7:00 PM	<p>WORKSHOPS There are light refreshments in Building A foyers, 5:30 - 5:45 pm.</p> <ol style="list-style-type: none"> 01. MS-Based Interactomics: Computational Resources and Tools for Studying the Physical Interactome (Bioinformatics MS Interest Group), <i>A402-403</i> 02. IMS: When Chromatography Just Won't Do (Ion Mobility MS Interest Group), <i>A404-405</i> 03. Clinical Applications: Standardization and Harmonization Efforts (Clinical Chemistry Interest Group), <i>A406-407</i> 04. Exposomics Workshop (Exposomics Interest Group), <i>A408</i> 05. MS-Based Process Analytical Technology (PAT): Testing & Control of CQAs (Pharmaceuticals Interest Group), <i>A410</i> 06. Endogenous Biomarkers: Measurement to Predict in vivo Drug-Drug Interactions (DMPK Interest Group), <i>A307</i> 07. The NIH and NSF Review and Funding Process, <i>A309</i> 08. Why You Should Submit Your Best Manuscripts to JASMS (and Introducing a New Publisher), <i>A311</i> 09. Metaproteomics for the Masses: Solutions, Opportunities and Challenges, <i>A312</i> 10. Bridging the Gap between Computational Biology and Biology: Matchmaking Session, <i>A313</i> 11. Ambient Ionization: Where We Stand Now and Go from Here, <i>A314</i> 12. The Proteomics Standards Initiative and ProteomeXchange: Supporting Open Data Practices in Proteomics, <i>A315</i> 13. Fundamentals: Structural Elucidation of Proteins (Fundamentals Interest Group), <i>A316</i> 14. Education: Teaching MS at the Undergraduate Level (Undergraduate Research in MS Interest Group), <i>A303</i> 15. New Ion Manipulations Prior to FT-MS (FTMS Interest Group), <i>A302</i> 16. Cannabis and Hemp Testing Requirements: How to Leverage with Mass Spectrometry, <i>A301</i> 17. Getting Started with R for Mass Spectrometry Data Analysis, <i>A305</i> 18. Career and Collaboration Opportunities in China, <i>A304</i>
7:00 - 8:00 PM	DINNER BREAK
AFTER 8:00 PM	CORPORATE HOSPITALITY SUITES , Omni CNN Center Hotel



THURSDAY

7:00 AM	CORPORATE BREAKFAST SEMINARS , Convention Center
7:30 AM - 5:00 PM	REGISTRATION , Building B Main Lobby
8:30 - 10:30 AM	<p>ORAL SESSIONS</p> <p>ThOA am: Informatics: Metabolomics, <i>Murphy Ballroom, Bldg. B, Level Five</i></p> <p>ThOB am: Fundamentals: Ion Spectroscopy, <i>B401-402</i></p> <p>ThOC am: Post-Translational Modifications: Qualitative and Quantitative Analysis, <i>B405-407</i></p> <p>ThOD am: Drug Discovery and Development: Quantitative Analysis, <i>B302-305</i></p> <p>ThOE am: Supramolecular and Macromolecular Complexes, <i>B308-309</i></p> <p>ThOF am: Clinical Analysis Using MS, <i>B312-314</i></p> <p>ThOG am: Informatics: Stable Isotope Labeling in MS: Applications, <i>Auditorium, Bldg. A</i></p> <p>ThOH am: Exposomics, Toxicology, and Human Health, <i>A411-412</i></p>
10:30 AM - 2:30 PM	<p>POSTER SESSION AND EXHIBITS, Thursday Posters, Poster/Exhibit Hall ground level</p> <p>Odd-number posters present: 10:30 - 11:30 am PLUS 12:30 – 2:30 pm</p> <p>Even-number posters present: 10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm</p>
2:30 - 4:30 PM	<p>ORAL SESSIONS</p> <p>ThOA pm: Informatics: Peptide and Protein Identification, Proteomics, <i>Murphy Ballroom, Bldg. B</i></p> <p>ThOB pm: Microorganisms and the Microbiome, <i>B401-402</i></p> <p>ThOC pm: Quantitative Proteomics in Systems Biology, <i>B405-407</i></p> <p>ThOD pm: Covalent Labeling and Chemical Crosslinking, <i>B302-305</i></p> <p>ThOE pm: Plant “omics”, <i>B308-309</i></p> <p>ThOF pm: Ion Mobility: Structure, <i>B312-314</i></p> <p>ThOG pm: Instrumentation: Innovations in Mass Analyzers, <i>Auditorium, Bldg. A</i></p> <p>ThOH pm: Fundamentals: Ion Activation and Dissociation, <i>A411-412</i></p>
4:45 - 5:30 PM	<p>PLENARY LECTURE, Murphy Ballroom, Bldg. B, Level Five</p> <div data-bbox="406 997 571 1201" data-label="Image"> </div> <p>Chemistry of Food and Soft Drinks</p> <p>Lilly D'Angelo <i>Global Food & Beverage Technology Associates</i></p>
6:30 - 9:00 PM	<p>CLOSING EVENT</p> <p>Georgia Aquarium. <i>Tickets (\$40) must be purchased in advance by Monday 12 noon.</i> Join us for an enchanting evening at the Georgia Aquarium. Dinner buffets close at 8:00 pm, dessert available until close. Ticket includes aquarium entry for our private event, dinner buffet and one drink ticket for soda, beer, or wine. Cash bars available until close</p> <div data-bbox="402 1432 1023 1839" data-label="Image"> </div>



SUNDAY EVENING AND MONDAY MORNING ORAL SESSIONS

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
B302-305 Level Three

5:00-6:30 pm Sunday
TUTORIAL SESSION I
Presiding: Susan Richardson (University of South Carolina)
Murphy Ballroom, Bldg B, Level Five



5:00-5:45 pm
Lipidomics
Stephen Blanksby
Queensland University of Technology
& **Gavin Reid**
University of Melbourne



5:45-6:30 pm
Targeted Imaging
Enrico Davoli
Mario Negri Institute

5:00-6:30 pm Sunday
TUTORIAL SESSION II
Presiding: Erin Baker (North Carolina State University)
B302-305 Level 3



5:00-5:45 pm
Native Mass Spectrometry
Michal Sharon
Weizmann Institute



5:45-6:30 pm
Data Independent Acquisition
Birgit Schilling
The Buck Institute

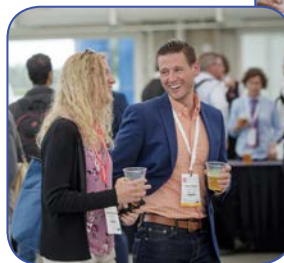
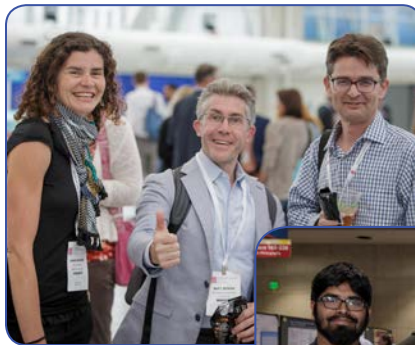
6:45- 7:45 pm Sunday
CONFERENCE OPENING
Presiding: Susan Richardson (University of South Carolina)
Murphy Ballroom, Bldg B, Level Five

Welcome, **Susan Richardson** *University of South Carolina*
ASMS Vice President for Programs



7:00-7:45 pm
Transitioning the World Energy for All Purposes
to Stable Electricity Powered by 100% Wind,
Water, and Sunlight
Mark Z. Jacobson
Stanford University

7:45-9:00 pm Sunday
WELCOME RECEPTION
Poster/Exhibit Hall (Level One)
Conference name badge is required.



MONDAY MORNING ORAL SESSIONS

From 7:00 am Monday
CORPORATE BREAKFAST SEMINARS
CONVENTION CENTER AND OMNI CNN CENTER HOTEL
See page 16 for detailed schedule. Reservation or
RSVP required.

8:30 - 10:30 am Monday
CANNABIS TESTING
Session Chair: Jack Henion (Advion, Inc.)
Murphy Ballroom, Bldg B, Level 5

MOA am 08:30 **Future Opportunities and Challenges in Mass Spectrometry Based Cannabis Analytical QC Testing and Research**; Scott Kuzdzal, Ph.D.¹; Andrew P. Fornadel, Ph.D.¹; Jeff H. Dahl, Ph.D.¹; Bob H. Clifford, Ph.D.¹; Nicole H. Lock¹; ¹Shimadzu Scientific Instruments, Inc., Columbia, MD

MOA am 08:50 **Novel HR-ESI-LC/MS and SHS-GC-MS/MS Methods for Comprehensive Metabolic Profiling of Phytocannabinoids and Terpenoids in Cannabis**; Paula Berman¹; Anna Shapira¹; Ben Yellin¹; Gil Lewitus¹; David Meiri¹; ¹Technion - Israel Institute of Technology, Haifa, Israel

MOA am 09:10 **Pesticide Residue Detection in Cannabis and Products using Liquid Chromatography-Mass Spectrometry/Mass Spectrometry (LC-MS/MS)**; Caley B Craven¹; Ping Jiang¹; Charles A. Lucy¹; Xing-Fang Li¹; ¹University of Alberta, Edmonton, Alberta

MOA am 09:30 **Cannabis Testing: Development, Validation, and Implementation of a Patient-centric Microsampling Assay for Analysis of Cannabinoids in Human Whole Blood**; Ganesh Moorthy; *The Children's Hospital of Philadelphia, Philadelphia, PA*



MOA am 09:50 **The Use of Mass Spectrometry for Quality Control and Understanding the Complex Chemistry of Cannabis and Its Therapeutic Effects;** Kaveh Kahen; *Sigma Analytical Services, Toronto, ON*

MOA am 10:10 **Specializing Cannabis Cultivation Quality Control with a Mobile Mass Spectrometry Lab;** Brigitte Simons¹; Afsoon Pajand Birjandi¹; Hesham Ghobarah²; Ping Jiang³; Hubert Marceau⁴; Alexis St-Gelais⁴; Tariq Akhtar⁵; Xing-Fang Li³; *¹Molecular Science Corp., Toronto, ON; ²Deep Dive Research Inc., Toronto, ON; ³University of Alberta, Edmonton, AB; ⁴Laboratoire PhytoChemia, Chicoutimi, QC; ⁵University of Guelph, Guelph, ON*

8:30 - 10:30 am Monday
GLYCOPEPTIDES AND GLYCOPROTEINS
Session Chair: Shujuan McDonald (Pfizer Inc.)
B401-402

MOB am 08:30 **Cost-Benefit Analysis of Stepped-Energy Collisional Dissociation and Electron Transfer Dissociation Approaches for Intact Glycopeptide Characterization;** Nicholas M Riley¹; Stacy A Malaker¹; Marc D Driessen¹; Carolyn R Bertozzi¹; *¹Stanford University, Stanford, CA*

MOB am 08:50 **Finding the Sweetspot of Prostate-Specific Antigen;** Guinevere S.M. Lageveen-Kammeijer¹; Alan B. Moran¹; Jan Nouta¹; Elena Dominguez-Vega¹; Manfred Wührer¹; *¹Leiden University Medical Center (LUMC), Leiden, Netherlands*

MOB am 09:10 **Advanced Data Acquisition and Processing Approach Increases Glycopeptide Identifications and Improves Confidence of Assignment;** Kevin Brown Chandler¹; Deborah R Leon¹; Catherine E Costello¹; *¹Department of Biochemistry, Boston University School of Medicine, Boston, MA*

MOB am 09:30 **Large Scale Human Glycoproteomics: Insights into Data Analysis;** Kathleen T. Grassmyer¹; Christopher J. Brown¹; Matthew L. MacDonald²; David E. Clemmer¹; Jonathan C. Trinidad¹; *¹Indiana University Bloomington, Bloomington, IN; ²University of Pittsburgh School of Medicine, Pittsburgh, PA*

MOB am 09:50 **Absolute Quantitation of the N-Linked Glycoforms of a Biotherapeutic IgG in Complex Mixtures by HILIC-MRM with an Isotopically Labeled Standard;** Ron Orlando^{1,2}; Marla Popov²; Stuart Haslam³; Tyler Fletcher¹; *¹University of Georgia, Athens, GA; ²Glycoscientific LLC, Athens, GA; ³Imperial College, London, United Kingdom*

MOB am 10:10 **Native Mass Spectrometry Analysis of Glycoprotein-Protein/Ligand Interactions;** Di Wu¹; Carol V. Robinson¹; *¹University of Oxford, Oxford, United Kingdom*

8:30 - 10:30 am Monday
MEMBRANE PROTEIN MS
Session Chair: Julien Marcoux (CNRS)
B405-407

MOC am 08:30 **Lipid-Composition Alters Protein Dynamics of Aquaporin Z Nanodisc;** Xin Shan Lim¹; Xin-Xiang Lim¹; Lili Wang¹; Qingsong Lin¹; Ganesh S Anand¹; *¹National University of Singapore, Singapore*

MOC am 08:50 **Detergent- and Chemical-Free Native Mass Spectrometry Reveals the Membrane Protein Complex Ensemble of Whole Membrane Fractions;** Dror Shlomo Chorev¹; Haiping Tang¹; Tom Durrant¹; Siyun Chen¹; Carol V. Robinson¹; *¹University of Oxford, Oxford, United Kingdom*

MOC am 09:10 **Revealing the Structural and Functional Environment of Sialylated Proteins on Cell**

MOC am 09:30 **Surfaces by Quantitative Oxidation Mapping;** Qiongyu Li¹; Yixuan (Axe) Xie¹; Gege Xu¹; Carlito B Lebrilla¹; *¹University of California, Davis, CA*

MOC am 09:50 **Localization and Activity of the Metal Centers of Membrane Complexes Using Micelles and Nanodiscs Coupled with Native Top-Down Mass Spectrometry;** Luis F. Schachner¹; Soo Y Roo¹; Christopher W Koo¹; Amy C Rosenzweig¹; Neil L Kelleher¹; *¹Northwestern University, Evanston, IL*

MOC am 10:10 **CellSurfer: An N-Glycoprotein-specific Analysis Platform for Semi-automated, Quantitative Discovery of Cell Surface Proteins;** Amanda Rae Buchberger¹; Linda Berg Luecke¹; Rachel A. Jones Lipinski¹; Ranjuna Weerasekera¹; Matthew Waas¹; Rebekah L. Gundry¹; *¹Medical College of Wisconsin, Milwaukee, WI*

8:30 - 10:30 am Monday
IMAGING: INSTRUMENTATION & METHOD DEVELOPMENT
Session Chair: Martina Marchetti-Deschmann (TU Wien)
B302-305

MOD am 08:30 **SPICing up your MALDI Image: Enhanced Ion Yields for Numerous Classes of Lipids via Single-Photon-Induced Chemical Ionization;** Christoph H. M. Bookmeyer¹; Jens Soltwisch^{1,2}; Ulrich Röhling³; Klaus Dreisewerd^{1,2}; *¹Institute for Hygiene, University of Münster, Münster, Germany; ²Interdisciplinary Center for Clinical Research (IZKF), University of Münster, Münster, Germany; ³Institute of Medical Physics and Biophysics, University of Münster, Münster, Germany*

MOD am 08:50 **Identification of Phosphatidylcholine Lipids in Imaging Mass Spectrometry Using Gas-Phase Charge Inversion Ion/Ion Reactions Enabled on an FT-ICR Mass Spectrometer;** Jonathan T. Specker^{1,2}; Steve L. Van Orden²; Boone M. Prentice¹; *¹Department of Chemistry, University of Florida, Gainesville, FL; ²Bruker Daltonics Inc., Billerica, MA*

MOD am 09:10 **Breast Cancer Tumor and Necrosis Associated Peptide and Glycan Co-Localizations in FFPE Tissues by MALDI-FTICR Imaging Mass Spectrometry;** Danielle A Scott¹; Laura Spruill¹; Peggy Angel¹; Richard Drake¹; *¹Medical University of South Carolina, Charleston, SC*

MOD am 09:30 **An Integrated Microfluidic Device for High-Resolution Nano-DESI Mass Spectrometry Imaging of Tissue Sections;** Xiangtang Li¹; Ruichuan Yin¹; Julia Laskin¹; *¹Purdue University, West Lafayette, IN*

MOD am 09:50 **LADI of All Trades: Imaging of Small-Molecule Spatial Distributions in Complex Matrices by a Novel Ambient Ionization Imaging Technique;** Kristen L Fowble¹; Rabi A Musah¹; *¹University at Albany-SUNY, Albany, NY*

MOD am 10:10 **Revealing Isobaric and Isomeric Substructure in Tissue: Advanced Multivariate Analysis for Ion Mobility Imaging Mass Spectrometry;** Raf Van de Plas^{1,2,3}; Lukasz Migas¹; Nathan Heath Patterson^{2,3}; Katerina V. Djambazova^{2,4}; Richard M. Caprioli^{2,3,4,5,6}; Jeffrey M. Spraggins^{2,3,4}; *¹Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; ²Mass Spectrometry Research Center,*



MONDAY MORNING ORAL SESSIONS

Vanderbilt University, Nashville, TN; ³Department of Biochemistry, Vanderbilt University, Nashville, TN; ⁴Department of Chemistry, Vanderbilt University, Nashville, TN; ⁵Department of Pharmacology, Vanderbilt University, Nashville, TN; ⁶Department of Medicine, Vanderbilt University, Nashville, TN

8:30 - 10:30 am Monday
LIPIDOMICS: TARGETED AND UNTARGETED
Session Chair: Peggi Angel
(Medical University of South Carolina)
B308-309

- MOE am 08:30 **A 'Systems-omics' Strategy to Uncover the Role of Brain Tissue Derived Exosomal Lipids in Alzheimer's Disease**; Huaqi (Kate) Su^{1,2}; Kevin J. Barnham^{1,2}; Laura J. Vella¹; Gavin E Reid²; ¹Florey Institute of Neuroscience and Mental Health, Parkville, Australia; ²University of Melbourne, Parkville, Australia
- MOE am 08:50 **Comprehensive Phospholipid Analysis Reveals Alternations in Extracellular Vesicles during Immune Responses**; Wenpeng Zhang^{1,2}; Ying Zhang³; Jiaqi Liang¹; Bing Shang¹; Hang Yin³; Yu Xia^{1,2}; ¹Department of Chemistry, Tsinghua University, Beijing, China; ²Department of Chemistry, Purdue University, West Lafayette, IN; ³School of Pharmaceutical Sciences, Tsinghua University, Beijing, China
- MOE am 09:10 **Localizing the Inflammatory Lipid Response to Structurally Engineered Lipopolysaccharide in Mouse Lung**; Alison J Scott^{1,2}; Shane R. Ellis²; Courtney E. Chandler¹; Sung Hwan Yoon³; Benjamin L Oyler⁴; David Robinson Goodlett¹; Ron M. A. Heeren²; Robert K. Ernst¹; ¹University of Maryland, Baltimore, Baltimore, MD; ²Maastricht Multimodal Molecular Imaging (M4I) Institute, Division of Imaging Mass Spectrometry, Maastricht, Netherlands; ³University of Maryland Baltimore, Baltimore, MD; ⁴Center for Food Safety and Applied Nutrition, FDA, Silver Spring, MD
- MOE am 09:30 **Next-Generation Imaging Technologies for 3-D Multimodal Lipid Atlases**; Jeffrey M Spraggins^{1,2}; Nathan Heath Patterson^{1,2}; David M. Anderson^{1,2}; Jamie Allen^{1,2}; William J. Perry^{1,2}; Martin Dufresne^{1,2}; Lukasz Migas⁴; Danielle Gutierrez^{1,2}; Eric P. Skaar⁵; Richard M. Caprioli^{1,2,3}; ¹Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; ²Vanderbilt University Department of Biochemistry, Nashville, TN; ³Vanderbilt University Department of Chemistry, Nashville, TN; ⁴Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; ⁵Vanderbilt University Medical Center Department of Pathology, Microbiology and Immunology, Nashville, TN
- MOE am 09:50 **Integrated Multidimensional Liquid Chromatography-Ion Mobility-Tandem Mass Spectrometry (LC-IM-MS/MS) Workflow for High Confidence Annotations in Global Untargeted Lipidomics**; Bailey S. Rose¹; Simona G. Codreanu¹; Jody C. May¹; Stacy D. Sherrod¹; John A. McLean¹; ¹Vanderbilt University, Nashville, TN
- MOE am 10:10 **In-Depth Lipidomic Profiling of the Australian Imaging Biomarker and Lifestyle Flagship Study of Aging**; Kevin Huynh¹; Wei Ling Florence Lim^{2,3}; Corey Giles⁴; Kaushala S Jayawardana⁴; Prathishtha Chatterjee^{2,5,6}; Natalie A Mellett⁴; Ian Martins^{2,3}; Simon M Laws^{3,7,8}; Ashley I Bush⁹; Christopher C Rowe^{9,10}; Victor L Villemagne^{9,10}; ¹¹David Ames¹²; Colin L Masters⁹; Brian G Drew¹;

Ralph N Martins^{2,3,5,6,13,14}; Peter J Meikle^{1,15}; ¹Baker Heart and Diabetes Institute, Melbourne, Australia; ²School of Medical and Health Sciences, Edith Cowan University, Perth, Australia; ³Cooperative Research Centre (CRC) for Mental Health, Perth, Australia; ⁴Baker Heart and Diabetes Institute, Melbourne, Australia; ⁵Department of Biomedical Sciences, Macquarie University, Sydney, Australia; ⁶KaRa Institute of Neurological Disease, Sydney, Macquarie Park, Sydney, Australia; ⁷Collaborative Genomics Group, School of Medical and Health Sciences, Edith Cowan University, Perth, Australia; ⁸School of Pharmacy and Biomedical Sciences, Faculty of Health Sciences, Curtin Health Innovation, Perth, Australia; ⁹Florey Department, University of Melbourne, Melbourne, Australia; ¹⁰Department of Nuclear Medicine and Centre for PET, Austin Health, Melbourne, Australia; ¹¹Department of Medicine, Austin Health, The University of Melbourne, Melbourne, Australia; ¹²National Ageing Research Institute, Parkville, Victoria, Australia; ¹³School of Psychiatry and Clinical Neurosciences, The University of Western Australia, Perth, Australia; ¹⁴Australian Alzheimer's Research Foundation, Nedlands, Perth, Australia; ¹⁵Monash University, Melbourne, Australia

8:30 - 10:30 am Monday
FUNDAMENTALS: ION MOBILITY AND MS
(IN MEMORY OF AL YERGEY)
Session Chair: Stephanie Cologna
(University of Illinois at Chicago)
B312-314

- MOF am 08:30 **Ultrahigh Resolution Ion Mobility Separations of Isotopologues and Isotopomers in Multi-Pass Traveling Wave-Based Structures Lossless Ion Manipulations (SLIM)**; Roza Wojcik¹; Gabe Nagy¹; Isaac K Attah¹; Sandilya V.B. Garimella¹; Yehia M Ibrahim¹; Richard D. Smith¹; ¹PNNL, Richland, WA
- MOF am 08:50 **Fundamental Principles and Experimental Performance of a Novel Counter Flow Ion Mobility Device: U-Shaped Mobility Analyzer**; Keke Wang¹; Qiao Jin¹; Xu Zhou¹; Lin Liu¹; Kent J. Gillig²; Xiaoqiang Zhang¹; Lei Wang³; Yilong Guo³; Wenjian Sun¹; ¹Shimadzu Research laboratory (Shanghai) Co. Ltd., Shanghai, China; ²Genomics Research Center, Academia Sinica, Taipei, Taiwan; ³Shanghai Institute of Organic Chemistry, Chinese Academy of Science, Shanghai, China
- MOF am 09:10 **Maximizing Signal to Noise Ratio for Voltage Sweep Multiplexing-Ion Mobility-Ion Trap Mass Spectrometry**; Tobias Reinecke¹; Pearl Kwantwi-Barima¹; Brian H. Clowers¹; ¹Department of Chemistry, Washington State University, Pullman, WA
- MOF am 09:30 **Collision Cross Sections of Phosphoric Acid Cluster Anions and their Use as Calibrants for Traveling Wave Ion Mobility**; Valentina Calabrese¹; Helene Lavanant¹; Frédéric Rosu²; Valérie Gabelica³; Carlos Afonso¹; ¹Normandie Univ, INSA Rouen, UNIROUEN, CNRS, COBRA, Rouen, France; ²CNRS, UMS 3033, Institut Européen de Chimie et Biologie (IECB), Pessac, France; ³University of Bordeaux, INSERM and CNRS, ARNA Laboratory, IECB, Bordeaux, France
- MOF am 09:50 **Combining Direct Metalation and Collision-Induced Unfolding Reveals Structure Changes of Metallothioneins During Ag⁺ Metalation**; Shiyu Dong¹; David H. Russell¹; ¹Texas A&M University, College Station, TX



MOF am 10:10 **Advanced Temporal Multiplexing and Peak Deconvolution for Improved Sensitivity and Resolution in Ion Mobility-Mass Spectrometry Analysis;** Jody C. May¹; Richard Knochenmuss²; John C. Fjeldsted³; John A. McLean¹; ¹Vanderbilt University, Nashville, TN; ²RKResearch, Seftigen, Switzerland; ³Agilent Technologies, Santa Clara, CA

**8:30 - 10:30 am Monday
INSTRUMENTATION: PORTABLE AND TRANSPORTABLE
MASS SPECTROMETERS**

**Session Chair: Essyllt Louarn (Université Paris-Sud)
Auditorium, Bldg A**

MOG am 08:30 **Miniature OzID Mass Spectrometer for Clinical Lipid Analysis;** Xinwei Liu¹; Wenbo Cao²; Xiaoxiao Ma²; Wenpeng Zhang³; Stephen J. Blanksby⁴; Yu Xia^{3,5}; Zheng Ouyang^{3,6}; ¹State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instruments, Tsinghua University, Beijing, China; ²State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instruments, Tsinghua University, Beijing, China; ³Department of Chemistry, Purdue University, West Lafayette, IN 47907; ⁴Central Analytical Research Facility, Queensland University of Technology, Brisbane, Australia; ⁵Department of Chemistry, Tsinghua University, Beijing, China; ⁶State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instruments, Tsinghua University, Beijing, China

MOG am 08:50 **MS2field: Automated Real-Time Water Quality Screening with a Transportable LC-HRMS;** Michael Stravs¹; Nicole Zehethofer²; Reto Bolliger³; Guenter Boehm³; Thomas Moehring²; Heinz Singer¹; Christian Stamm¹; Christoph Ort¹; ¹Eawag, Duebendorf, Switzerland; ²Thermo Fisher Scientific, Bremen, Germany; ³CTC Analytics AG, Zwingen, Switzerland

MOG am 09:10 **Pulse-sampling Assisted Flash Heating Desorption Miniature Ion Trap Mass Spectrometry with Photoionization for Sensitivity and On-Site Identification of Illegal Drugs;** Keyong Hou¹; shuang Wang¹; Weimin Wang¹; Haiyang Li¹; ¹Dalian Institute of Chemical Physics, Chinese Academy of Science, Dalian, China

MOG am 09:30 **Development and Validation of a Simple Headspace Needle-Trap Method for Quantitative Estimation of Butylated Hydroxytoluene from Cosmetic by Hand-Portable GC/MS;** Chiranjit Ghosh¹; Jonathan Grandy¹; Varoon Singh¹; Janusz Pawliszyn¹; ¹University of Waterloo, Waterloo, ON

MOG am 09:50 **Designing a Magnetic Sector for a Cycloidal Mass Analyzer in a Miniature Mass Spectrometer;** Kathleen L Horvath¹; Tanouir Aloui¹; Raul Vyas¹; Maria Luisa Sartorelli¹; Yuriy Zhilichev²; Roger P Sperline³; M Bonner Denton³; Patrick Keelan⁴; David Koester¹; Jeffrey T Glass¹; Jason J Amsden¹; Jesko A von Windheim¹; ¹Duke University, Durham, NC; ²Independent, Durham, NC; ³University of Arizona, Tucson, AZ; ⁴PFT Technology, Long Island, NY

MOG am 10:10 **Demonstration and Verification of the Pyrolysis and Derivatization GCMS Capabilities of the Mars Organic Molecule Analyzer (MOMA) Mass Spectrometer;** Desmond A. Kaplan^{1,2}; Melissa Guzman³; Fabien Stalport⁴; Noel Grande⁴; Cyril Szopa^{3,5}; Caroline Freissinet⁶; Arnaud Buch⁷; Andrej Grubisic²; Ryan M. Danell⁸; Friso Van Amerom⁹; Xiang Li^{2,10}; Stephanie A.

Getty²; William B. Brinckerhoff²; Paul R. Mahaffy²; ¹KapScience LLC, Tewksbury, MA; ²NASA Goddard Space Flight Center, Greenbelt, MD; ³LATMOS/IPSL, Université Versailles St Quentin, UPMC Université Paris 06, CNRS, Guyancourt, France; ⁴Laboratoire Interuniversitaire des Systèmes Atmosphériques (LISA), Paris, France; ⁵Institut Universitaire de France, Paris, France; ⁶LATMOS/IPSL, UVSQ Université Paris-Saclay, Paris, France; ⁷CentraleSupélec, Paris, France; ⁸Danell Consulting, Inc., Winterville, NC; ⁹Mini-Mass Consulting, Inc, Hyattsville, MD; ¹⁰University of Maryland, College Park, MD

**8:30 - 10:30 am Monday
BIOMARKERS: QUALITATIVE ANALYSIS
Session Chair: Jason Hogan (Bristol-Myers Squibb)
A411-412**

MOH am 08:30 **Proteomic Assessment of Synapses with Rich Associated Clinical Data Highlight Potential Targets for Mediating Alzheimer's Pathology and Cognitive Decline;** Becky C Carlyle^{1,2}; Savannah E. Kandigian¹; Bianca A. Trombetta¹; Wilhelm Haas^{1,2}; Steven E. Arnold^{1,2}; ¹Massachusetts General Hospital, Charlestown, MA; ²Harvard Medical School, Boston, MA

MOH am 08:50 **Proteome Profiling of Multiple Sclerosis Cerebrospinal Fluid by Data Independent Acquisition Reveals Disease Biomarkers;** David R. Spiciarich¹; Christopher T. Harp¹; Ann E. Herman¹; W. Rodney Mathews¹; Veronica G. Anania¹; ¹Genentech, Inc., South San Francisco, CA

MOH am 09:10 **Urine Metabolomics of Children with Autism Spectrum Disorder (ASD) Treated with Sulforaphane;** Roshanak Aslebagh¹; Kanwaljit Singh²; Michelle L. Dubuke¹; Andrew W. Zimmerman²; Scott A. Shaffer¹; ¹Department of Biochemistry and Molecular Pharmacology, University of Massachusetts Medical School, Worcester, MA; ²Department of Pediatrics (Neurology), University of Massachusetts Medical School, Worcester, MA

MOH am 09:30 **Unraveling a Complex Immunoprotein Profile in Multiple Myeloma with Middle-Down de novo Sequencing and Native Mass Spectrometry;** Valerie J Winton^{1,2}; W Ian Deighan³; Lissa C. Anderson⁴; Rafael D. Melani^{1,2}; Luis F. Schachner¹; Feargal P McNicholl³; John P. McGee¹; Romain Huguet⁵; Philip M Remes⁵; Christopher Mullen⁵; Paul M Thomas^{1,2}; Neil L Kelleher^{1,2}; ¹Northwestern University, Evanston, IL; ²Proteomics Center of Excellence, Northwestern University, Chicago, IL; ³Altnagelvin Hospital, Londonderry, United Kingdom; ⁴National High Magnetic Field Laboratory, Tallahassee, FL; ⁵Thermo Fisher Scientific, San Jose, CA

MOH am 09:50 **Proteogenomic Analyses of Peptide Ancestry Informative Markers in Uterine Neoplasms from Women of European, African and Asian Descent;** Nicholas W Bateman^{1,2}; Brian Hood¹; Christopher Tarney¹; Michael Kessler³; Zhou Ming⁴; Alexander Wong¹; Anthony R Soltis⁵; Xijun Zhang⁵; Clifton Dalgard⁵; Mathew Wilkerson⁵; Kathleen Darcy^{1,2}; Yovanni Casablanca^{1,2}; George Larry Maxwell^{1,2,4}; Timothy O'Connor³; Thomas P. Conrads^{1,2,4}; ¹Gynecologic Cancer Center of Excellence, Annandale, VA; ²John P. Murtha Cancer Center, Bethesda, MD; ³Institute for Genome Sciences and the Department of Medicine University of Maryland



MONDAY MORNING AND AFTERNOON ORAL SESSIONS

MOH am 10:10 *School of Medicine, Baltimore, MD; ⁴Inova Schar Cancer Institute, Annandale, VA; ⁵The American Genome Center, Uniformed Services University, Bethesda, MD*
BloodKB: An Open Community-Scale Knowledge Base for Blood-Related Proteome and Peptidome Diversity; Benjamin Pullman¹; Julie S Wertz¹; Nuno Bandeira¹; ¹University of California, San Diego, La Jolla, CA

**10:30 am-2:30 pm Monday
MONDAY POSTER SESSION**
Poster/Exhibit Hall ground level
Lunch concessions are open 11:00 am - 2:00 pm

Odd-number posters present:
 10:30 am - 11:30 am **PLUS** 12:30- 2:30 pm

Even-number posters present:
 10:30 am - 12:30 pm **PLUS** 1:30- 2:30 pm
 Poster Pick-Me-Up Snacks served at 1:30 pm

**11:30 am - 1:00 pm
Undergraduate Students**
 "Meet the Experts" at tables reserved for you.

MONDAY AFTERNOON ORAL SESSIONS

2:30 - 4:30 pm Monday
INFORMATICS: MULTIOMICS INTEGRATION AND APPLICATIONS
Session Chair: Ewy Mathe (Ohio State University Medical Center)
Murphy Ballroom, Bldg B, Level 5

MOA pm 02:30 **ProteomicsDB: A Big-Data, Multi-Omics, Multi-Organism Resource for Life Science Research;** Patroklos Samaras¹; Tobias Schmidt¹; Pia Bothe¹; Martin Frejno¹; Siegfried Gessulat^{1,2}; Jana Zecha¹; Anna Jarzab¹; Maria Reinecke¹; Julia Mergner¹; Piero Giansanti¹; Johannes Rank³; Harald Kienegger³; Helmut Krcmar³; Hans-Christian Ehrlich²; Stephan Aiche²; Bernhard Kuster^{1,4}; Mathias Wilhelm¹; ¹Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; ²SAP SE, Potsdam, Germany; ³Chair for Information Systems, Technical University of Munich, Munich, Germany; ⁴Bavarian Center for Biomolecular Mass Spectrometry, Freising, Germany

MOA pm 02:50 **Cognitive Re-Analysis of Metabolomics Data Reveals Newly-Associated Metabolite Biological Functions and Mechanistic Predictions of Activity;** Erica Majumder¹; Elizabeth M Billings¹; H. Paul Benton¹; Richard L Martin²; Amelia Palermo¹; Carlos Guijas¹; Markus M Rinschen¹; Xavier Domingo-Almenara¹; J. Rafael Montenegro-Burke¹; Gary Siuzdak¹; ¹The Scripps Research Institute, La Jolla, CA; ²IBM Watson Health, Cambridge, MA

MOA pm 03:10 **Data Integration of Proteomics and Metabolomics from Sugarcane Leaves upon Water Deficit;** Ilara Gabriela Frasson Budzinski¹; Fabrício Edgar de Moraes¹; Thais Regiani Cataldi¹; Livia Maria Franceschini¹; Carlos Alberto Labate¹; ¹ESALQ, Piracicaba, Brazil

MOA pm 03:30 **Linking Cell Lines to Proteotypes: A Proteome-Level Analysis of Protein Interactions, Expression Levels, and Post-Translational Modifications;** Edward L. Huttlin¹; Raphael J Bruckner¹; Jose Navarrete-Perea¹; David Nusinow¹; Brandon M. Gassaway¹; Fana Gebreab¹; Kurt Baltier¹; Melanie Gygi¹; Laura Pontano Vaites¹; Joao A. Paulo¹; J. Wade Harper¹; Steve Gygi¹; ¹Harvard Medical School, Boston, MA

MOA pm 03:50 **A Web-based Platform for Data Exploration and Its Application to Multi-omic Profiling of a Large CRISPR Knockout Collection;** Dain Ryan Brademan¹; Evgenia Shishkova¹; Jarred Rensvold²; Paul D Hutchins¹; Sean Peters¹; Adam Jochem²; Alexander S. Hebert¹; Nicholas W Kwiecien¹; Ian J

Miller¹; Michael S Westphall¹; David J Pagliarini²; Joshua J Coon^{2,3,4,5}; ¹University of Wisconsin - Madison, Madison, WI; ²Morgridge Institute for Research, Madison, WI; ³Genome Center of Wisconsin, Madison, WI; ⁴Department of Chemistry, University of Wisconsin, Madison, WI; ⁵Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI

MOA pm 04:10 **More Than Just a List: An Accessible and Flexible Informatics Environment for Proteogenomic Data Processing, Interpretation and Hypothesis-Generation;** Timothy J. Griffin¹; Praveen Kumar^{1,2}; James E. Johnson³; Thomas McGowan³; Ray W. Sajulga¹; Subina Mehta¹; Pratik D. Jagtap¹; ¹University of Minnesota, Minneapolis, MN; ²Bioinformatic and Computational Biology Program, University of Minnesota, Rochester, MN; ³Minnesota Supercomputing Institute, University of Minnesota, Minneapolis, MN

2:30 - 4:30 pm Monday
HOMELAND SECURITY: CHEMICAL/BIOLOGICAL DEFENSE
Session Chair: Carolyn Koester
(Lawrence Livermore National Laboratory)
B401-402

MOB pm 02:30 **Infrared Thermal Desorption DART-MS of Trace Explosive Fuel-Oxidizer Mixtures: Powders, Propellants, and Pyrotechnics;** Thomas P. Forbes¹; Jennifer R. Verkouteren¹; Edward Sisco¹; Matthew Staymates¹; ¹National Institute of Standards and Technology, Gaithersburg, MD

MOB pm 02:50 **Screening of Chemical Warfare Agent Simulants and Hydrolysis Products in Soil Using Paper Spray Mass Spectrometry;** Sarah Dowling¹; Trevor Glaros²; Nicholas Manicke¹; ¹IUPUI, Indianapolis, IN; ²ECBC, Aberdeen Proving Ground, MD

MOB pm 03:10 **Traceable Opioid Material Kits for Mass Spectrometric Opioid Detection in U.S. Laboratories;** Mike A Mojica¹; Melissa Carter¹; Samantha L Isenberg¹; Cody I Sheppard¹; Elizabeth I. Hamelin¹; Rebecca L. Shaner¹; Craig Seymour¹; Rudolph C. Johnson¹; ¹CDC, Atlanta, GA

MOB pm 03:30 **Mass Spectrometric Detection and Characterization of Botulinum Neurotoxins;** Suzanne R. Kalb¹; John R. Barr¹; ¹CDC, Atlanta, GA

MOB pm 03:50 **Fast and Efficient Immuno-MALDI Proteomics for Reliable Quantification of Abrin Toxin in Complex Food Matrices;** Sandrine Livet¹; Sylvia Worbs²; Eva Hansbauer¹; Hervé Volland³; Stéphanie



Simon³; Christophe Junot⁴; François Fenaille¹; Brigitte Dorner²; [Francois Becher](#)¹; ¹CEA Saclay, Service de Pharmacologie et Immunoanalyse (SPI) - Laboratoire d'Etude du Métabolisme des Médicaments, Gif-Sur-Yvette, France; ²Robert Koch Institute, Biological Toxins - Centre for Biological Threats and Special Pathogens, Berlin, Germany; ³CEA Saclay, Service de Pharmacologie et Immunoanalyse (SPI) - Laboratoire d'Etude et de Recherche en Immunoanalyse, Gif Sur Yvette, France; ⁴CEA Saclay, Service de Pharmacologie et Immunoanalyse (SPI), Gif Sur Yvette, France

MOB pm 04:10 **Highly Accurate Classification of Biological Spores by Culture Medium for Forensic Attribution Using Multiple Chemical Signature Types and Machine Learning**; [Paul J. Ippoliti](#)¹; Michael Crenshaw¹; Michael Sworin¹; Frances E. Nargi¹; Tara L. Boettcher¹; Matthew E. Walsh¹; Amanda M. Casale¹; Jason J. Han¹; Joshua R. Dettman¹; ¹MIT Lincoln Laboratory, Lexington, MA

2:30 - 4:30 pm Monday
FOOD SAFETY & CHEMISTRY: FOODOMICS, ALLERGENS, BACTERIA, FOODS, AND SUPPLEMENTS
Session Chair: Michelle Colgrave (CSIRO)
B405-407

MOC pm 02:30 **Towards a Proper Drop Time for Coffee Beans during Roasting with Maximized Antioxidant Capacity Using Photoionization Mass Spectrometry**; [Jan Heide](#)¹; Hendryk Czech¹; Patrick Martens¹; Michael Wendler¹; Sven Ehler¹; Andreas Walte²; Ralf Zimmermann¹; ¹University of Rostock, Rostock, Germany; ²Photonion GmbH, Schwerin, Germany

MOC pm 02:50 **A PRM-based MS Method for Detection of Milk-Derived Ingredients from a Processed Food Matrix**; [Bini Ramachandran](#)¹; Shyamali Jayasena¹; Charles T Yang²; Melanie Downs¹; ¹Food Allergen Research and Resource Program, University of Nebraska, Lincoln, NE; ²Thermo Fisher Scientific, San Jose, CA

MOC pm 03:10 **Development of an Encyclopedia of Food Carbohydrates: A Rapid-Throughput LC-MS Based Approach to Global Carbohydrate Analysis of 1000 Foods**; [Matthew Amicucci](#)¹; Eshani Nandita¹; Ace G. Galermo²; Thai-Thanh T Vo²; Megan Lee²; Carlito B Lebrilla²; Yiyun Liu²; ¹University of California Davis, CA; ²University of California, Davis, CA

MOC pm 03:30 **A Novel Dereplication Strategy for Comprehensive Studying the Unique Composition of Saponins in Taiwan Quinoa Using High-Resolution Mass Spectrometry**; [Hong-jhang Chen](#)¹; Gui-ru Xie¹; ¹National Taiwan University, Taipei, Taiwan

MOC pm 03:50 **A Novel, Step-Wise Nutrimetabolomics Approach Reveals Small Molecule-Associated Changes in a DASH-Diet Study**; [Nichole Reisdorph](#)¹; MInghua Tang¹; Audrey Hendricks¹; Katrina Doenges¹; Richard Reisdorph¹; Brian Tooker¹; Kevin Quinn¹; Wayne Campbell²; Nancy Krebs¹; ¹University of Colorado Anschutz Medical Campus, Aurora, CO; ²Purdue University, West Lafayette, IN

MOC pm 04:10 **Fast Profiling and Classification of Wines and Wine Quality via SAWN-MS**; Alina Astefanei¹; Roselina Medico¹; Lauren Pintabona¹; Petra Jansen¹; [Garry Corthals](#)¹; ¹University of Amsterdam, Amsterdam, Netherlands

2:30 - 4:30 pm Monday
THERAPEUTIC PROTEINS, ANTIBODIES, AND ANTIBODY/DRUG CONJUGATES
Session Chair: Dhanashri Bagal (Amgen)
B302-305

MOD pm 02:30 **Characterizing and Quantitating Biotransformation of Larger Atypical Antibody Therapeutics Using Affinity Capture and SampleStream™ for Intact Protein Mass Spectrometry**; [John C. Tran](#)¹; Hae-Min Park²; Wenjing Li¹; Neha Srikumar¹; Cong Wu¹; Phillip Y. Chu¹; William S. Sawyer¹; Yichin Liu¹; Philip D. Compton³; ¹Genentech, South San Francisco, CA; ²Proteomics Center of Excellence, Northwestern University, Chicago, IL; ³Integrated Protein Technologies, Inc., Evanston, IL

MOD pm 02:50 **Discovery of Bioactive Proteins Derived from Scorpion Venom using Two Dimensional Mass Spectrometry**; [Meng Li](#)¹; Pui Yiu Lam¹; Peng Chen²; Remy Gavard¹; Kung Ching Cookson Chiu¹; Qiong Wu²; Christopher A. Wootton¹; Mark P. Barrow¹; Hongzheng Fu²; Peter B. O'Connor¹; ¹University of Warwick, Coventry, United Kingdom; ²Peking University, Beijing, China

MOD pm 03:10 **Intact Protein Mass Spectrometry Guiding Cell Line Development for Tri-specific Antibodies**; [Fateme Tousei](#)¹; Yan Jiang¹; Susan Elliott¹; Anthony Paiva¹; Karen Albee¹; Karen Lee¹; ¹Sanofi, Framingham, MA

MOD pm 03:30 **Cation-Exchange Chromatography – Mass Spectrometry and Top-Down Analysis of Therapeutic Proteins**; [Rachel Liuqing Shi](#)¹; Gang Xiao¹; Thomas M Dillon¹; Margaret S Ricci¹; Pavel V. Bondarenko¹; ¹Amgen, Inc., Thousand Oaks, CA

MOD pm 03:50 **Direct Determination of Antibody Chain Pairing by Top-Down Mass Spectrometry Using Electron Capture Dissociation and Ultraviolet Photodissociation**; Weijing Liu¹; Neha Malhan¹; Yury V. Vasil'ev^{2,3}; Joseph S. Beckman^{2,3}; Valery G. Voinov^{2,3}; [Jared B. Shaw](#)¹; ¹Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA; ²e-Msion Inc., Corvallis, OR; ³Linus Pauling Institute, Oregon State University, Corvallis, OR

MOD pm 04:10 **Collision Induced Unfolding Enables the Rapid Analysis of Stressed Monoclonal Antibodies and Biosimilars**; [Daniel D Vallejo](#)¹; Daniel A. Polasky¹; Jukyung Kang²; Kathryn D. Kulju¹; Alexander Benet²; Ruwan T Kurulugama³; John C. Fjeldsted³; Anna Schwendeman²; Brandon T. Ruotolo¹; ¹University of Michigan, Ann Arbor, MI; ²Department of Pharmaceutical Science, University of Michigan, Ann Arbor, MI; ³Agilent Technologies, Inc., Santa Clara, CA

2:30 - 4:30 pm Monday
LIPIDOMICS: NEW MS TECHNOLOGIES AND APPLICATIONS
Session Chair: Christina Jones (NIST)
B308-309

MOE pm 02:30 **Quantitative Lipidomics Profiling Reveals Metabolic Subphenotypes in a Cross-Sectional Human Cohort**; [Daniel Hornburg](#)¹; Kevin Contrepoint²; Sara Ahadi³; Kegan Moneghetti³; Si Wu³; Ming-Shian Tsai²; Eric Wei²; Jennifer Quijada²; Francois Haddad²; Michael Snyder²; ¹Stanford, Palo Alto, CA; ²Stanford University, Stanford, CA; ³Stanford University, Palo Alto, CA

MOE pm 02:50 **Genome-Guided Lipid Identification - A Novel Aid for Hopeless Cases**; [Vanessa Linke](#)¹; Ian J Miller^{1,2}; Dain Ryan Brademan¹; Paul D Hutchins¹; Edna A Trujillo¹; Thiru R Reddy³; Jason D Russell³; Kathryn



MONDAY AFTERNOON ORAL SESSIONS

- MOE pm 03:10 L Schueler¹; Donald S Stapleton¹; Mary E Rabaglia¹; Mark P Keller¹; Daniel M Gatti⁴; Greg Keele⁴; Duy Pham⁴; Gary A Churchill⁴; Alan D Attie¹; Joshua J Coon^{2,3,5,6}; ¹University of Wisconsin, Madison, WI; ²Genome Center of Wisconsin, Madison, WI; ³Morgridge Institute for Research, Madison, WI; ⁴The Jackson Laboratory, Bar Harbor, ME; ⁵Department of Chemistry, University of Wisconsin, Madison, WI 53706; ⁶Department of Biomolecular Chemistry, University of Wisconsin-Madison, WI
- MOE pm 03:30 **Rapid and Simple Differentiation of Lipid Regioisomers in Complex Biological Samples;** Johan Lilljå¹; Kyle D. Duncan¹; Pontus Gieselsson²; Fredrik Palm¹; Ingela Lanekoff¹; ¹Uppsala University, Uppsala, Sweden; ²Lund University, Lund, Sweden
- MOE pm 03:50 **Conformational Lipid Atlas for High Confidence Lipidomics;** Katrina L. Leaprot¹; Jody C. May¹; James N. Dodds²; John A. McLean¹; ¹Vanderbilt, Nashville, TN; ²North Carolina State University, Raleigh, NC
- MOE pm 04:10 **A Novel Solid Phase Sample Preparation Method for Lipidomic Analysis of Plasma Samples;** James A. Apffel¹; Limian Zhao²; Mark Sartain¹; ¹Agilent Laboratories, Santa Clara, CA; ²Agilent Technologies, Wilmington, DE
- MOE pm 04:10 **Laser-Ablation Rapid Evaporative Ionization Mass Spectrometry (LA-REIMS) for Fast Lipidomic Analysis of Genetically Modified CHO Cells in Ambient Conditions;** Stefania Maneta-Stavarakaki¹; Alvaro Perdones-Montero¹; Simon Cameron¹; Julia Abda¹; Yuen-Ting Chim²; Paloma Diaz-Fernandez²; Zoltán Takáts¹; ¹Imperial College London, London, United Kingdom; ²GSK, Stevenage, United Kingdom
- 2:30 - 4:30 pm Monday**
BIOMARKERS: QUANTITATIVE ANALYSIS
Session Chair: Suraj Saraswat (ARUP Lab)
B312-314
- MOF pm 02:30 **Targeted Metabolomic Analysis of Urine for Validating Diagnostic Biomarkers of Asthma and COPD;** Mona M. Khamis¹; Hanan Awad¹; Darryl J Adamko²; Nancy Klemm³; Teagan Holt¹; Mays Al-Dulaymi⁴; Anas El-Aneed¹; ¹College of Pharmacy and Nutrition, University of Saskatchewan, Saskatoon, Saskatchewan; ²Department of Pediatrics, College of Medicine, Saskatoon, Saskatchewan; ³Brandenburg University of Technology Cottbus-Senftenberg, Senftenberg, Germany; ⁴Department of Pediatrics, College of Medicine, Saskatoon, Saskatchewan
- MOF pm 02:50 **Development and Quantitative Characterization of a Reproducible Method for Proteomic Analysis of Circulating Extracellular Vesicles;** Patrick Vanderboom¹; Gregory N Ruegsegger¹; Katherine A Klaus¹; Dawn M Morse¹; Surendra Dasari¹; Ian R Lanza¹; Sreekumaran Nair¹; ¹Mayo Clinic, Rochester, MN
- MOF pm 03:10 **The Role of Mass Spectrometry in Newborn Screening for Krabbe Disease;** Sara E Smith¹; Jim DiPerna¹; Melissa Longua¹; Erica L Fox¹; ¹PerkinElmer Genomics, Pittsburgh, PA
- MOF pm 03:30 **An Innovative Multi Point Internal Calibrator (MPIC) Isotopic Dilution Strategy for Biomarker Quantitation by LC-MS/MS;** Shaoxia Yu¹; Guowen Liu¹; Thomas Roddy¹; Max Lein¹; Dongwei Zhu¹; Rohini Narayanaswamy¹; Unnati Kapadnis¹; Hua Yang¹; Jose Castro-Perez¹; ¹Agios Pharmaceuticals, Cambridge, MA
- MOF pm 03:50 **SASP Atlas: A Database of Senescent Cell Secretomes;** Nathan Basisty¹; Abhijit Kale¹; Okhee Jeon¹; Chisaka Kuehnemann¹; Therese Payne¹; Chirag Rao¹; Anja Holtz¹; Samah Shah¹; Judith Campisi^{1,2}; Birgit Schilling¹; ¹The Buck Institute for Research on Aging, Novato, CA; ²Lawrence Berkeley Laboratory, Berkeley, CA
- MOF pm 04:10 **One Injection Does It All: Small Molecule Drug Pharmacokinetics (PK), Drug Metabolites, and Pharmacodynamics (PD) Biomarkers;** Steven Gernhardt¹; Brendan Tierney²; Gang Xing³; Amit Kalgutkar³; Christopher Holliman²; Ragu Ramanathan²; ¹Pfizer, Groton, CT; ²Pfizer Inc., Groton, CT; ³Pfizer WRD, Cambridge, MA
- 2:30 - 4:30 pm Monday**
INSTRUMENTATION: NEW DEVELOPMENTS IN IONIZATION AND SAMPLING
Session Chair: Emmanuelle Claude (Waters Corporation)
Auditorium, Bldg A
- MOG pm 02:30 **iTrEnDi on Biomolecules and Beyond: Enhancing MS-Based Quantitative Analyses Using New in Situidiazoalkane Chemistry;** Samuel W Shields¹; Peter Pallister¹; Christian Rosales¹; Carlos R Canez^{1,2}; Karl V Wasslen¹; John Rivada¹; Chelsey Aulenback¹; Joshua Roberts¹; Fraser Colquhoun¹; Jeff Manthorpe¹; Jeffrey C. Smith¹; ¹Carleton University, Ottawa, ON; ²University of Alberta, Edmonton, AB
- MOG pm 02:50 **Integration of a Picodroplet Microfluidic Chip with Mass Spectrometry - A Step towards High Throughput Directed Evolution Screening;** Emily E. Kempa¹; Clive A. Smith²; Xin Li²; Perdita E. Barran¹; ¹The University of Manchester, Manchester, United Kingdom; ²Sphere Fluidics Limited, Cambridge, United Kingdom
- MOG pm 03:10 **Deep-ultraviolet Laser Ablation Sampling for Mass Spectrometry;** Remilekun O. Lawal¹; Fabrizio Donnarumma¹; Kermit K. Murray¹; ¹Louisiana State University, Baton Rouge, LA
- MOG pm 03:30 **Direct Thermal Analysis Methods as Sample Introduction for High-Resolution Mass Spectrometry – Molecular Level Description of Heavy Petroleum Fractions;** Christopher Paul Rüger^{1,2,3}; Uwe Käfer^{2,4}; Johann Le Maître^{3,5}; Anika Neumann^{1,2}; Oscar Lacroix Andrivet³; Marie Hubert-Roux³; Benoit Paupy⁵; Sabrina Marceau⁵; Thomas Gröger⁴; Martin Sklorz^{2,4}; Carlos Afonso³; Pierre Giusti³; Ralf Zimmermann^{1,2,4}; ¹University of Rostock, Institute of Chemistry, Division of Analytical and Technical Chemistry, Rostock, Germany; ²Joint Mass Spectrometry Centre, University of Rostock, Rostock, Germany; ³Normandy University, COBRA laboratory, Mont Saint Aignan, France; ⁴Joint Mass Spectrometry Centre, Comprehensive Molecular Analytics, Helmholtz Zentrum München, Neuherberg, Germany; ⁵Total Research & Technology Gonfreville, Harfleur, France
- MOG pm 03:50 **More Inclusive Ionization Demonstrated for Direct Bacteria Differentiation by Combining Automated ESI, MAI, and SAI Methods;** Charles N McEwen¹; Darrell Marshall²; Santosh Karki^{2,3}; Milan Pophristic²; Khoa Hoang¹; Sarah Trimpin³; Adetoun Adeniji-Adele¹; John W Tomsho¹; ¹Univ. of the Sciences, Philadelphia, PA; ²MSTM, LLC, Newark, DE; ³Wayne State University, Detroit, MI
- MOG pm 04:10 **T-MALDI-2-Orbitrap MS: Sensitive Ion Imaging with Sub-Micrometer Resolution and ppm Mass Accuracy;** Marcel Niehaus¹; Jens Soltwisch^{1,2}; Mikhail Belov³; Klaus Dreisewerd^{1,2}; ¹Institute of



Hygiene, University of Münster, Münster, Germany;
²Interdisciplinary Center for Clinical Research
(IZKF), University of Münster, Münster, Germany;
³Spectrograph, LLC, Kennewick, WA

2:30 - 4:30 pm Monday
ART, ARCHAEOLOGY, AND PALEONTOLOGY

Session Chair: Julie Arslanoglu
(The Metropolitan Museum of Art)
A411-412

MOH pm 02:30 **New Molecular Evidence of Restoration Treatments Applied to Historic Coptic Manuscripts Using Protein Crosslinking and Top Down Proteomics;** Francesca Galluzzi^{1,2}; Catherine M. Rawlins^{1,2}; Stéphane Claverol²; Federica Pozzi³; Maria Fredericks⁴; Franck Trujillo⁴; Caroline Tokarski^{1,2}; ¹Institute of Chemistry and Biology of Membrane and NanoObjects, UMR CNRS 5248, Bordeaux, France; ²Proteome Platform, Center of Functional Genomics of Bordeaux, University of Bordeaux, Bordeaux, France; ³Department of Scientific Research, The Metropolitan Museum of Art, New York, NY; ⁴Thaw Conservation Center, The Morgan Library & Museum, New York, NY

MOH pm 02:50 **A Minimally Invasive and Portable Tool for MS Identification of Proteins in Ancient Paintings;** Georgia Ntasi¹; Paola Cicatiello¹; Gennaro Marino^{1,2}; Paola Giardina¹; Leila Birolo¹; ¹Dept. Chemical Sciences, University of Naples Federico II, Naples, Italy, Naples, Italy; ²BIOGEM Institute, Ariano Irpino (AV), Italy, Ariano Irpino (AV), Italy

MOH pm 03:10 **Early Pleistocene (1.8 million years old) Enamel Proteome Sequences Resolve Stephanorhinus phylogeny;** Enrico Cappellini¹; Frido Welker¹; Jazmin Ramos Madrigal¹; Diana Samodova²; Patrick L. Ruether²; Jesper V. Olsen²; David Lordkipanidze³; Eske Willerslev¹; ¹Natural History Museum of Denmark, Copenhagen, Denmark; ²NNF Center for Protein Research University of Copenhagen, Copenhagen, Denmark; ³Georgian National Museum, Tbilisi, Georgia

MOH pm 03:30 **Single-Pot Solid-Phase-Enhanced Sample Preparation (SP3) for Bone Paleoproteomics;** Timothy Cleland; Museum Conservation Institute, Smithsonian Institution, Suitland, MD

MOH pm 03:50 **DeamiDATE 1.0: Site-Specific Deamidation as a Tool to Assess Authenticity of Members of Ancient Proteomes;** Abigail Ramsøe^{1,2}; Vivian van Heekeren¹; Ian Barnes²; Camilla Speller³; Matthew J Collins^{4,5}; ¹BioArCh, Department of Archaeology, University of York, York, United Kingdom; ²Department of Earth Sciences, Natural History Museum, London, United Kingdom; ³Department of Anthropology, University of British Columbia, Vancouver, BC; ⁴EvoGenomics Section, Natural History Museum of Denmark, University of Copenhagen, Copenhagen, Denmark; ⁵McDonald Institute for Archaeological Research, Downing St, Cambridge, United Kingdom

MOH pm 04:10 **A Proteomic Workflow to Extract, Concentrate, Digest, and Enrich Peptides from Fossils with High Humic Content for Mass Spectrometry Analyses;** Elena R. Schroeter¹; Kevin Blackburn²; Michael B. Goshe¹; Mary H. Schweitzer¹; ¹North Carolina State University, Raleigh, NC; ²Waters Corporation, Milford, MA

4:45-5:30 pm Monday
AWARD LECTURE
Richard A. Yost (University of Florida), presiding
Murphy Ballroom, Bldg B, Level 5

Presentation of the AI Yergey MS Scientist Award
Jeffrey Shabanowitz, University of Virginia



John B. Fenn Award for a Distinguished Contribution in Mass Spectrometry

John R. Yates III
The Scripps Research Center

5:45 - 7:00 PM MONDAY WORKSHOPS

There will be light refreshments in Building A foyers. All workshops are in Building A.

01 High Spatial Resolution 2D and 3D Mass Spectrometry Analysis: Current Trends
Presiding: Francisco Fernandez-Lima, Christopher Anderson, Gregory Fisher
A402-403

Advances on 2D and 3D Mass Spectrometry analysis currently drive research in biological, biomedical, materials, environmental and forensic sciences. With the development of new and the incorporation of hyphenated techniques during 2D and 3D MS analysis, the MS community needs to further develop universal analysis and data processing protocols; definitions; reference guidelines; standard reference materials; and inter-laboratory comparisons.

In this third workshop, we will provide a short overview of the state of the art from experts in the field and provide ample time for discussion focused on the definitions of and protocols for testing performance metrics; strategies for sample preparation; data analysis, data processing and data reporting workflows.

A preliminary list of topics will include:

- i) Fundamentals of high spatial resolution in 2D and 3D MS analysis (tutorial)
- ii) Overview of current and new imaging modalities: challenges and perspectives
- iii) Influence of instrument settings and use of standards for 2D and 3D MS imaging
- iv) 2D and 3D MS imaging data in public repositories: vendor and user's perspectives

The workshop encourages the participation and presentations of new investigators, postdocs and graduate students. A combination of short presentations (2-3 slides/group) from representatives of the 2D and 3D MS imaging techniques, with a balance between academic, national laboratories and industrial researchers will be followed by an open discussion forum. One of the goals of this workshop is to gather researchers and enable the discussion towards the development of an interest group within the ASMS community to address these new scientific challenges.



There will be light refreshments in Building A foyers. All workshops are in Building A.

**02 Enhancing MS-Based Glycomics and Glycoproteomics
Toolbox: Round-table Discussion
Presiding: Yehia Mechref
A404-405**

Glycosylation is a prevalent posttranslational modification of proteins in mammalian cells. Many proteins act through oligosaccharide recognition. Glycosylation of proteins is one of the most common protein posttranslational modifications. The glycans of the membrane or secreted glycoproteins are responsible for modulating and controlling many of the biological roles of these glycoproteins, including cell signaling, adhesion, and communication. Protein folding, stability, and localization are dependent on protein glycosylation. A correlation between changes in the glycans of glycoproteins and many mammalian diseases, such as hereditary disorders, immune deficiencies, cardiovascular disease, and cancer has been suggested. This and the biological roles of glycans have created a demand for reliable glycomics and glycoproteomics strategies, permitting sensitive monitoring of glycans in biological systems. Mass spectrometry-based glycomics and glycoproteomics methods, glycan and glycoproteins standards and bioinformatics tools are continuously being introduced. However, glycomics and glycoproteomics strategies are far from being routine or automated as proteomics strategies. This workshop will focus on discussing and highlighting what needs to be done to attain complete automation of glycomics and glycoproteomics analyses. The workshop will have a roundtable format and will not include any presentations. The workshop will be addressing questions to be solicited from glycomics and glycoproteomics experts in advance of the meeting, including but not limited to, what is hindering the automation of glycome and glycoproteome analysis, why are glycomics and glycoproteomics strategies not as routinely used as proteomics strategies, how can we overcome the lack of reliable standards, and why a uniform bioinformatics tools are lacking.

**03 MassIVE Translation of Public Mass Spectrometry Big Data
into Reusable Community Resources
Presiding: Nuno Bandeira, Mingxun Wang
A406-407**

The productive reutilization of the very large volumes of public proteomics and metabolomics mass spectrometry data continues to be hindered by significant challenges in the limited findability, accessibility and integration of datasets and reanalysis results. This workshop will focus on approaches addressing these challenges by i) systematically reanalyzing public data using open-source advanced algorithms, ii) reorganizing reanalysis results into open community-scale knowledge bases, and iii) integrating global results into freely-accessible data analysis workflows available free of charge to all research labs.

This workshop is designed to be highly interactive and will aim to inform as well as to promote discussion about ways in which public mass spectrometry big data can be made most useful for the community as a whole.

**04 Mass Spectrometry in the Developing World: Supporting
Education and Research
Presiding: Kym Faull, Giles Edwards
A408**

This will be a follow-up to the workshops on the same topic presented at the 2017 and 2018 Indianapolis and San Diego ASMS meetings. The point will be to report on progress and interest during the preceding 12 months. Students in developing nations learn about mass spectrometry from text books. They rarely if ever get to actually see one, and never get to use them. Old but working instruments that are replaced with new versions could be made available to Universities and research organizations in developing countries to be used for research and teaching purposes. This would entail shipping, installation, training and maintenance which would all require funding and support. Some aspects of maintenance and training could probably be handled remotely via email, Skype, etc. This would be a noble aspiration for ASMS to embrace. It would improve our relations with the developing

world and perhaps provide an example for other organizations (e.g. the NMR Society, etc) to follow. The Presiders will begin with a brief description of their personal experiences that stimulated them to organize this workshop. There is a need to formulate a plan of action that will assist with moving this initiative forward in the USA. There is a lot of interest but a way of cutting through the various layers of red tape that is currently impeding the mission is needed. All those interested are invited to join in a friendly and constructive discussion on this topic.

**05 Ion Trap Mass Spectrometry: Latest Trends
(Ion Trap MS Interest Group)
Presiding: Glen Jackson, Desmond Kaplan
A410**

The Ion Trap Interest Group Meeting will cover the latest trends in instrumentation and applications in ion trap mass spectrometry. Instrumentation topics will cover some of the latest developments in instrument design, miniaturization, hybrid instruments and scanning methods. Applications will cover some of the latest trends in MSn, ion/molecule and ion/ion reaction methods. The workshop will consist of lightning-fast talks to introduce the topics and extended question and answer sessions to discuss, among other details, the limitations to commercialization of new advances.

**06 FAIMS/DIMS/DMS Technology and its Impact on Current Day
MS Analyses
Presiding: Sue Abbatiello
A307**

The goal of this workshop is to provide a forum for people interested in High-field Asymmetric Waveform Ion Mobility Spectrometry (FAIMS) and Differential Ion Mobility Spectrometry (DIMS or DMS). We will go over the basics and fundamentals of how FAIMS/DIMS/DMS works, differences in hardware, the effects of different parameters on performance, and how it is different than Drift-Tube Ion Mobility (DT-IMS). Examples of applications benefiting from FAIMS/DIMS/DMS will be discussed, and attendees are invited to bring their questions and experiences of success, uncertainty, and even bad luck, to share with the community. Discussion will be led by several subject matter experts.

**07 Food Safety and Quality Applications: Tools for Putting MS
Methods into Practice
(Flavor Fragrance & Foodstuff Interest Group)
Presiding: Melanie Downs, James Redwine
A309**

Mass spectrometry can be used to solve a number of different types of food safety and quality issues, but validation and implementation of methods across diverse food products and individual scenarios can be challenging. This workshop will discuss tools currently available and in development for food safety and quality MS analysis applications, including reference materials, method validation schemes, and other resources. The format of the workshop will include brief introductory presentations from selected resource developers and users, followed by a panel discussion moderated by the interest group co-chairs.

**08 Automation for Proteomics Sample Preparation
Presiding: Michael Ford, Michael Knierman
A311**

The performance of modern mass spectrometers and liquid chromatography systems is enabling proteomics experiments with previously unobtainable throughput and sensitivity. The analysis of cohorts of 50 or more samples, with acquisition timelines of a week or so, is now routine in many labs. Combined with robust sample preparation workflows and turnkey data processing proteomics is delivering on the promise and approaching a new level of usefulness. Assay and sample type aside it is fair to say, for proteomics experiments, the bottleneck is still instrument time. That said sample preparation is a significant use of human resources and with the scale of experiments expanding so too is the associated time and investment in labor. A practical solution to ease the growing sample preparation burden is automation.



There will be light refreshments in Building A foyers. All workshops are in Building A.

Automated sample preparation solutions are not new to the field of proteomics, look back ten years or so and 2D gel spot picking and in-gel digestion robots were common. Presently, and looking ahead, however the requirements of the field have changed; solution digestion, target enrichment at the protein and proteome level and sample clean-up are a few of the time-consuming tasks that would benefit from automation. Vendors have stepped up to deliver automation solutions such as the Agilent AssayMap, ThermoFisher KingFisher and more recent low cost OpenTrons OT2. This workshop is an opportunity to get together with like-minded scientists and discuss the emerging role of automation in sample preparation for proteomics experiments and to share practical experience with automation.

09 MS Software: Peak Picking - Paramount Practises and Perilous Pitfalls

Presiding: Magnus Palmblad, Jeff Agar
A312

The MS Software workshop is aimed at anyone who either writes MS software or is interested in learning how to. In this workshop, we will discuss the state of the art in peak picking, existing solutions, and common pitfalls.

Peak picking is a vital step in the interpretation of mass spectrometry data. Peak picking algorithms and their parameters influence your abundance accuracy, your false negative (missed peaks) and false positive (noise peaks erroneously detected that go on to be assigned) rates, and can even affect your mass accuracy. Peak shapes and the concept of spectral accuracy can be used to detect chimeric, unresolved, peaks and to help define instrument performance.

Peak picking, in the simplest sense, is the process of determining the mass-to-charge ratio (m/z) and abundance of peaks in mass spectra. When MS is hyphenated with other separation techniques, peak picking can be done on multidimensional data including tandem m/z , retention time or mobility. For the purposes of the discussion in this workshop, we will focus on the one-dimensional case of peaks in a mass spectrum.

When planning this year's workshop, we polled a number of stakeholders in the community. Peak picking was the most popular topic among those suggested. Learning from the feedback from the 2018 workshop, we will allocate most of the time to discussions and have only a short introduction to the topic. We will also discuss reference datasets with ground truth suitable for evaluating peak picking algorithms.

10 Solid Phase Microextraction Approaches Applied with Mass Spectrometry Techniques

Presiding: Janusz Pawliszyn
A313

The workshop is targeted at both new and current solid phase microextraction (SPME) users. The primary goal of this workshop is to provide interested participants with deeper insight into the main principles of this technique, which will ultimately enhance the productivity and quality of the analytical results. This workshop will be of interest to analytical and clinical chemists, laboratory supervisors, scientists and industry regulators in the environmental, food and beverage, pharmaceutical, clinical, forensic, cosmetic, and industrial hygiene fields. High throughput capabilities of the technology will be emphasized in the discussions including direct coupling to mass spectrometry via direct analysis in real time (DART), coated blade spray (CBS), microfluidic open interface (MOI) and others. The unique features of in vivo SPME sampling technologies will be of particular interest to researchers in biomedical, neurobiological and life sciences.

Agenda/Speakers

- Introduction to SPME and Bio-SPME; Janusz Pawliszyn (University of Waterloo)
- Ambient Ionization and SPME: A Perfect Complement; Robert B. (Chip) Cody (JEOL USA, Inc.)

- Rapid Determination of β -agonists in Animal Urine by Coated Blade Spray - Mass Spectrometry; Marco Blokland (RIKILT Wageningen University)
- Coated Blade Spray - Mass Spectrometry (CBS-MS) for Clinical Toxicology Testing in Urine; Shirin Hooshfar (University of California, San Francisco)
- *In vivo* SPME of Eicosanoids in Brain; Dajana Vuckovic (Concordia University)
- Determination of Cannabinoids using SPME Coupled to MS/LEI via MOI Interface; Achille Cappiello (University of Urbino)

12 LC-MS Jeopardy - I'll Take Increasing Throughput for \$200 (LCMS & Related Topics Interest Group)

Presiding: Erik Soderblom, Will Thompson
A315

Need a break from formal talks? Already an expert in LC-MS and want to impress your friends? Not an expert and want to learn something about LC-MS? Just like games where you win "cash"? Well, this workshop is for you! Although the Jeopardy board has been cleared and refreshed from last year, the LC-MS and Related Topics Interest Group Workshop will remain focused on audience-driven discussions around various aspects of Proteomics, Pharmacokinetics, Metabolomics, Laboratory Automation, and Increasing Sample Throughput, all in a "Jeopardy" format! Early rounds will provide an opportunity to share, learn about, and discuss new and emerging strategies and applications in these various areas. Later rounds will be specific scenarios or analytical problems which are in need of solutions! Not only will creative, insightful, and thought provoking considerations be discussed, but will earn you and your team ASMS Jeopardy Cash (redeemable for free beers at ASMS Hospitality Suites).

13 Art and Cultural Heritage: Mass Spec Applications

Presiding: Mehdi Moini
A316

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.

14 Photoionization (APPI/PI) - Bridging the Gap between Academic and Industrial Research (Photoionization MS Interest Group)

Presiding: Sven Ehlert, Eleanor Riches, Matthias Lorenz
A303

Photoionization is a powerful tool for soft ionization mass spectrometry (PI-MS) in research and routine analytical applications. After concentrating on the fundamentals of atmospheric pressure (APPI) and vacuum (SPI and REMPI) photoionization for mass spectrometry in the last year's workshop, we want to turn our view to the future of photoionization and discuss with the attendees challenges, ideas and new approaches. One or two key thought leaders will address the topic to stimulate discussion. The focus will be on the interface between academic and industrial research - what are the specific needs, capabilities and perspectives to bridge the gap with (AP)PI MS?

As a result of last year's workshop survey, we put the focus of this workshop on the discussion between participants. If it is appropriate and there is sufficient time, there will also be the chance for attendees to share novel and exciting developments with the PI community. Furthermore, we want to give attendees with different experience levels the opportunity to get in contact to discuss challenges as well as ask questions to the experts and more experienced users.



There will be light refreshments in Building A foyers. All workshops are in Building A.

Together with the attendees, we want to reveal the advantages, capabilities and diversity of photoionization mass spectrometry to support its dissemination into laboratories worldwide.

15 MS-Based Multi-Attribute Method (MAM): The Future of Biotherapeutic Development Analytics (Biotherapeutics Interest Group)
Presiding: Andrew Dawdy, Hao Zhang

A302

Join our panel of experts to discuss the future of MAM, an emerging mass spectrometry-based methodology with the potential to significantly transform standard analytical practice for biotherapeutic development across the biopharma industry. In the development of biotherapeutics, a thorough understanding of a molecule's product quality attributes (PQAs) and their effect on its structure and function is essential for ensuring safety and efficacy of the clinical trial material. Numerous routine chromatographic and electrophoretic assays, intended for batch release, are used to characterize and monitor the PQAs that contribute to product-related heterogeneity such as N-glycosylation, charge isoforms, oxidation, fragmentation, and aggregation. However, execution of multiple routine methods for batch release, stability time-points, and process/formulation development support becomes time and resource intensive, and often provides an indirect measure of biologically-relevant PQAs. Recently, a liquid chromatography-mass spectrometry-based multi-attribute method (MAM) has arisen (Rogers et al., AAPS J, 2017) as an improved means for detecting, identifying, and quantitating a multitude of PQAs in an automated fashion by a single assay. In its short public lifespan, MAM's popularity has exploded as evidenced by the formation of an industry-wide MAM Consortium, assessment of its suitability by the FDA, and the rapid growth in MAM-centric products from numerous vendors. MAM is poised to revolutionize the biopharmaceutical industry if fully embraced and adopted. This workshop will provide a forum to discuss the status of MAM and address existing challenges. Topics may include sample preparation, instrumentation, software/data processing, hotspot characterization, new peak detection, regulatory acceptance, qualification and validation, and more.

16 MS Career Options: How to Kick Start Your Career (Young Mass Spectrometrists Interest Group)
Presiding: Veronica Anania, Sharon Pitteri

A301

This workshop features a panel discussion on professional development in the area of mass spectrometry. Topics will be focused on career planning and management, fundamental training, industrial internship, job search tools and interview strategies. The panel, consisting of representatives from industrial and academic organizations, will share their knowledge and practices on career prospects.

17 Membrane Proteins, Nanodiscs, and Beyond: MS Analysis in Academia and Industry
Presiding: Iain Campuzano, Michael Marty

A305

Membrane proteins make up over 50% of possible "druggable" targets, making them very attractive targets for academic and industrial research. Membrane proteins are inherently insoluble in aqueous solvents and require the presence of lipid or detergent to remain soluble, which makes their analysis by many biophysical techniques such as native mass spectrometry (MS) and x-ray crystallography very challenging. However, over the past 10 to 15 years, researchers have begun to overcome such hurdles and are now producing native intact mass spectra for membrane protein complexes of ion channels, membrane bound receptor molecules, transporters, and fully assembled lipoprotein nanodiscs.

Most of this pioneering work has been focused on native MS in the academic environment. Native MS analysis of membrane proteins within the pharmaceutical industry is still in its infancy compared to established structural biology techniques such as x-ray diffraction and cryo-EM.

Within this workshop, we will discuss MS experiments for characterizing intact membrane proteins under denaturing and native conditions, focusing on current protocols used within both academia and industry for native MS analysis of membrane protein solubilized in "MS-friendly" detergents. We will also discuss how these techniques can be used to support the structural biology and drug discovery efforts within the pharmaceutical industry.

The workshop will be a panel discussion format where general and detailed topics can be discussed.

A preliminary list of discussion topics will include:

- MS determination of membrane proteins using denaturing LC and MS conditions
- Membrane protein purification and detergent screening for optimal MS analysis
- Native MS instrumentation and analysis of membrane proteins
- New frontiers in membrane mimetics: nanodiscs and beyond
- The industrial perspective on membrane protein MS

18 Energy, Petroleum, and Biofuels MS: Targeted Analysis, Fingerprinting and Speciation in Complex Mixtures (Energy Petroleum & Biofuels Interest Group)
Presiding: Marianny Combariza, Amy McKenna

A304

Fossil- and bio- fuels are complex mixtures containing thousands of compounds with different molecular compositions; which in turn determine macroscopic properties. In petroleum chemistry, for instance, low MW components of low and medium polarity are well studied and understood. However, trace amounts of heavier and polar components, less known compositionally, are usually very reactive and responsible for many problems. For instance, asphaltene, naphthenic acids and metal complexes can cause aggregate formation, corrosion and catalyst poisoning, during transport, storage and refining of petroleum. Yet, due to lower ionization efficiencies than their low MW counterparts, these compounds remain undetected in direct infusion MS analysis of the whole oil.

Correlating compositional data to macroscopic behavior is paramount to future energy research, with HRMS playing a vital role at providing molecular information. Complex organic mixture analysis by MS has prompted development of novel ionization sources and techniques, off- and on-line chromatographic methods, and data processing algorithms. Despite many efforts to overcome the limitation of ion suppression in these polydisperse systems, compound classes present in low concentration still remain undetected. Often, these species are responsible for performance issues of final products derived from the raw feeds. Therefore, targeted analysis, fingerprinting and selective speciation of chemical functional groups is emerging as the next big advancement in MS of complex mixtures. In this workshop, practitioners from these areas will present the development and applicability of their strategies of analysis, and will participate in a panel discussion with the audience.

Topics: Selective ionization, selective fractionation, derivatization, structure-related separation.



From 7:00 am Tuesday
CORPORATE BREAKFAST SEMINARS
CONVENTION CENTER AND OMNI CNN CENTER HOTEL
See page 16 for detailed schedule. Reservation or RSVP required.

8:30 - 10:30 pm Tuesday
INFORMATICS: INNOVATIONS

Session Chair: David Stranz (Sierra Analytics, Inc.)
Murphy Ballroom, Bldg B, Level 5

- TOA am 08:30 **Differential Mass Spectra (ΔS) and Differential Ion Currents ($\Delta I C$) for Smarter Mass Spectrometer Operation and Data Interpretation;** Changtong Hao¹; Thomas Lee Collier^{1,2}; Lawrence Klecha¹; Simon Prosser¹; Daniel Eikel¹; ¹Advion Inc., Ithaca, NY; ²Harvard Medical School, Boston, MA
- TOA am 08:50 **XNet: A Bayesian Approach to Extracted Ion Chromatogram Clustering for Precursor Mass Spectrometry Data;** Mathew M Gutierrez¹; Kyle Handy¹; Rob Smith¹; ¹University of Montana Missoula, MT
- TOA am 09:10 **KairosMS: Processing of Complex Mixture Data Analyzed by Hyphenated Ultrahigh Resolution Mass Spectrometry;** Remy Gavar¹; Hugh E. Jones¹; Diana Catalina Palacio Lozano¹; Mary J. Thomas¹; David Rossell^{1,2}; Simon E. F. Spencer¹; Mark P. Barrow¹; ¹University of Warwick, Coventry, United Kingdom; ²Universitat Pompeu Fabra, Barcelona, Spain
- TOA am 09:30 **Zero-Knowledge *de novo* and the Alphabet Projection of Spectra;** Patrick Kreitzberg¹; Marshall Bern²; Oliver Serang¹; ¹University of Montana, Missoula, MT; ²Protein Metrics Inc., San Carlos, CA
- TOA am 09:50 **Fast and Accurate Estimation of Relative Molecule Abundance and Resolution of Overlapping Isotopic Envelopes Using Optimal Transport Theory;** Michał Aleksander Ciach^{1,2}; Grzegorz Skoraczynski¹; Szymon Majewski³; Błażej Miasojedow¹; Michał Piotr Startek¹; Dirk Valkenborg^{2,4,5}; Anna Gambin¹; ¹Faculty of Mathematics, Informatics and Mechanics, University of Warsaw, Warsaw, Poland; ²Centre for Statistics, Hasselt University, Diepenbeek, Belgium; ³Mathematical Institute of the Polish Academy of Sciences, Warsaw, Poland; ⁴UA-VITO Center for Proteomics, University of Antwerp, Antwerp, Belgium; ⁵Applied Bio and Molecular Systems, Flemish Institute for Technological Research (VITO), Mol, Belgium
- TOA am 10:10 ***ab initio* Prediction of Peptide Tandem Mass Spectra;** Kaiyuan Liu¹; Sujun Li¹; Lei Wang¹; Yuzhen Ye¹; Haixu Tang¹; ¹Indiana University, Bloomington, IN

8:30 - 10:30 pm Tuesday
FUNDAMENTALS: PHOTOIONIZATION AND PHOTODISSOCIATION

Session Chair: Hendrik Kersten (University of Wuppertal)
B401-402

- TOB am 08:30 **APPI-MS Analysis of Endohedral Fullerenes;** Julie Herniman¹; G. John Langley¹; Sally Bloodworth¹; Richard J Whitby¹; Gabriela Sitinova¹; ¹University of Southampton, Southampton, United Kingdom
- TOB am 08:50 **Right-Angle Ion Mirror-Prism (RAIMP): First Experiments with the Novel Time-of-Flight Mass Analyzer;** Igor V. Veryovkin¹; Raveendra C. Wickramasinghe¹; Igor L. Bolotin¹; Jason M. Gross¹; C. Emil Tripa¹; Luke Hanley¹; ¹University of Illinois at Chicago (UIC), Chicago, IL

- TOB am 09:10 **Improved Top-Down *de novo* Sequencing of Denatured and Native Proteins Using Hybrid Ion Activation Methods;** Weijing Liu¹; Kira Vyatkina²; Jared B. Shaw¹; ¹Pacific Northwest National Laboratory, Richland, WA; ²St. Petersburg Academic University, St. Petersburg, Russia
- TOB am 09:30 **Peptide and protein fragmentation using 193 nm UVPD on a Q-IM-TOF platform;** Alyssa Q. Stiving^{1,2}; Sophie R. Harvey^{1,2}; Benjamin J. Jones^{2,3}; Bruno Bellina⁴; Perdita E. Barran⁵; Jeffery M. Brown⁶; Vicki H. Wysocki^{2,3}; ¹The Ohio State University, Columbus, OH; ²Resource for Native Mass Spectrometry Guided Structural Biology, The Ohio State University, Columbus, OH; ³The Ohio State University, Columbus, OH; ⁴Manchester Institute of Biotechnology, University of Manchester, United Kingdom; ⁵Manchester Institute of Biotechnology, University of Manchester, United Kingdom; ⁶Waters Corporation, Wilmslow, United Kingdom
- TOB am 09:50 **Enhanced Characterization of Membrane Protein Complexes Using Ultraviolet Photodissociation;** Sarah N Sipe¹; John W Patrick²; Arthur Laganowsky²; Jennifer S Brodbelt¹; ¹Department of Chemistry, University of Texas, Austin, TX; ²Department of Chemistry, Texas A&M University, College Station, TX
- TOB am 10:10 **Chiral Analysis Base on Mass Spectrometry and Photodissociation Spectroscopy in the Gas Phase: from IR to UV;** Xianglei Kong; Nankai University, Tianjin, China

8:30 - 10:30 pm Tuesday
NATIVE MS IN STRUCTURAL BIOLOGY

Session Chair: Rita Grandori (University of Milano-Bicocca)
B405-407

- TOC am 08:30 **Native MS-Based Platform for Screening Optimal Conditions in Preparing Intact Macromolecular Assemblies for cryo-EM Analysis;** Paul Dominic B. Olinares¹; Courtney Chiu²; Jin Young Kang²; Eliza Llewellyn²; James Chen²; Ruth Saecker²; Elizabeth Campbell²; Seth Darst²; Brian T. Chait¹; ¹Laboratory of Mass Spectrometry & Gaseous Ion Chemistry, The Rockefeller University, New York, NY; ²Laboratory of Molecular Biophysics, The Rockefeller University, New York, NY
- TOC am 08:50 **Exploring the Structure and Specificity of Antimicrobial Peptides in Lipid Nanodiscs by Native MS;** Larry Walker¹; Elaine Marzluff²; Marius Kostelic¹; Julia Townsend¹; Michael Thomas Marty¹; ¹University of Arizona, Tucson, AZ; ²Grinnell College, Grinnell, IA
- TOC am 09:10 **Interaction of Metals with Amyloid Beta and Alpha-Synuclein Studied by Native FTICR-MS with Advanced Dissociation Methods;** Frederik Lermyte¹; Francesca Bellingeri¹; James Everett²; Jake Brooks¹; Yuko P. Y. Lam¹; Christopher A. Wootton¹; Mark P. Barrow¹; Peter J. Sadler¹; Neil D. Telling²; Joanna F. Collingwood¹; Peter B. O'Connor¹; ¹University of Warwick, Coventry, United Kingdom; ²Keele University, Stoke-on-Trent, United Kingdom
- TOC am 09:30 **Development of High Throughput Online Native LC/MS;** Chris Nortcliffe¹; Esme Candish²; Sibylle Heidelberger³; Ferran Sanchez⁴; Sean McCarthy²; ¹AB Sciex UK Ltd, Warrington, United Kingdom; ²Sciex, Framingham, MA; ³SCIEX, Warrington, United Kingdom; ⁴SCIEX, Darmstadt, Germany



TUESDAY MORNING ORAL SESSIONS

TOC am 09:50 **Analysis of Diubiquitin Chains by Variable-Temperature Electrospray Ionization Provides Evidence for Seven Non-Native Solution States and Stabilities;** Lucas W. Henderson¹; Tarick J. El-Baba¹; Shannon A. Raab¹; Christopher J. Brown¹; Daniel W. Woodall¹; David E. Clemmer¹; ¹Department of Chemistry, Indiana University, Bloomington, IN

TOC am 10:10 **Multistage Native MS Enables Direct Identification of Unknown Ligands Bound to Protein Assemblies;** Joseph F. Gault¹; Ildir Liko²; Michael Landreh³; Hsin-Yung Yen²; Denis Shutin¹; Rosa Viner⁴; Romain Huguet⁴; Christopher Mullen⁴; John E. P. Syka⁴; Jesse D Canterbury⁴; Philip M Remes⁴; Graeme McAlister⁴; Carol V. Robinson¹; ¹Oxford University, Oxford, United Kingdom; ²OMass Therapeutics, Oxford, United Kingdom; ³Karolinska Institutet, Stockholm, Sweden; ⁴Thermo Fisher Scientific, San Jose, CA

8:30 - 10:30 pm Tuesday

IMAGING: PHARMACEUTICALS, METABOLITES, AND LIPIDS

Session Chair: Uwe Karst (University of Münster)

B302-305

TOD am 08:30 **High-Performance MS Strategies Provide Detailed Insights into Neglected Tropical Diseases and Infection Mechanisms;** Bernhard Spengler¹; Stefanie Gerbig¹; Patrik Kadesch¹; Parviz Ghezellou¹; Simone Häberlein²; Christoph G. Greveling²; Katja Becker³; Anja Taubert²; Carlos Hermosilla²; ¹Analytical Chemistry, Giessen, Germany; ²Institute of Parasitology, Giessen, Germany; ³Biochemistry and Molecular Biology, Giessen, Germany

TOD am 08:50 **MALDI Mass Spectrometry Imaging of Alzheimer's Disease Human Brain Tissue Reveals Distributions of Functionally Important Metabolites;** Abby S. Gelb^{1,2}; Nivedita Bhattacharya²; Weiming Xia^{1,2}; Catherine E. Costello²; ¹Edith Nourse Rogers Memorial Veterans Hospital, Geriatric Research Education & Clinical Center, Bedford, MA; ²Boston University School of Medicine, Boston, MA

TOD am 09:10 **Lessons Learned from Mice and Cheese: Investigating Diffusion Processes by MALDI MS Imaging;** Julia Kokesch-Himmelreich¹; Alan M. Race¹; Axel Treu¹; Claus Schlicht²; Ulrich Busch²; Kerstin Walter³; Christoph Hölscher³; Andreas Römpf¹; ¹University of Bayreuth, Bayreuth, Germany; ²Bavarian Health and Food Safety Authority, Oberschleißheim, Germany; ³Research Center Borstel, Borstel, Germany

TOD am 09:30 **Simultaneous Lipids/Metabolites Imaging (1 µm Resolution) of Traumatic Brain Injury Tissue Using Gas Cluster Ion Beam Secondary Ion Mass Spectrometry (GCIB-SIMS);** Hua Tian¹; Louis J. Sparvero^{2,3}; Andrew A. Amoscato^{2,4}; Valerian E. Kagan^{2,4,5}; Hülya Bayir^{2,4,6}; John C. Vickerman⁷; Peter J. Cumpson⁸; Nicholas Winograd¹; ¹Department of Chemistry, Pennsylvania State University, University Park, PA; ²Department of Environmental and Occupational Health, University of Pittsburgh, Pittsburgh, PA; ³Center for Free Radical and Antioxidant Health, Pittsburgh, PA; ⁴Center for Free Radical and Antioxidant Health, University of Pittsburgh, Pittsburgh, PA; ⁵Departments of Chemistry, Pharmacology and Chemical Biology, Radiation Oncology, University of Pittsburgh, Pittsburgh, PA; ⁶Department of Critical

Care Medicine, and Safar Center for Resuscitation Research, University of Pittsburgh, Pittsburgh, PA; ⁷School of Chemical Engineering and Analytical Science, The University of Manchester, Manchester, United Kingdom; ⁸Mark Wainwright Analytical Centre, the University of New South Wales, Sydney, Australia

TOD am 09:50 **Dual Mode Mass Spectrometry Imaging to Probe the Inflammatory Properties of Nanoparticle Stabilized Capsules;** Kristen Sikora¹; Joseph M Hardie¹; Vincent M Rotello¹; Richard W. Vachet¹; ¹University of Massachusetts, Amherst, MA

TOD am 10:10 **Correlated Chemical Mapping of Multiple Compounds and Metabolites in Rat Tissues;** Gary J Van Berkel¹; Thomas R. Covey²; Chang Liu²; Bryce Young²; Robert Johnson³; Christopher DeBenedetto³; Danielle Diaz³; Adam Bentley³; James Glick³; Jimmy Flarakos³; ¹Gary Van Berkel LLC, Oak Ridge, Tennessee; ²SCIEX, Concord, ON; ³Novartis Institutes for BioMedical Research, East Hanover, NJ

8:30 - 10:30 pm Tuesday

ENVIRONMENTAL: EMERGING CONTAMINANTS

(IN HONOR OF RON HITES)

Session Chair: Susana Y. Kimura (University of Calgary)

B308-309

TOE am 08:30 **Nontargeted Identification of Antioxidants in the Environment;** Ronald A. Hites¹; Yan Wu¹; Marta Venier¹; ¹Indiana University, Bloomington, IN

TOE am 08:50 **Stable Isotopic Labeling and Nontargeted Identification of ng/L Amino-Contaminants in Water;** Zhongshan Liu¹; Guang Huang¹; Ping Jiang¹; Lindsay Jmaiff Blackstock¹; Xing-Fang Li¹; ¹University of Alberta, Edmonton, AB

TOE am 09:10 **Organic Pollutants in the Snow of Franz Joseph Land. Expedition 2017;** Dmitrii Mazur^{1,2}; Dmitrii Kosyakov²; Aleksandr Kozhevnikov²; Thomas Latkin²; Evgeniy Varakin²; Oleg Khoroshev²; Albert T Lebedev¹; ¹Moscow State University, Moscow, Russia; ²Lomonosov Northern (Arctic) Federal University, Centre of collective usage "Arctica", Arkhangelsk, Russia

TOE am 09:30 **Design and Initial Findings of EPA's Non-Targeted Analysis Collaborative Trial (ENTACT);** Jon R Sobus¹; Elin Ulrich²; Jarod Grossman^{3,4}; Alex Chao³; Randolph Singh^{5,6}; Christopher Grulke⁷; Ann Richard⁷; Andrew McEachran⁵; Seth Newton²; Mark Strynar²; Kamel Mansour^{5,6}; Antony Williams⁷; ¹US EPA, Research Triangle Park, NC; ²US EPA, National Exposure Research Laboratory, Research Triangle Park, NC; ³Student Contractor, US EPA, Research Triangle Park, NC; ⁴Agilent Technologies, Inc., Santa Clara, CA; ⁵ORISE Participant, US EPA, Research Triangle Park, NC; ⁶University of Luxembourg · Luxembourg Centre for Systems Biomedicine (LCSB), Luxembourg City, Luxembourg; ⁷US EPA, National Center for Computational Toxicology, Research Triangle Park, NC; ⁸Integrated Laboratory Systems, Inc., Contractor to National Toxicology Program, National Institute of Environmental Health Sciences, Morrisville, NC

TOE am 09:50 **Multidimensional Fractionation and Molecular Characterization of Lingering Oil Compounds in Coastal Sediments: A Nine Year Evolution;** Amy McKenna¹; Huan Chen¹; Cameron C. Davis¹; Donald F Smith¹; Sydney Niles^{1,2}; Chad R. Weisbrod¹; Gregory T. Blakney¹; Aixin Hou³; Qianxin Lin³; Ryan P. Rodgers^{1,2}; ¹National High Magnetic Field



- Laboratory, Florida State University, Tallahassee, FL; ²Florida State University, Tallahassee, FL; ³Louisiana State University, Baton Rouge, LA
- TOE am 10:10 **Advancing a Full Picture on Water-Soluble Synthetic Polymers in Wastewater- Different Ionization Strategies for Homologue Series Detection**; [Teresa Mairinger](#)¹; Martin Loos²; Juliane Hollender^{1,3}; ¹EAWAG: Swiss Federal Institute of Aquatic Science and Technology, Dübendorf, Switzerland; ²looscomputing, Zurich, Switzerland; ³Institute of Biogeochemistry and Pollutant Dynamics, ETH Zurich, Zurich, Switzerland
- 8:30 - 10:30 pm Tuesday**
PROTEIN-LIGAND INTERACTIONS
Session Chair: Justin Benesch (University of Oxford)
B312-314
- TOF am 08:30 **Semi-Tryptic Peptide Enrichment Strategy for Protein-Ligand Interaction Analysis on the Proteomic Scale Using Limited Proteolysis**; [Michael C. Fitzgerald](#)¹; Renza Ma¹; Do-Yeon Kwon¹; Tesia Stevenson¹; Hyeri Park¹; Jiyong Hong¹; ¹Duke University, Durham, NC
- TOF am 08:50 **Interactions between Integrin and Ligands: Conformational Changes upon Binding to RDG-type receptors**; [Roxana E. Iacob](#)¹; Yang Su²; Timothy A. Springer³; John R. Engen¹; ¹Northeastern University, Boston, MA; ²Harvard Medical School, Boston, MA; ³Harvard Medical School, Boston, MA
- TOF am 09:10 **A Single Experiment (LITPOMS) Reveals Composite Conformational Changes, Order of Binding, and Affinities for Calcium Binding to Calmodulin**; [Roger \(Xiaoran\) Liu](#)¹; Mengru Zhang¹; Don L. Rempel¹; Michael L. Gross¹; ¹Washington University, St. Louis, MO
- TOF am 09:30 **Ion Mobility-Mass Spectrometry of Peptidomimetic- α Complexes: Towards Generalized Amyloid Inhibitors**; [Yilin Han](#)¹; Neha Jain²; Varun V. Gadkari³; Elizabeth Gichana³; Fredrick Almqvist⁴; Magdalena I. Ivanova³; Matthew T. Chapman³; Brandon T. Ruotolo³; ¹University of Michigan, Ann Arbor, MI; ²Ahmedabad University, Ahmedabad, India; ³University of Michigan, Ann Arbor, MI; ⁴Umeå University, Umeå, Sweden
- TOF am 09:50 **Combining Native Mass Spectrometry with Ion Mobility and Top-Down Approaches Provides Unique Insights into the Dynamics of Protein-RNA Interactions**; [Rebecca J. D'Esposito](#)¹; Alice Sosic¹; [Daniele Fabris](#)¹; ¹The RNA Institute, University at Albany, Albany, NY
- TOF am 10:10 **Quantifying Soluble Protein Interactions with Glycolipids in Model Membranes**; [Ling Han](#)¹; Michele Richards¹; Elena N Kitova¹; John Klassen¹; ¹University of Alberta, Edmonton, AB
- 8:30 - 10:30 pm Tuesday**
MS IN THE QC LAB
Session Chair: Richard Rogers (Just Biotherapeutics)
Auditorium, Bldg A
- TOG am 08:30 **A Software Tool for Automated, Fast, Flexible and Comprehensive Quality Control Analysis of Shotgun Proteomics Raw-Files**; [Christian D. Kelstrup](#)¹; Martin Rykaer¹; Jeppe Madsen¹; Jesper V. Olsen¹; ¹CPR, University of Copenhagen, Copenhagen N, Denmark
- TOG am 08:50 **QC Benchmark: A Streamlined Web Application to Comprehensively Evaluate Instrument Performance and Direct Troubleshooting**; [Benjamin Neely](#)¹; Magnus Palmblad²; ¹National Institute of Standards and Technology, Charleston, SC; ²Leiden University Medical Center, Center for Proteomics and Metabolomics, Leiden, Netherlands
- TOG am 09:10 **Multi-Attribute Method Evaluation of the High Resolution X500B Quadrupole Time-of-Flight System**; [Monica Sadek](#)¹; Frank Macchi¹; Chengfeng Ren¹; Benjamin Moore¹; ¹Genentech, Inc., South San Francisco, CA
- TOG am 09:30 **Meeting the Challenges of Implementing Accurate-Mass Mass Spectrometry for Biotherapeutic Development in Regulated/ Non-Regulated Environments**; [Henry Shion](#)¹; Mellisa Ly²; Nilini Ranbaduge¹; Ximo Zhang¹; Yun Adelyunas¹; Jonathan Pugh³; Robert Lewis³; Jill Lord³; Mark Halifax³; Nick Tomczyk³; Ying-Qing Yu¹; Jason Rouse²; Weibin Chen¹; ¹Waters Corporation, Milford, MA; ²Pfizer, Andover, MA; ³Waters Corporation, Wilmslow, United Kingdom
- TOG am 09:50 **Understanding Biotherapeutic Product Quality Attributes through a Multi-Attribute Method (MAM) Lab-of-the-Future**; [Andrew William Dawdy](#)¹; Kristin Boggio²; Keith Lutke¹; Anastasiya Manuilov²; Tiffany Medwid¹; Halyna Narepekha¹; Wenqin Ni²; Nataliya Parahuz¹; Himakshi Patel²; Thomas Powers¹; David Ripley²; Amy Schmidt²; Justin Sperry¹; Matthew Thompson²; Joshua Woods¹; Ying Zhang²; Richard Cornell²; Sonia Taktak²; Carly Daniels¹; Keith Johnson²; Olga Friese¹; Jason Rouse²; ¹Pfizer, Chesterfield, MO; ²Pfizer, Andover, MA
- TOG am 10:10 **Strategies and Practices for Implementing Multi-Attribute Method (MAM) in GMP Environment**; [Da Ren](#); Amgen Inc., Thousand Oaks, CA
- 8:30 - 10:30 pm Tuesday**
NUCLEIC ACIDS AND OLIGONUCLEOTIDES
Session Chair: Satoko Akashi (Yokohama City University)
A411-412
- TOH am 08:30 **Nucleic Acids Biophysics by In-Solution HDX/ Native MS**; [Eric Lary](#)¹; Laura Fricot¹; Anaïs Ferrer¹; Valérie Gabelica¹; ¹Université de Bordeaux, INSERM U1212, CNRS UMR 5320, IECB, Pessac, France
- TOH am 08:50 **Duplex and Triplex siRNA-mAb Conjugate Product Confirmation for Pharma: Positive or Negative Native nESI MS**; [Iain D G Campuzano](#)¹; Carter Lantz²; Chawita Netirojanakul³; Sara C Humphreys⁴; Mai B Thayer⁴; Joseph A Loo²; ¹Amgen Inc., Thousand Oaks, CA; ²UCLA, Los Angeles, CA; ³Amgen, Inc., Thousand Oaks, CA; ⁴Amgen, South San Francisco
- TOH am 09:10 **Combining Different Solution Denaturation Techniques to Expand the Limits of Top-Down Analysis of Large Ribonucleic Acids**; [Will McIntyre](#)¹; Thomas Kenderdine¹; Botros Toro¹; Ryan Treen¹; Alice Sosic¹; Daniele Fabris¹; ¹SUNY Albany, NY
- TOH am 09:30 **Using Nucleic Acid Stable Isotope Labeling Mass Spectrometry (NAIL-MS) to Unlock the Mysteries Surrounding RNA Modifications**; [Kayla Borland](#)¹; Felix Hagelskamp¹; Valentin Reichle¹; Matthias Heiss¹; Stefanie Kellner¹; ¹Ludwig-Maximilians-University, Munich, Germany
- TOH am 09:50 **The Landscape of Post-Transcriptional Modifications in Human tRNA**; [Hendrik Weisser](#)¹; Jack Rogan¹; Byron Andrews¹; ¹STORM Therapeutics Limited, Cambridge, United Kingdom



TUESDAY MORNING AND AFTERNOON ORAL SESSIONS

TOH am 10:10 **The Role of Bioanalytical Assays in Supporting the Development of a siRNA Nanoparticle Drug;** Uma Kavita¹; Neil Mathias¹; Fulya Akpinar¹; Giridhar S. Tirucherai¹; Renuka C. Pillutla¹; Qin C. Ji¹; ¹Bristol-Myers Squibb Co., Princeton, NJ

10:30 am - 2:30 pm Tuesday

TUESDAY POSTER SESSION

Poster/Exhibit Hall ground level

Lunch concessions are open 11:00 am - 2:00 pm

Odd-number posters present:

10:30 am - 11:30 am PLUS 12:30 - 2:30 pm

Even-number posters present:

10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

Poster Pick-Me-Up Snacks served at 1:30 pm



TUESDAY AFTERNOON ORAL SESSIONS

2:30 - 4:30 pm Tuesday

INFORMATICS: DATA-INDEPENDENT ACQUISITION

Session Chair: Bernd Wollschäe (Institute of Molecular Systems Biology, ETH Zürich)

Murphy Ballroom, Bldg B, Level 5

TOA pm 02:30 **Mobi-DIK (Ion Mobility DIA Analysis Kit): Targeted Analysis Software for diaPASEF Data Improves Proteome Coverage;** Annie Ha¹; Max Frank¹; Florian Meier²; Andreas-David Brunner²; Stephanie Kaspar-Schönefeld³; Scarlet Koch³; Markus Lubeck³; Oliver Raether³; Ben C Collins⁴; Ruedi Aebersold⁴; Matthias Mann^{2,5}; Hannes Röst¹; ¹Donnelly Centre for Cell and Molecular Research, University of Toronto, Toronto, ON; ²Max Planck Institute of Biochemistry, Martinsried, Germany; ³Bruker Daltonik GmbH, Bremen, Germany; ⁴ETH Zurich, Zurich, Switzerland; ⁵NNF Center for Protein Research University of Copenhagen, Copenhagen, Denmark

TOA pm 02:50 **“Library-Free” DIA Analysis: Using Proteome-Wide in-silico Generated Spectral Libraries by ProSift for DIA Data Analysis;** Tobias Schmidt¹; Daniel P Zolg¹; Siegfried Gessulat^{1,2}; Oliver M. Bernhardt³; Tejas Gandhi³; Patroklos Samaras¹; Martin Frejno¹; Hans-Christian Ehrlich²; Lukas Reiter³; Bernhard Kuster¹; Mathias Wilhelm¹; ¹Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; ²SAP SE, Potsdam, Germany; ³Biognosys, Schlieren, Switzerland

TOA pm 03:10 **Increasing the Dynamic Range of Data Independent Acquisition (DIA) by Fusing BoxCar MS1 With Segmented MS2;** Florian Meier¹; Roland Bruderer²; Oliver M. Bernhardt²; Tabiwang N. Arrey³; Tejas Gandhi²; Yue Xuan⁴; Oliver Lange³; Alexander Makarov³; Alexander Harder³; Lukas Reiter²; Matthias Mann¹; ¹Max Planck Institute of Biochemistry, Martinsried, Germany; ²Biognosys AG, Schlieren, Switzerland; ³Thermo Fisher Scientific, Bremen, Germany; ⁴Thermo Fisher Scientific, Bremen, Germany

TOA pm 03:30 **Avant-Garde: Your DIA Data Sommelier to Assess and Improve Quantitative Suitability in Large Datasets;** Sebastian Vaca¹; Karen E. Christianson¹; Nicholas Schulman²; Karsten Krug¹; Katherine C. DeRuff¹; Ryan Peckner¹; Malvina Papanastasiou¹; Michael J. MacCoss²; Jacob D. Jaffe¹; Steven A. Carr¹; ¹Broad Institute of MIT and

Harvard, Cambridge; ²University of Washington, Seattle, WA

TOA pm 03:50 **ISObaric Modification Extraction and Resolvment (ISOMER);** Zuofei Yuan¹; Simone Sidoli¹; Katarzyna Kulej^{1,2}; Benjamin A. Garcia¹; ¹University of Pennsylvania, Philadelphia, PA; ²The Children's Hospital of Philadelphia, Philadelphia, PA

TOA pm 04:10 **An Open Searching Strategy for Identification and Quantification of Expressed Variants in Serum and Plasma;** Matthew Foster¹; Emily Ko¹; J. Will Thompson¹; Sunil Suchindran¹; Sarah Rains¹; Rose Asrican¹; L. Gayani Tillekeratne¹; Matthew Rubach¹; Thomas Burke¹; Elizabeth Petzold¹; Christopher Woods¹; M. Arthur Moseley¹; ¹Duke University, Durham, NC

2:30 - 4:30 pm Tuesday

GC/MS, GCXGC/MS, GC-MS/MS, AND GC/HRMS

Session Chair: David Touboul (CNRS-ICSN) B401-402

TOB pm 02:30 **Enantiomeric Profiling of Terpenes in Plant Material Using Gas Chromatography-Mass Spectrometry;** Seamus Riordan-short¹; Don Nguyen¹; Thu-Thuy Dang¹; Rob O'Brien¹; Matthew Noestheden¹; ¹Supra R&D, Kelowna, BC

TOB pm 02:50 **Evaluating the Volatile Constituents of Different Cannabis Varieties using Solventless Sample Preparation and Orbitrap Based MS Detection;** Gyorgy Vas¹; VasAnalytical, Flemington, NJ

TOB pm 03:10 **Covalent Adduct Chemical Ionization (CACI)-MS/MS for Assignment of Double Bond Position without Standards on a Shimadzu Triple Quadrupole MS;** Tom Brenna¹; Hui Gyu Park¹; Zhen Wang¹; Dong Hao Wang¹; Riki Kitano²; ¹University of Texas, Austin, TX; ²Shimadzu Scientific Instruments, Inc., Columbia, MD

TOB pm 03:30 **Extending the Range of Compounds Amenable for GC-MS Analysis with Cold EI – Recent Applications;** Aviv Amirav¹; Alexander B. Fialkov¹; Ksenia Kladchenko¹; Tal Alon¹; ¹Tel-Aviv University, Tel-Aviv, Israel

TOB pm 03:50 **Large Scale Breath Monitoring for Asthma Phenotyping;** Jean-François Focant¹; Delphine Zanella¹; Pierre-Hugues Stefanuto¹; Florence Schleich²; Renaud Louis²; ¹Liège University, Liège, Belgium; ²Liège University Hospital, Liège, Belgium



TOB pm 04:10 **GNPS GC Enables Automated Processing, Annotation and Visualization of Large Scale GC-MS Metabolomics Datasets**; Alexander Aksenov¹; Ivan Laponogov²; Mingxun Wang³; Dennis Veselkov⁴; Zheng Zhang³; Louis Felix Nothias³; Alexey Melnik³; Pieter Dorrestein³; Kirill Veselkov²; ¹UCSD, La Jolla, CA; ²Imperial College London, London, United Kingdom; ³University of California San Diego, La Jolla, CA; ⁴Intelligify Limited, London, United Kingdom

2:30 - 4:30 pm Tuesday

TOP DOWN PROTEIN ANALYSIS

Session Chair: **Ryan Kelly (Brigham Young University)**
B405-407

TOC pm 02:30 **Large-Scale Top-Down Proteomics Across Two-Dozen Cell Types from Human Blood and Bone Marrow**; Rafael D Melani¹; Robert V Gerbasi¹; Jacek W Sikora¹; Josiah E Hutton¹; Jeannie M Camarillo¹; Timothy Toby¹; Kristina Srzentić¹; Richard D Leduc¹; Ryan T Fellers¹; Joseph B Greer¹; Andy I Kokajić²; Lissa C Anderson³; Christopher L. Hendrickson³; Paul M Thomas¹; Neil L Kelleher¹; ¹Northwestern University, Evanston, IL; ²STEMCELL Technologies Inc., Vancouver, BC; ³NHMFL-FSU, Tallahassee, FL

TOC pm 02:50 **Direct Mass Spectrometry Analysis of Protein Complexes and Intact Proteins Up to 70 kDa from Tissue**; Helen Cooper¹; Rian Griffiths¹; Albert Konijnenberg²; Rosa Viner³; ¹University of Birmingham, Birmingham, United Kingdom; ²Thermo Fisher Scientific, Eindhoven, Netherlands; ³Thermo Fisher Scientific, San Jose, CA

TOC pm 03:10 **Advancing High-Throughput Top-Down Analysis of Proteoforms up to 60 kDa using a Modified Orbitrap Tribrid Mass Spectrometer**; Michael W. Senko¹; Romain Huguet¹; Kristina Srzentić²; Vlad Zabrouskov¹; Jesse D. Canterbury¹; Christopher Mullen¹; John E. P. Syka¹; Luca Fornelli³; ¹Thermo Fisher Scientific, San Jose, CA; ²Thermo Fisher Scientific, Cambridge, MA; ³University of Oklahoma, Norman, OK

TOC pm 03:30 **Capillary Zone Electrophoresis-Tandem Mass Spectrometry with Activated Ion Electron Transfer Dissociation and Ultraviolet Photodissociation for Large-Scale Top-Down Proteomics**; Eli McCool¹; Jean Lodge²; Yansheng Liu³; Joshua J Coon²; Liangliang Sun¹; ¹Michigan State University, East Lansing, MI; ²University of Wisconsin, Madison, WI; ³Yale University School of Medicine, West Haven, CT

TOC pm 03:50 **Extending the Upper Mass Range Available to Top-Down Proteomics with 21 T-FTICR MS**; Lissa C. Anderson¹; Chad R. Weisbrod¹; David S. Butcher¹; Christopher L. Hendrickson¹; ¹NHMFL-FSU, Tallahassee, FL

TOC pm 04:10 **The Use of Top-Down Sequencing in the Evaluation of Enzyme Specificity of Streptococcal Cysteine Protease SpeB on Human IgG2**; Anja Resemann¹; Waltraud Evers¹; Robert Kane²; Fredrik Olsson³; Guillaume Tremintin⁴; Lars Vorwerk¹; Detlev Suckau¹; ¹Bruker Daltonics, Bremen, Germany; ²Bruker Daltonics Inc., Billerica, MA; ³Genovis AB, Lund, Sweden; ⁴Bruker Scientific, San Jose, CA

2:30 - 4:30 pm Tuesday

DRUG TARGET IDENTIFICATION BY MS

Session Chair: **Angela I. Calderon (Auburn University)**
B302-305

TOD pm 02:30 **Proteome Wide Unbiased Target Identification for Radiation Mitigating Drug Candidate Using Thermal Proteome Profiling**; Kate Liu¹; Constance Yuen¹; William H. McBride¹; Robert Damoiseaux¹; Julian P. Whitelegge¹; Joseph A. Loo¹; ¹UCLA, Los Angeles, CA

TOD pm 02:50 **Development of a Novel Drug Target Identification Platform Based on Size (DTIPS)**; Yanting Guo¹; Zhe Wang¹; Dahang Yu¹; Kellye A Cupp-Sutton¹; Si Wu¹; ¹University of Oklahoma, Norman, OK

TOD pm 03:10 **The Good, the Bad and the Ugly - Thermal Stability Changes for Targets, Off-Targets and Non-Targets of Small Molecule Drugs**; Alexey Chernobrovkin¹; Cindy Caceres Körner¹; Tomas Friman¹; Johan Lengqvist¹; Maria Thastrup²; Matilda Degn Vinther²; Daniel Martinez Molina¹; ¹Pelago Bioscience AB, Solna, Sweden; ²Rigshospitalet, Copenhagen, Denmark

TOD pm 03:30 **Integrative Mass Spectrometry and RNA-Sequencing Identifies DLK1 as a Candidate Immunotherapeutic Target in Neuroblastoma**; Amber K. Weiner^{1,2}; Alexander B. Radaoui²; Simone Sidoli¹; Karina L. Konkrite²; Zalman Vaksman²; Komal S. Rathi²; Pichai Raman²; Jo Lynne Harenza-Rokita²; Dan Martinez²; Tricia Bhatti²; Matthew Tsang²; Bruce Pawel²; Benjamin A. Garcia¹; John M. Maris^{1,2}; Sharon J. Diskin^{1,2}; ¹University of Pennsylvania, Philadelphia, PA; ²Children's Hospital of Philadelphia, Philadelphia, PA

TOD pm 03:50 **Mechanism and Dynamics of SAMT Analog Inactivation of HIV-1 Gag Polyprotein**; Lisa M. Miller Jenkins¹; Elliott L. Paine¹; Lalit Deshmukh^{2,3}; Herman Nikolayevskiy²; Gaelyn C. Lyons¹; John M. Louis²; Robert J. Gorelick⁴; David E. Ott⁴; G. Marius Clore²; Daniel H. Appella²; ¹National Cancer Institute, Bethesda, MD; ²National Institute of Diabetes and Digestive and Kidney Diseases, Bethesda, MD; ³University of California San Diego, La Jolla, CA; ⁴Frederick Nat'l Lab for Cancer Research, Frederick, MD

TOD pm 04:10 **Illuminating the Druggable Proteome: Deconvolution of Drug Action by Multi-Omics, Thermal Profiling and High-Content Screening**; Doug Chapnick¹; Christopher Ebmeier¹; Kerri Ball¹; Stephen Coleman¹; Jeremy Jacobsen¹; Kristofor Webb¹; Travis Nemkov²; Xuedong Liu¹; Michael Stowell¹; Angelo D'Alessandro²; William Old¹; ¹University of Colorado Boulder, Boulder, CO; ²University of Colorado, Denver - Anschutz, Aurora, CO

2:30 - 4:30 pm Tuesday

FOOD SAFETY & CHEMISTRY: INNOVATIONS

Session Chair: **Christine Fisher (US Food & Drug Administration)**
B308-309

TOE pm 02:30 **Sensitive Multi-Mycotoxin Biomonitoring in Breast Milk by LC-MS/MS**; Dominik Braun¹; Maximilian Eiser¹; Doris Marko¹; Benedikt Warth¹; ¹University of Vienna, Faculty of Chemistry, Department of Food Chemistry and Toxicology, Vienna, Austria

TOE pm 02:50 **Formation of Toxic Iodinated Disinfection Byproducts during the Cooking of Pasta with Iodized Table Salt**; Huiyu Dong^{1,2}; Ilona Nordhorn¹; Karsten Lamann¹; Danielle C. Westerman¹; Hannah K Liberatore¹; Susan D. Richardson¹; ¹University of



TUESDAY AFTERNOON ORAL SESSIONS

- TOE pm 03:10 *South Carolina, Columbia, SC;* ²*Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences, Beijing, China*
Rapid Retrospective Assessment of Exposure of Cattle to Pesticides, Growth Promoters, Antibiotics by Use of In-House Developed Software Tools; Marco Blokland¹; Arjen Lommen¹; Robin Wegh¹; Frederike van Tricht¹; Hans Mol¹; Michel W.F. Nielsen¹; ¹*RIKILT, Wageningen, Netherlands*
- TOE pm 03:30 **Utilization of the MasSpec Pen for Rapid and Direct Investigation of Meat Fraud;** Abigail Gatmaitan¹; Jialing Zhang¹; John Q. Lin¹; Livia S Eberlin¹; ¹*University of Texas, Department of Chemistry, Austin, TX*
- TOE pm 03:50 **Ambient Ionization Coupled with a Miniature Mass Spectrometer for Rapid Analysis of Adulterated Additives in Food;** Xianshuang Meng¹; Qiang Ma¹; ¹*Chinese Academy of Inspection and Quarantine, Beijing, China*
- TOE pm 04:10 **Innovations in Food Safety Assessment of Genetically Modified Crops – the Deregulation of a Sustainable Source of Omega-3 Oils;** Michelle Colgrave; *CSIRO, St Lucia, Australia*

**2:30 - 4:30 pm Tuesday
CANCER RESEARCH**
**Session Chair: Erik Cressman (MD Anderson)
B312-314**

- TOF pm 02:30 **Proteomic Profiling of Cancer Cell Exosomes;** Kelly Servage¹; Karoliina Stefanius¹; Kim Orth¹; ¹*UT Southwestern Medical Center, Dallas, TX*
- TOF pm 02:50 **MALDI Detection of Exosomes for Cancer Studies;** Hubert H. Girault¹; Yingdi Zhu¹; ¹*Ecole Polytechnique Fédérale de Lausanne (EPFL), Sion, Switzerland*
- TOF pm 03:10 **Live Single Cell Mass Spectrometry Reveals Cancer-Specific Metabolic Profiles of Circulating Tumor Cells;** Yasmine Abouleila¹; Kaoru Onidani²; Ahmed Ali¹; Eiso Hiyama³; Yoshihiro Shimizu¹; Kazafumi Honda²; ¹*RIKEN, Osaka, Japan;* ²*National Cancer Institute, Tokyo, Japan;* ³*Hiroshima University, Hiroshima, Japan*
- TOF pm 03:30 **Tumor and CD8 T Cells Metabolism and Consumption in the Tumor Microenvironment;** Lauranne Poncelet^{1,2}; Rima Ait-Belkacem¹; Pierre Levy³; Maarten Ligtenberg³; Daniel Peeper³; Jonathan Stauber⁴; ¹*Imabiotech, Loos, France;* ²*Université de Lille, Lille, France;* ³*Netherlands Cancer Institute, Molecular oncology and Immunology department, Amsterdam, Netherlands;* ⁴*ImaBiotech Corp, Boston, MA*
- TOF pm 03:50 **Multisite Multimodal Mass Spectrometry Imaging of Organoids, Cell Extracts, and GEMMs to Explore Metabolic Changes in Colorectal Cancer Mutants;** Chelsea J Nikula¹; Rory T. Steven¹; Alex Dexter¹; Efstathios A. Elia¹; Teresa I. Murta¹; Bin Yan¹; Andrew D. Campbell²; Arafath K. Najumudeen²; Gregory Hamm³; David Gay²; Lucas Zeiger²; Aurelien Tripp⁴; Vincen Wu⁵; James S. McKenzie⁵; Paolo Inglese⁵; Jean-Luc Vorng¹; Seyma Turkseven⁵; Simon Cameron⁵; Stefania Maneta-Stavarakaki⁵; Spencer A. Thomas¹; Adam J. Taylor¹; Ala Al-Afeef¹; Tingting Fu¹; Kenneth N. Robinson¹; Weiwei Zhou¹; Xavier Loizeau¹; Ian S. Gilmore¹; Richard J.A. Goodwin³; George Poulgiannis⁴; Zoltan Takats⁵; Owen J. Sansom²; Josephine Bunch^{1,5}; ¹*National Physical Laboratory,*

- London, United Kingdom;* ²*Cancer Research UK Beatson Institute, Department of Invasion and Metastasis, University of Glasgow, United Kingdom;* ³*AstraZeneca, iMED, United Kingdom;* ⁴*Institute of Cancer Research, Division of Cancer Biology, United Kingdom;* ⁵*Imperial College London, Department of Surgery and Cancer, United Kingdom*
- TOF pm 04:10 **Interim Proteomic Analysis of Ovarian Cancer by the US Cancer Moonshot's Applied Proteogenomic Organizational Learning and Outcomes (APOLLO) Program;** Nicholas Bateman^{1,2}; Kathleen Darcy^{1,2}; Emmanuel Petricoin³; Brian Hood¹; Ming Zhao⁴; Kelly Conrads¹; Christopher Tarney¹; Christine Rojas¹; Guisong Wang¹; Craig Shriver²; Yovanni Casablanca^{1,2}; George Larry Maxwell^{1,2,4}; Thomas P. Conrads^{1,2,4}; ¹*Gynecologic Cancer Center of Excellence, Annandale, VA;* ²*John P. Murtha Cancer Center, Bethesda, MD;* ³*Center for Applied Proteogenomics, George Mason University, Manassas, VA;* ⁴*Inova Schar Cancer Institute, Annandale, VA*

**2:30 - 4:30 pm Tuesday
INSTRUMENTATION: INNOVATIVE SEPARATIONS APPROACHES
COUPLED TO MS**

**Session Chair: Xing-Fang Li (University of Alberta)
Auditorium, Bldg A**

- TOG pm 02:30 **The N-glycome Development Plan during Vertebrate Embryogenesis;** Yanyan Qu¹; Zhenbin Zhang¹; Michael Westphal²; Paul Huber¹; Josh Coon²; Norman Dovichi¹; ¹*University of Notre Dame, Notre Dame, IN;* ²*University of Wisconsin, Madison, WI*
- TOG pm 02:50 **Novel Capillary Columns for Bottom-Up and Top-Down Strategies Based Proteome Analysis;** Yu Liang¹; Yutong Jing²; Lihua Zhang¹; Yukui Zhang¹; Ying Ge²; ¹*Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China;* ²*University of Wisconsin, Madison, WI*
- TOG pm 03:10 **Improved Sensitivity for Single Cell Proteomics Using micro-Chip Pillar Arrays;** Karl Mechtler^{1,2}; Claudia Ctorteca^{1,2}; Jeff Op Beck³; Paul Jacobs³; Gert Van Raemdonck³; Gabriela Krssakova^{1,2}; Johannes Stadlmann^{1,2}; ¹*Research Institute of Molecular Pathology (IMP), Vienna, Austria;* ²*IMBA Institute of Molecular Biotechnology of the Austrian Academy of Sciences, Vienna, Austria;* ³*PharmaFluidics, Ghent, Belgium*
- TOG pm 03:30 **Comprehensive Target and Non-Target Analysis of Unregulated Disinfection Byproducts with High Resolution Mass Spectrometry in Drinking Water;** Susana Y Kimura Hara¹; Amy A. Cuthbertson²; Raphael Acabaya^{1,3}; Cassiana Montagner Raimundo³; Susan D. Richardson²; ¹*University of Calgary, Calgary, AB;* ²*University of South Carolina, Columbia, SC;* ³*Campinas University, Campinas, Brazil*
- TOG pm 03:50 **Coupling Advanced Chromatographic Methods for Analysis of Petroleum Products and Asphaltenes with On-line Detection by 21 T FT-ICR MS;** Jonathan Putman^{1,2}; Donald F. Smith¹; Chad R. Weisbrod¹; Steven M Rowland¹; Martha L. Chacón-Patiño¹; Yuri E. Corilo¹; Greg T. Blakney¹; Christopher L. Hendrickson^{1,2}; Ryan P. Rodgers^{1,2}; Alan G. Marshall^{1,2}; ¹*National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL;* ²*Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL*



TOG pm 04:10 **High-Throughput Analysis of Phospholipid Isomers by Online Photochemical Derivatization and RPLC-MS;** Wenpeng Zhang^{1,2}; Bing Shang^{1,3}; Qinhua Chen³; Zheng Ouyang⁴; Yu Xia^{1,2}; ¹Department of Chemistry, Tsinghua University, Beijing, China; ²Department of Chemistry, Purdue University, West Lafayette, IN 47907; ³Affiliated Dongfeng Hospital, Hubei University of Medicine, Shiyan, China; ⁴State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instruments, Tsinghua University, Beijing, China

**2:30 - 4:30 pm Tuesday
ENERGY, PETROLEUM, AND BIOFUELS: INSTRUMENTATION
AND APPLICATIONS**

**Session Chair: Amy McKenna
(National High Magnetic Field Laboratory)
A411-412**

TOH pm 02:30 **Pseudo-Quantitative Approach for Molecular Nitrogen Compounds Analysis in Gas Oils and Vacuum Gas Oils Using FT-ICR/MS, GCxGC-NCD and GCxGC/HRMS;** Julie Guillemant¹; Florian Albriex¹; Luis Pereira de Oliveira¹; Marion Lacoue-Nègre¹; Ludovic Duponchel²; Jean-François Joly¹; ¹Institut Français du Pétrole et Energies Nouvelles, Solaize, France; ²LASIR, Lille, France

TOH pm 02:50 **Extending the Application Range of a GCxGC High-Resolution TOF-MS platform for Fuel Analysis by Hyphenation to Thermal Analysis Techniques;** Uwe Kafer^{1,2}; Christopher Paul Rüger²; Thomas Gröger¹; Mohammad Saraji-Bozorgzad³; Thomas Wilharm⁴; Ralf Zimmermann^{1,2}; ¹Joint Mass Spectrometry Centre, Comprehensive Molecular Analytics, Helmholtz Zentrum München, Neuherberg, Germany; ²Joint Mass Spectrometry Centre, Chair of Analytical Chemistry, University of Rostock, Rostock, Germany; ³Photonion GmbH, Schwerin, Germany; ⁴ASG Analytik-Service Gesellschaft mbH, Neusäss, Germany

TOH pm 03:10 **Case Studies in Oil Spill Forensics: Finding Petroleum Biomarkers with GCxGC-TOFMS;** Christina Kelly¹; Joseph E Binkley¹; Lorne M Fell¹; Robert K Nelson²; Christopher M Reddy²; ¹LECO Corporation, Saint Joseph, MI; ²Woods Hole Oceanographic Institution, Woods Hole, MA

TOH pm 03:30 **Structural Analysis of Compounds Refractory to the Hydrodenitrogenation Process of Heavy Oil Fractions by Ion Mobility Coupled with Mass Spectrometry;** Johann Le Maître^{1,2}; Marie Hubert-Roux¹; Benoit Paupy²; Sabrina Marceau²; Christopher Rüger¹; Carlos Afonso¹; Pierre Giusti²; ¹Normandy University, COBRA laboratory, Mont Saint Aignan, France; ²Total Research & Technology Gonfreville, Harfleur, France

TOH pm 03:50 **Obtaining Tandem Mass Spectra of Individual Crude Oil Compounds within Narrow m/z Windows Using Cyclic Ion Mobility Mass Spectrometry;** Eunji Cho¹; Eleanor Riches²; Martin Palmer²; Kevin Giles²; Jakub Ujma²; Yunju Cho³; Sunghwan Kim^{1,3}; ¹Kyungpook National University, Daegu, South Korea; ²Waters Corporation, Wilmslow, United Kingdom; ³Green-Nano Materials Research Center, Daegu, South Korea

TOH pm 04:10 **Recent Developments in Petroleum Characterization by Advanced Chromatography and Mass Spectrometry;** Kuangnan Qian; ExxonMobil Research Engineering, Annandale, NJ

**4:45-5:30 pm Tuesday
BIEMANN MEDAL LECTURE
Richard A. Yost (University of Florida), presiding
Murphy Ballroom, Bldg B, Level 5**

Presentation of Research Award at Primarily Undergraduate Institution (PUI)

- Award sponsored by Agilent Technologies presented by Bryan Miller to Callie Cole (Fort Lewis College)

Presentation of the Research Awards

- Award sponsored by Bruker presented by Rohan A. Thakur to James F. Davies (University of California, Riverside).
- Award sponsored by Thermo Scientific presented by Iain Mylchreest to Nicolas L. Young (Baylor College of Medicine).
- Award sponsored by Waters Corporation presented by Lance Nicolaysen to Eleanor Browne (University of Colorado, Boulder)



Biemann Medal

Sarah Trimpin
Wayne State University

5:45 - 7:00 PM TUESDAY WORKSHOPS

There will be light refreshments in Building A foyers. All workshops are in Building A.

**01 Top Down Proteomics: Advancing Widespread Adoption and Expanding Applications
(Top-Down Proteomics Interest Group)
Presiding: Nicolas Young, Frederik Lermyte
A402-403**

Top-down protein mass spectrometry allows comprehensive characterization of proteoforms from complex mixtures and avoids many of the pitfalls associated with traditional bottom-up workflows. While the top-down approach is conceptually simple, a number of significant technical challenges must be overcome in order to successfully perform a top-down experiment. This combination of utility and difficulty has led to the creation and rapid expansion of the multinational Consortium for Top-Down Proteomics in 2012. In this workshop, we will bring together experienced and novice top-down mass spectrometry users in order to promote the development and democratization of these methods. The primary emphasis will be open discussion and debate. The selected topics and formal introductions will serve primarily to educate and provide greater accessibility to novice participants and induce discourse

from a wide range of voices. We will discuss the following topics: Introduction to top-down proteomics and practical implementation in your laboratory; community initiatives and standardization; metrics for identification and accurate quantitation in biomedical research; and native mass spectrometry and native top-down proteomics. Each topic will be introduced by a 5-minute lightning talk, followed by approximately 10 minutes of audience discussion and debate. Thus, the majority of the workshop will be audience participation and a lively discussion amongst attendees. Contact workshop chairs if you are interested in presenting an introduction to spark the discussion of a topic.

**02 Networking for Scientists: Celebrating Women Mass Spectrometrists (Year 2)
Presiding: Erin Baker, Anumita Saha
A404-405**

In our second year of the Celebrating Women Mass Spectrometrists Workshop, we will utilize feedback from last year to refine our workshop. Due to the desire for more networking, this year we will start with a



There will be light refreshments in Building A foyers. All workshops are in Building A.

panel of ~6 women mass spectrometrists who have excelled in diverse careers in academia, industry and government. The session will kick off with panelists introducing themselves and giving a brief summary of their career paths. Then we will allow questions from the audience until there is ~30 min left in the workshop. At this time, the panelists will disperse in the room for one-on-one interaction with the audience. We feel this will give anyone who would like to attend, the chance to meet these women and ask them specific questions about their career paths in a social and non-threatening environment.

03 Say No to Drugs: Forensic Applications Outside of Traditional Illicit Drug Analysis
(Forensics & Homeland Security Interest Group)
Presiding: Christopher Mulligan, Brittany Casey
A406-407

As almost any chemical species could be potential evidence and/or a threat, given that it was involved in or alludes to criminal activities, the fields of forensic science and homeland security are some of the most demanding and comprehensive. To further complicate the issue, the large breadth of chemical targets can be found in various states of matter, as residues on many different substrates, or in the presence of complex chemical/biological matrices. Thus, forensic and security science has matured concurrently with advancements in analytical chemistry, and almost all processing of chemical substances incorporates some aspect of instrumental analysis.

Of the commonly-utilized instrumentation in these areas, mass spectrometry has a prominent role and is considered to be a "gold standard" technique (in the form of GC/MS) for illicit substance analysis. While much emphasis and effort (as evidenced by the recent Census of Publicly Funded Forensic Crime Laboratories by the Bureau of Justice Statistics) goes towards illicit drugs, the sensitivity and selectivity of MS-based methods are employed in many other areas of interest. This year, the workshop will move away from abused drugs to highlight other application areas of critical importance to forensic science and homeland security, such as chemical threats/CWAs, explosives/firearms, toxicology, etc. Through discussions with a panel of scientists from the federal, private and academic sectors, the audience will gain insight into how researchers employ MS strategies in these important areas.

04 Proteoform Identification and Quantification Using Toppic Suite
Presiding: Xiaowen Liu, Si Wu, Liangliang Sun
A408

Top down mass spectrometry (MS) has gained increasing attention in the past decade because of its capability to sequence whole proteoforms with post-translational modifications (PTMs) and other alterations. Although many computational methods have been developed for top-down MS data analysis, it is still challenging for MS labs to efficiently identify and quantify proteoforms because of the complexity of the data and methods. TopPIC suite is an open source software package that is routinely used for proteoform identification and characterization by top-down MS. In this workshop, we will present the computational methods of the tools in TopPIC suite for spectral deconvolution and the identification of proteoforms with unknown alterations and those with multiple variable PTMS, and demonstrate new functions such as proteoform quantification and data visualization. We will give tutorials on applying the tools to various research problems ranging from phosphorylated proteoform identification to native proteomics. We will discuss with users and collect their feedback and suggestions for further improvement of the tools.

05 Protein Biomarkers Method Development & Validation by LCMS, HRMS and Hybrid LBA/LCMS: Recent Advancements (Regulated Bioanalysis Interest Group)
Presiding: Jian Wang, Dian Su, Fabio Garofolo
A410

The 2019 Regulated Bioanalysis Interest Group (RBIG) Workshop is focused on recent advancements in protein biomarkers method development strategies and regulated Biomarker Assays Validation (BAV) by LCMS, HRMS and hybrid LBA/LCMS. This workshop will develop further mass spectrometry community discussions and consensus on the recently published recommendations on this topic including:

- Neubert, Song, Lee et al. - 2017 White Paper in Bioanalysis - <https://www.future-science.com/doi/pdf/10.4155/bio-2017-4973>
- Neubert, Olah, Lee et al. - 2018 White Paper in Bioanalysis - <https://www.future-science.com/doi/pdf/10.4155/bio-2018-0285>
- "[...]Accessibility and innovative integration of advanced technologies have accelerated the development of hybrid LBA/LCMS, which has become an important bioanalytical platform to verify novel targets in discovery and confirm promising targets and biomarkers in early clinical development [...] Protein immunoaffinity techniques linked to MS (hybrid LBA/LCMS) have solidified their impact in translational research and in clinical analysis[...] This technique has been on an incredible journey in recent years that enabled growing adaptation through its use by an increasing number of practitioners and experts due to improved assay sensitivity and throughput, new reagents for capture approaches and automation of key steps, to name a few factors [...] Bioanalysts have advanced the ability from measuring soluble proteins to target engagement, moved from plasma to tissues including small biopsies, from soluble proteins to structural and membrane bound proteins and from concentration analysis to measuring protein synthesis rates." - excerpts from Bioanalysis (2017) 9(23) 1902-1903

Invited experts in this field will informally provide a wide range of perspectives on biomarkers method development and BAV by mass spectrometric techniques to stimulate an interactive & all-inclusive discussion with the audience

06 Improving Scientific Writing Skills
Presiding: Chris Petucci
A307

"The difference between the almost right word and the right word is really a large matter. It's the difference between the lightning bug and the lightning (Mark Twain)." A scientist's ability to clearly communicate ideas in written form has a major impact on his or her scientific reputation, obtaining grants, and publishing manuscripts. This workshop will be a hands-on session that includes essential grammar for scientists, writing grammatically correct sentences, and principles of logical paragraph development. At the conclusion of this workshop, you will have an increased knowledge of vital writing skills to prepare high quality manuscripts and other documents.

07 Metal Ions and Non-Threshold Ion Activation in Biomolecules (Metal Ion Coordination Chemistry Interest Group)
Presiding: Franklin E. Leach III
A309

Biomolecular ions can interact with metal species in a variety of ways ranging from cofactors in metalloproteins to exchange with acidic protons. These interactions lead to structural changes that can be deduced by mass spectrometry and can affect the utility of specific MS/MS approaches to provide sufficient structural information. The workshop will focus on the application of non-threshold ion activation approaches (ExD, UVPD, CTD, etc.) to determine structure in biomolecules that interact with metal ions. Short presentations (~8-10 mins) from the community that demonstrate a fundamental understanding or unique application of these MS/MS approaches in



There will be light refreshments in Building A foyers. All workshops are in Building A.

metal ion systems will be given followed by time for discussion along with a series of lightning talks for any late breaking presentations of interest.

08 Protein Imaging - Are We There? Are All Issues Solved?
(Imaging MS Interest Group)
Presiding: Martina Marchetti-Deschmann, Peggi Angel
A311

MS Imaging allows to obtain detailed images of the spatial distribution of proteins in tissue and has tremendously progressed over the years. In this workshop experts will shortly introduce the participants to state-of-the-art protein imaging, covering aspects of specificity, dynamic range, protein identification and data interpretation. The speakers will foster discussions about potentials and limitations of protein imaging. This workshop is addressing everyone in the field, from beginners to experts and also those who are just interested in the method.

We moreover strongly encourage students and early stage researchers to give a short presentations (5 min/2-3 slides) on their perspectives of protein imaging, including insights or any challenges and limitations they face in this area. If you are interested in participating or have any questions, please contact us via email:
martina.marchetti-deschmann@tuwien.ac.at; angelp@musc.edu

09 Metabolomics: Points of Agreement and Disagreement
(Metabolomics Interest Group)
Presiding: Gary Patti, Jon Sobus
A312

The field of metabolomics emerged nearly twenty years ago, and targeted methods to measure metabolites were in place decades before. Given the tens of thousands of studies that are now available on metabolite profiling, there has been increasing clarity on best practices to quantitate small molecules with mass spectrometry. The purpose of this workshop is to review such analytical procedures, while also discussing practices in which disagreement persists. Moderators will first present themes from the literature representing perspectives they feel are widely shared by many researchers in the community. This will include sample preparation, metabolite extraction, and data processing steps. Focus will be dedicated to analytical strategies that may not have been agreed upon 10-15 years ago, but where progress has been made towards consensus. To contrast generally shared perspectives, moderators will also present views where varying opinions still exist among the community. Some examples may include: (i) what experimental data should constitute various confidence levels when identifying a metabolite? (ii) what are the minimal requirements for data sharing? (iii) how should databases be organized? Critical to the workshop will be the participation of the audience, whose input will help reflect the broader opinion of the community. At the end of the workshop, we hope participants will have a clearer sense of some basic ideas where there is general agreement and disagreement in the field of metabolomics.

10 Environmental MS: Detection of Emerging Contaminants
(Environmental Applications Interest Group)
Presiding: Chris Gill
A313

New classes of compounds and contaminants emerge every decade, encouraging analytical scientists to come up with state-of-the-art methodologies for their analysis. New instrumentation in mass spectrometry is driving the field of unequivocal identification (accurate mass techniques) and lower detection limits (super sensitive instrumentation). This workshop will be focused broadly on discussing the best techniques and analytical approaches, including sample preparation, for the determination of important emerging contaminants that require generation of new methods, such as nanoparticles, microplastics and perfluorinated compounds (PFOS/PFOA). Presentations will be limited to briefly introduce the topic to prioritize active discussion among environmental scientists.

11 Visualization, Comparison and Accessibility of Large Data Sets
(Analytical Lab Managers Interest Group)
Presiding: David Quilici, Samuel Mackintosh
A314

Analytical laboratories face significant challenges related to the analysis and storage of large data sets on behalf of principal investigators, many of whom have little experience with data analysis themselves. These investigators need to be able to understand what they are looking at, search their data easily, and extract useful information. In addition, analytical labs have the responsibility to maintain consistent standards for data analysis and to store and share large data sets appropriately and economically. The 2019 ASMS Analytical Lab Managers Workshop will focus on potential solutions to some of these challenges. Specifically, the workshop will cover data visualization techniques, standards for data normalization and comparison, and approaches to data storage and sharing. Three fifteen-minute presentations will be given, with each talk followed by a ten-minute discussion period.

12 Advances in Polymer Mass Spectrometry - Architecture
(Polymeric Materials Interest Group)
Presiding: Christina Mastromatteo, Jessica Hoskins
A315

This year's meeting will consist of three distinct sections; a workshop, student poster elevator talks, and an open forum.

To start with, we will have two short tutorials on analysis of polymer architecture:

- KMD applications to polymer analysis
- Hydrogel crosslinking studied by mass spectrometry

Secondly, we will host a series of short Polymer Section poster presentations (3-5 min each) by any students / presenters regarding their upcoming posters. This will provide each presenter an opportunity to promote their work externally to a professional scientific audience in their specialized field.

There will then be an open forum, in which attendees are invited to ask about any particular issues or questions that they would like to ask for help with. In addition, input will be sought for future Workshop topics.

13 (Emotional) Intelligence Gathering
(Career Development Interest Group)
Presiding: Lucinda Hittle, Charles Veltri
A316

Have you ever wondered how to improve your ability to think on your feet, resolve conflicts with others, and manage your emotions more effectively? Emotional intelligence may be one of the most underestimated elements of a successful career. This workshop will take participants through a brief assessment of their emotional intelligence quotient (EQ) then break out into small group discussions facilitated by veteran scientists across diverse sectors including industry, government and non-profit agencies, and academia. The goals of this workshop will be to foster relationships across the society that span the boundaries of geography, age, level of experience, and academic training as well as enabling networking and small group discussions. No experience required, but imagination and an open mind are pre-requisites!

14 MS in Extractable and Leachable Analysis
Presiding: Kate Comstock, Gyorgy Vas
A303

Mass spectrometry plays an essential role in extractable and leachable (E&L) analysis. Complete E&L profiles require GC-MS, LC-MS, and ICP-MS analysis. The advancements in mass spectrometry instrumentation and new techniques provide new and much-needed tools for confident and comprehensive E&L profiling.



There will be light refreshments in Building A foyers. All workshops are in Building A.

Currently, the increasing demands for E&L analysis are driven by growth in medical devices, single-use systems (SUS), continuous processing in bioproduction, etc. The variation in materials, applications, and interactions with contact media of these products pose new challenges for E&L analysis. Furthermore, the existing E&L regulations are lacking in clarification of acceptance for these new products.

There are many techniques and new developments for E&L analysis in terms of sample preparations, chromatographic separations, and data acquisitions by various mass spectrometry instruments. In addition, the data processing and interpretation often are rate-limiting factors, and there is an urgent need for efficient, easy-to-use data processing software, E&L database and spectral libraries, and result reports generator.

This workshop will provide a venue for E&L analysis scientists to discuss all the above issues, exchange practices, also present problems and challenges concerning mass spectrometry instrumentation, methodologies, and data processing. Through this workshop, E&L scientists will have direct open discussion and information exchange, establish and expand networks. It will promote good science and advancement of mass spectrometer's usage in E&L analysis.

15 HDX, Covalent Labeling & Cross-Linking: Status of Community-Initiatives and New Developments and Applications (HDX Covalent Labeling & Cross Linking Interest Group)

Presiding: Kasper Rand, Jim Bruce

Recent innovations in MS instrumentation, sample preparation strategies, cross-linking and chemical labeling reagents, and bioinformatics tools have significantly facilitated the developments and applications of HDX, covalent labeling and cross-linking approaches in protein structural and interaction analysis. In order to allow robust data evaluation and result comparison among experiments and across laboratories, data acquisition, analysis and interpretation need to be standardized. Since the last workshop, community-wide efforts have focused on these topics and in the first part of the workshop, one panelist from each community will present current status and highlights from this work for the benefit of beginners and experts alike. In addition, interactive discussions among audience members will be stimulated by the panelists, regarding to future perspectives for other topics that need to be harmonized within each fields. The second part of the workshop will focus on most recent technical developments or new areas of application within HDX/XL/CL-MS. Exciting and promising new developments will be highlighted by 5 min talks from invited members of the community, with a focus on current applicability and limitations. The invited speakers will form a panel for this second part of the workshop and there will be ample time for questions and answers including an opportunity for novices/students to contribute anonymous questions on fundamentals.

16 Lipidomics: Path to Clinical Utility (Lipids & Lipidomics Interest Group)

Presiding: John Bowden, Kim Ekroos, A301

The field of lipidomics is rapidly evolving, driven by high expectation in its ability to afford new opportunities for studying lipids in health and disease and in many other fields of research. As such, in this lipidomics workshop, we aim to discuss the current status of lipidomics in the clinical arena. The workshop will be designed to stimulate discussion on several key questions, including: what are the current roadblocks preventing the universal adaptation of lipidomics in the clinical setting, which lipids/disease states already show clinical promise and which should we be focusing on next, and moving forward within the clinic, how much effort should be placed on those lipids that are historically difficult to measure but might have clinical promise? At present, the field is currently challenged by large disparities in methodologies and technologies and in how users apply them, resulting in an increasing number of publications of varying quality. Two potential reasons for

this are the lack of a common language and the lack of community-accepted best practice guidelines, both stalling the future development and true utilization of lipidomics in clinical research and diagnostics. This workshop will review the current challenges and discuss strategies moving forward, including the community-wide harmonization (and standardization) of lipidomics. A group of experts will share their experience and answer any questions, and views from the audience will be discussed.

17 Data Independent Acquisition: Expanding the Scope of DIA Strategies for Quantitative Mass Spectrometry (Data Independent Acquisition Interest Group)

Presiding: Hannes Röst, Birgit Schilling, A305

In quantitative proteomics, the fundamental aim is to accurately identify and quantify analytes across various conditions. Data independent acquisition (DIA) has recently emerged as a promising method to accurately quantify analytes in complex samples, allowing consistent detection and quantification of thousands of proteins across large sample cohorts. Utilizing MS2-based quantification (as in SRM/PRM) in high throughput workflows (as in DDA) has led to impressive results with highly consistent and accurate quantitative data matrices suitable for systems biology, systems medicine and personalized medicine applications. However, most current methods focus on accurate protein quantification using a label-free approach. However, the DIA approach can readily be applied to other MS-based questions and can be beneficial if high-quality fragment ion data is essential for correct analyte characterization. This workshop will discuss novel technological and software innovations in the field of DIA: How can novel advances in computer science (deep learning) advance the field of DIA and which novel analysis methods do they make available? What specific challenges await when expanding the scope of DIA beyond unmodified peptides (PTMs, SAV, lipids, small molecules)? How can ion mobility be integrated with DIA? How can very short gradients be exploited in DIA? This workshop will focus on existing and emerging approaches using novel technology and software in DIA and discuss some unique challenges, and opportunities, of translating the recently developed DIA approaches (such as targeted extraction) to these fields.

18 Trans-Proteomic Pipeline: Recent Advances and Future Directions

Presiding: Luis Mendoza, David Shteynberg, Eric Deutsch, A304

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 four 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: proteogenomics & PEFf applications, analyzing PTMs with PTMProphet, cross-linking analysis with Kojak 2.0, and deploying the TPP using Docker containers & cloud computing platforms. Each topic will be introduced with a brief summary of features and ideas. Then feedback and discussion by the workshop participants will be promoted.





From 7:00 am Wednesday
CORPORATE BREAKFAST SEMINARS
CONVENTION CENTER AND OMNI CNN CENTER HOTEL
See page 16 for detailed schedule. Reservation or RSVP required.

8:30 - 10:30 am Wednesday

METABOLOMICS: NEW TECHNOLOGIES AND APPLICATIONS

Session Chair: Nichole Reisdorph (University of Colorado
Anschutz Medical Campus)

Murphy Ballroom, Bldg B, Level 5

- WOA am 08:30 **Uncovering the Role of Autophagy Impairment on Dysregulated Lipid Metabolism in Skeletal Muscle Aging through Multi-Platform Metabolomics Analysis**; Christian Toonstra¹; Zoe Maxwell¹; Heather Brown¹; Michelle Kuhns¹; Edgar Arriaga¹; ¹University of Minnesota, Minneapolis, MN
- WOA am 08:50 **Metabolically Labeled Ribonucleotides Enable Multiplexed Quantitative Analysis of the Effects of Stress and Viral Infection by High Resolution Mass Spectrometry**; Thomas J Kenderdine¹; Reza Nemati²; Rachel Netzband^{1,3}; Molly FitzGibbon⁴; Will McIntyre¹; Cara T. Pager^{1,3}; Daniele Fabris^{1,3}; ¹SUNY Albany, Albany, NY; ²Biogen, Cambridge, MA; ³The RNA Institute, University at Albany, Albany, NY; ⁴University of California, San Diego, CA
- WOA am 09:10 **Native ESI-MS Based Metabolomics Enables the Search for Metal-Binding Molecules**; Allegra Aron^{1,2}; Daniel Petras^{2,3,4}; Julia M Gauglitz^{1,2}; Hui Zhi⁵; Manuela Raffatellu^{2,5,6}; Pieter C. Dorrestein^{1,3}; ¹University of California San Diego, Collaborative Mass Spectrometry Innovation Center, La Jolla, CA; ²University of California San Diego, Center for Microbiome Innovation, La Jolla, CA; ³University of California San Diego, Collaborative Mass Spectrometry Innovation Center, La Jolla, CA; ⁴University of California San Diego, Scripps Institution of Oceanography, La Jolla, CA; ⁵University of California San Diego Division of Host-Microbe Systems & Therapeutics, Department of Pediatrics, La Jolla, CA; ⁶Chiba University-University of California San Diego Center for Mucosal Immunology, Allergy, and Vaccines (CU-UCSD cMAV), La Jolla, CA
- WOA am 09:30 **Creation and Annotation of a Recurrent Spectral Library of Cho Cell Metabolites and Media Components**; Kelly H. Telu¹; Ramesh Marupaka¹; Nirina R. Andriamaharavo¹; Yamil Simón-Manso¹; Yuxue Liang¹; Yuri A. Mirokhin¹; Xinjian Yan¹; Tallat H. Bukhari¹; Stephen E. Stein¹; ¹NIST, Gaithersburg, MD
- WOA am 09:50 **Quantitative Sub-Cellular acyl-CoA Analysis Using SILEC Internal Standards**; Sophie Trefely¹; Katharina Huber²; Joyce Liu²; Mary Doan³; Helen Jiang³; Jay Singh³; Kenneth C Bedi²; J. Eduardo Rame²; Kathryn E. Wellen²; Nathaniel W Snyder³; ¹University of Pennsylvania, Philadelphia, PA; ²University of Pennsylvania, Philadelphia, PA; ³Drexel University, Philadelphia, PA
- WOA am 10:10 **Chemical Isotope Labeling LC-MS for Studying the Metabolic Response of Single Cells to Heat Shock**; Wan Chan¹; Michael C. Schultz¹; Liang Li¹; ¹University of Alberta, Edmonton

8:30 - 10:30 am Wednesday

CARBOHYDRATES

Session Chair: Ron Orlando (University of Georgia)
B401-402

- WOB am 08:30 **CUPRA-ZYME: A Novel ESI-MS Method for Measuring Carbohydrate-Active Enzyme Activities and Profiling their Substrate**

Specificities; Zhixiong Li¹; Pavel I Kitov¹; Erick Bolivar¹; Elena N Kitova¹; John Klassen¹; ¹Department of Chemistry, University of Alberta, Edmonton, AB

- WOB am 08:50 **Analysis of N-Glycans Released from Monoclonal Antibodies by Combining Ultra High-Resolution Ion Mobility Spectrometry and Cryogenic Ion Spectroscopy**; Natalia Yalovenko¹; Ahmed Ben faleh¹; Stephan Warnke¹; Thomas R. Rizzo¹; ¹Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland
- WOB am 09:10 **Dissecting Fragment Ion Structures of Protonated Oligosaccharides by MSn, Ion Mobility Spectrometry, and Gas-Phase Hydrogen/Deuterium Exchange Mass Spectrometry**; Abhigya Mookherjee¹; Sanjit Singh Uppal¹; Miklos Guttman¹; ¹University of Washington, Seattle, WA
- WOB am 09:30 **A Simplified Approach to N-Glycan Profiling of Cultured Cells Using MALDI Imaging Mass Spectrometry**; Janet Saunders¹; Cassandra L Clift¹; Anand S. Mehta¹; Richard R. Drake¹; Peggi Angel¹; ¹Medical University of South Carolina, Charleston, SC
- WOB am 09:50 **Comparison of Charge Transfer Dissociation (CTD) and Electron Detachment Dissociation (EDD) for the Structural Analysis of Glycosaminoglycans**; Lauren Pepi¹; Zachary J Sasiene²; Praneeth M Mendis²; Glen P Jackson^{2,3}; I. Jonathan Amster¹; ¹University of Georgia, Athens, GA; ²West Virginia University, C. Eugene Bennett Department of Chemistry, Morgantown, WV; ³Department of Forensic and Investigative Science, West Virginia University, Morgantown, WV
- WOB am 10:10 **NanoPGC-LC-EED-MS/MS Analysis of N-linked Glycans in Human Serum**; Yang Tang¹; Juan Wei¹; Catherine E. Costello¹; Cheng Lin¹; ¹Boston University, Boston, MA

8:30 - 10:30 am Wednesday

FUNDAMENTALS FOR EVERYONE: PEPTIDES AND PROTEINS

Session Chair: Cheryl Lichti (Washington University in St. Louis)
B405-407

- WOC am 08:30 **Robust Methods for Endogenous Proteoform Characterization by Immunoprecipitation and Subsequent Targeted Top-Down Proteomic Analysis**; Caroline DeHart¹; Luca Fornelli²; Lauren M Adams³; Jacek W Sikora¹; Vincent Gerbasi¹; Ryan T Fellers¹; Richard D Leduc¹; Paul M Thomas¹; Philip D. Compton¹; Neil L Kelleher¹; ¹Proteomics Center of Excellence, Northwestern University, Evanston, IL; ²University of Oklahoma, Norman, OK; ³Northwestern University, Evanston, IL
- WOC am 08:50 **Ion Mobility Separations of Proteins at Extreme Fields with Dipole Alignment Tunable by Changing the Gas Pressure**; Alexandre A. Shvartsburg¹; Roch Andrzejewski²; Andrew Entwistle²; Roger Giles²; ¹Wichita State University, Wichita, KS; ²Shimadzu Corporation, Manchester, United Kingdom
- WOC am 09:10 **Nanodroplet Sample Processing, Ultra-Low-Flow nanoLC and Next-Generation Tribid MS Enable In-Depth, Label-Free Profiling of Single Mammalian Cells**; Yongzheng Cong¹; Ying Zhu²; Yiran Liang¹; Maowei Dou²; Greg Foster³; Daniel Lopez-Ferrer³; Yufeng Shen⁴; Ryan T. Kelly^{1,2}; ¹Brigham Young University, Provo, UT; ²Pacific Northwest National Laboratory, Richland, WA; ³Thermo Fisher Scientific, San Jose, CA; ⁴CoAnn Technologies, LLC, Richland, WA



WEDNESDAY MORNING ORAL SESSIONS

- WOC am 09:30 **FAIMS Enables Increased Proteome Coverage on a Q Exactive Platform with Short LC Gradients;** Dorte Breinholdt Bekker-Jensen¹; Patrick L. Ruether²; Christian D. Kelstrup²; Jesper V. Olsen²; ¹University of Copenhagen, NNF CPR, Copenhagen N, Denmark; ²University of Copenhagen NNF CPR, Copenhagen N, Denmark
- WOC am 09:50 **Multimodal Approaches for Non-targeted Discovery of Endogenous D-amino Acid Containing Peptides;** David H. Mast¹; James W. Checco¹; Elena V. Romanova¹; Jonathan V. Sweedler¹; ¹University of Illinois at Urbana Champaign, Urbana, IL
- WOC am 10:10 **Two Dimensional Mass Spectrometry (2DMS) – the Next Dimension in Proteomics;** Pui Yiu Lam¹; Christopher A. Wootton¹; Kung Ching Cookson Chiu¹; Tomos E. Morgan¹; Remy Gavard¹; Meng Li¹; Mark P. Barrow¹; Peter B. O'Connor¹; ¹University of Warwick, Coventry, United Kingdom

8:30 - 10:30 am Wednesday

MICRODOSING AND MICROSAMPLING: ANALYTICAL CHALLENGES

Session Chair: Uliana Danilenko (CDC)
B302-305

- WOD am 08:30 **Rapid, Untargeted Metabolomic Profiling of Single Cells in Their Native Environment Using Single-Cell Printer-Liquid Vortex Capture-Mass Spectrometry;** John F. Cahill¹; Julian Riba^{2,3}; Vilmos Kertesz¹; ¹Oak Ridge National Laboratory, Oak Ridge, TN; ²University of Freiburg, 79110, Germany; ³Cytena GmbH, 79108, Germany
- WOD am 08:50 **“Dip and Go”: High-Throughput Direct Bioassays by Inductive nESI;** Zhenwei Wei¹; Zhuoer Xie¹; Reshma Kuvelkar²; Vinit Shah²; Kevin P. Bateman²; David G. McLaren²; Graham R. Cooks¹; ¹Purdue University, West Lafayette, IN; ²Merck & Co. Inc., Kenilworth, NJ
- WOD am 09:10 **High Speed System for Analysis of Biological Samples that Corrects for ESI Ionization Suppression in Real Time;** Thomas R. Covey¹; Peter Kovarik¹; Chang Liu¹; ¹SCIEX, Concord, ON
- WOD am 09:30 **On-Line Spatially Resolved Surfaces Sampling Capillary Electrophoresis Mass Spectrometry;** Ingela Lanekoff¹; Kyle D Duncan¹; ¹Uppsala University, Uppsala, Sweden
- WOD am 09:50 **Inter-Laboratory Validation of Solid-Phase Microextraction-Based Protocol for Untargeted Profiling of Lipids in Rat Brain;** Mariola Olkowicz¹; Cian Monnin²; Nathaly Reyes-Garcés^{1,3}; Sofia Lendor¹; Ezel Bojaci^{1,4}; Miao Yu^{1,5}; German Augusto Gomez-Rios^{1,3}; Clement Hamani⁶; Barbara Bojko^{1,7}; Dajana Vuckovic²; Janusz Pawliszyn¹; ¹University of Waterloo, Waterloo, ON; ²Concordia University, Montreal, Qc; ³Restek Corporation, Bellefonte, PA; ⁴Department of Chemistry, Middle East Technical University, Ankara, Turkey; ⁵Icahn School of Medicine at Mount Sinai, New York, NY; ⁶Sunnybrook Health Sciences Centre, Toronto, ON; ⁷Nicolaus Copernicus University, Torun, Poland
- WOD am 10:10 **Controlling Variance for Self-collected Plasma; Anatomy, Analysis and Accuracy;** Russell Grant¹; Bradley Collier¹; Jennifer Pollock¹; Julia Hannon¹; Matthew Crawford¹; ¹Labcorp., Burlington, NC

8:30 - 10:30 am Wednesday

ENVIRONMENTAL: INNOVATIVE APPROACHES AND INSTRUMENTATION

Session Chair: Pierangela Palma (University of Urbino)
B308-309

- WOE am 08:30 **Mass Spectrometry of Single Picoliter Droplets to Explore the Chemistry of Atmospheric Aerosol;** James F Davies; *UC Riverside, Riverside, CA*
- WOE am 08:50 **Byproducts Formation in a VOC Air Cleaning System: Real-Time Analysis Using a Compact FTICR in a Model Plasma Reactor;** Sébastien Thomas¹; Nicole Blin-Simiand²; Joel Lemaire³; Michel Héninger³; Héléne Mestdagh³; Lionel Magne²; Stéphane Pasquiers²; Essyllt Louarn⁴; ¹CSNSM – CSNCM - UMR8609 – Univ. Paris-Sud, CNRS, Univ. Paris-Saclay, Orsay, France; ²LPGP - UMR8578 - Univ. Paris-Sud, CNRS, Univ. Paris-Saclay, Orsay, France; ³LCP - UMR8000 - Univ. Paris-Sud, CNRS, Univ. Paris-Saclay - Orsay, Orsay, France; ⁴LCP - UMR8000 - Univ. Paris-Sud, CNRS, Univ. Paris-Saclay, Orsay, France
- WOE am 09:10 **MALDI-TOF Imaging and LC-HRMS: New tools for Degradation Studies of Polymer Probes Exposed to Different Waste Water Environments;** Damia Barcelo¹; Antoni Ginebreda¹; Maria Vila Costa¹; Bozo Zonja¹; Nicola Montemurro¹; A Martinez Varela¹; Sandra Perez¹; Daniel Rivas¹; ¹IDAEA-CSIC, Barcelona, Spain
- WOE am 09:30 **Iodinated X-ray Contrast Media as a Source of Iodine for the Formation of Iodinated DBPs upon Chlorination during Wastewater Treatment;** Caroline O. Granger¹; Hannah K. Liberatore¹; Susan D. Richardson¹; Mark Ferrey²; ¹University of South Carolina, Columbia, SC; ²Minnesota Pollution Control Agency, St. Paul, Minnesota
- WOE am 09:50 **Dissolved Organic Matter Molecular Composition to Optical Properties Relations as Determined by Ultra-High Resolution Mass Spectrometry;** Alexander Zhrebker¹; Evgeny Shirshin²; Oleg Kharybin¹; Irina Perminova²; Eugene (evgeny) Nikolaev¹; ¹Skolkovo institute of science and technology, Moscow Region, Russian Federation; ²Moscow State University, Moscow, Russian Federation
- WOE am 10:10 **Chemical or Electron Ionization? The Application of GC×GC HRT in Environmental Research with Source-Specific Molecular Markers;** Ulrich M Hanke¹; Robert K Nelson¹; Christina Kelly²; Bruno Glaser³; Christopher M Reddy¹; ¹Woods Hole Oceanographic Institution, Woods Hole, MA; ²LECO Corporation, St Joseph, MI; ³Martin-Luther-University Halle-Wittenberg, Halle / Saale, Germany

8:30 - 10:30 am Wednesday

ION MOBILITY: NEW DEVELOPMENTS & APPLICATIONS

Session Chair: Helen Cooper (University of Birmingham)
B312-314

- WOF am 08:30 **Segmented Ion Fractionation and High Field Asymmetric Waveform Ion Mobility Spectrometry Expands Proteome Coverage to Uncover Sequence Variants;** Eric Bonneau¹; Sibylle Pfammatter^{1,2}; Pierre Thibault^{1,2}; ¹IRIC-Université de Montréal, Montréal, QC; ²Department of Chemistry, Université de Montréal, Montréal, QC
- WOF am 08:50 **A Novel Cyclic Ion Mobility Enabled Method for Data Enrichment, Selectivity and Sensitivity Enhancement in MS/MS Experiments;** Eleanor Riches¹; Martin Palmer¹; Jakub Ujma¹; Kevin Giles¹;



- Sunghwan Kim²; ¹Waters Corporation, Wilmslow, United Kingdom; ²Kyungpook National University, Daegu, South Korea
- WOF am 09:10 **A Drift-Tube Ion Mobility-Mass Spectrometer for Native Mass Spectrometry: High Resolution Ion Mobility, Collision Induced Unfolding, and Electron Capture Dissociation;** Varun Gadkari¹; Ruwan T Kurulugama²; John C. Fjeldsted²; Brandon T. Ruotolo¹; ¹University of Michigan, Ann Arbor, MI; ²Agilent Technologies, Inc., Santa Clara, CA
- WOF am 09:30 **Top-Down Sequencing of Mobility-Selected Glycoprotein Complexes Using Tandem Trapped Ion Mobility Spectrometry – Mass Spectrometry (Tandem-TIMS/MS);** Fanny C Liu¹; Mark E. Ridgeway²; Melvin A. Park²; Christian Bleiholder¹; ¹Florida State University, Tallahassee, FL; ²Bruker Daltonics Inc., Billerica, MA
- WOF am 09:50 **Trapped Ion Mobility Mass Spectrometry as a Tool for Neuropeptide Analysis;** Geert Baggerman^{1,2}; Kristina Marx³; Harshavardhan Budamgunta²; Gerben Menschaert⁴; Kurt Boonen^{2,5}; ¹Vito, Mol, Belgium; ²Uantwerpen, Antwerpen, Belgium; ³Bruker Daltonik GmbH, Bremen, Germany; ⁴UGent, Gent, Belgium; ⁵Vito, Mol, Belgium
- WOF am 10:10 **Broad Targeted Phosphoproteomics analysis Using Structures for Lossless Ion Manipulations (SLIM) Ion Mobility-MS;** Yi-Ting Wang¹; Gabe Nagy¹; Adam Hollerbach¹; Chia-Feng Tsai¹; Karin Rodland¹; Tujin Shi¹; Richard Smith¹; Tao Liu¹; ¹Biological Science Division, Pacific Northwest National Laboratory, Richland, WA
- 8:30 - 10:30 am Wednesday**
FUNDAMENTALS FOR EVERYONE: STRUCTURAL ELUCIDATION
Session Chair: Albert T. Lebedev (Moscow State University)
Auditorium, Bldg A
- WOG am 08:30 **Structural Elucidation of Metabolites Using Accurately Computed Fragmentation Patterns and Searches in Databases of 2D Molecular Structures;** Bela Paizs^{1,2}; Zoltan Takats^{2,3}; ¹Bangor University, Bangor, United Kingdom; ²deshape Ltd, Bangor, United Kingdom; ³Imperial College, London, United Kingdom
- WOG am 08:50 **Gas-Phase Ion/Ion Chemistry for the Detailed Structural Analysis and Relative Quantitation of Unsaturated Lipids;** Caitlin E. Randolph¹; David J. Foreman¹; Stephen J. Blanksby²; Scott A McLuckey¹; ¹Purdue University, West Lafayette, IN; ²Central Analytical Research Facility, Institute for Future Environments, Queensland University of Technology, Brisbane, Australia
- WOG am 09:10 **IRMPD Ion Spectroscopy and Ion-Molecule Reactions as Structure Elucidation Tools for Peptide Radical Ions;** Victor Ryzhov; Northern Illinois University, DeKalb, IL
- WOG am 09:30 **Characterization of Small Molecule Unknowns Using the AcquireX Data Acquisition Strategy;** Seema Sharma¹; Stephanie N. Samra¹; Caroline Ding¹; Kate J. Comstock¹; Reiko Kiyonami¹; Scott M. Peterman¹; Graeme McAlister¹; Mark Sanders¹; Vlad Zabrouskov¹; ¹Thermo Fisher Scientific, San Jose, CA
- WOG am 09:50 **Cationized Glycan Fragmentation Chemistry;** Benjamin Bythell; Univ. of Missouri-St. Louis, St. Louis, MO
- WOG am 10:10 **Comparative Study of 'Ortho-' and 'Para-' Effects in EI Spectra Of Silyl, Acyl, Mesyl and Tosyl Derivatives of tert-Butylphenols / Thiophenols;** Anzor Mikaia¹; Nino Todua^{1,2}; Levan Megutnishvili¹; ¹National Institute of Standards and Technology, Gaithersburg, MD; ²Stratavia, Largo, MD
- 8:30 - 10:30 am Wednesday**
SYNTHETIC POLYMERS
Session Chair: Rainey Patterson Garland (Eastman Chemical Co.)
A411-412
- WOH am 08:30 **High-Throughput Screening of Polysorbates by High Resolution Mass Spectrometry with Rapid H/D Exchange;** Kui Yang¹; Asha Hewarathna¹; Ilan Geerluf-Vidavsky¹; Connie Ruzicka¹; David Keire¹; ¹FDA, St. Louis, MO
- WOH am 08:50 **Analysis of Biocompatible Synthetic Polymers with Electron Capture Dissociation and Two-Dimensional Mass Spectrometry;** Tomos E. Morgan¹; Sean H. Ellacott¹; Andrew Kerr¹; Christopher A. Wootton¹; Bryan P. Marzullo¹; Maria van Agthoven¹; Mark P. Barrow¹; Anthony W. T. Bristow²; Sebastien Perrier¹; Peter B. O'Connor¹; ¹University of Warwick, Coventry, United Kingdom; ²AstraZeneca, Macclesfield, United Kingdom
- WOH am 09:10 **Probing the Reaction Mechanisms of Troger's Base Polymers of Intrinsic Microporosity;** Anthony P. Gies¹; Robert E. Hefner¹; Nathan J. Rau¹; Praveenkumar Boopalachandran¹; ¹The Dow Chemical Company, Lake Jackson, TX
- WOH am 09:30 **Secured Communications with Sequence-Controlled Synthetic Polymers: Decoding by Tandem Mass Spectrometry, Decrypting by Ion Mobility Spectrometry;** Jean-Arthur Amalian¹; Gianni Cavallo²; Abdelaziz Al Ouahabi²; Jean-François Lutz²; Laurence Charles¹; ¹Aix-Marseille University, Marseille Cedex 20, France; ²Institut Charles Sadron, University of Strasbourg, Strasbourg, France
- WOH am 09:50 **Determination of Gas Phase Ion Structures of Polar Homopolymers through Ultra-High Resolution Ion Mobility Spectrometry-Mass Spectrometry;** Xi Chen^{1,2}; Shannon A. Raab³; Timothy Poe¹; David E. Clemmer³; Carlos Larriba Andaluz¹; ¹IUPUI, Indianapolis, IN; ²Purdue University, West Lafayette, IN; ³Indiana University, Bloomington, IN
- WOH am 10:10 **Charge Detection Mass Spectrometry with an Orbitrap Analyzer;** Jared O. Kafader¹; Rafael D. Melani¹; Bryan P. Early¹; Kenneth R. Durbin¹; Neil L. Kelleher¹; Philip D. Compton¹; Steven C. Beu²; Deven L. Shinholt³; Joshua T. Maze³; Alexander A. Makarov⁴; Vlad Zabrouskov⁵; Michael W. Senko⁵; ¹Northwestern University, Evanston, IL; ²S.C. Beu Consulting, Austin, TX; ³Thermo Fisher Scientific, Austin, TX; ⁴Thermo Fisher Scientific, Bremen, Germany; ⁵Thermo Fisher Scientific, San Jose, CA

10:30 am - 2:30 pm Wednesday
WEDNESDAY POSTER SESSION
Poster/Exhibit Hall ground level
Lunch concessions are open 11:00 am - 2:00 pm

Odd-number posters present:
10:30 am - 11:30 am PLUS 12:30 - 2:30 pm

Even-number posters present:
10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

Poster Pick-Me-Up Snacks served at 1:30 pm



WEDNESDAY AFTERNOON ORAL SESSIONS

2:30 - 4:30 pm Wednesday

METABOLOMICS: UNTARGETED PROFILING

Session Chair: Elizabeth J. Want (Imperial College)

Murphy Ballroom, Bldg B, Level 5

- WOA pm 02:30 **Determining the Metabolic Fate of Nitrogen Oxide Species Using Isotopic Tracing and High Resolution Mass Spectrometry**; Steven Mullett¹; Stacy L. Wendell²; ¹University Of Pittsburgh, Pittsburgh; ²University of Pittsburgh, Pittsburgh, PA
- WOA pm 02:50 **Single-Cell Metabolomic Analysis of Metastatic and Non-Metastatic Cell Line Pairs Using Mass Spectrometry**; Shelby R Beasley¹; Mei Sun¹; Zhibo Yang¹; ¹University of Oklahoma, Norman, OK
- WOA pm 03:10 **Enhancing Untargeted Metabolomics with Fast-Scanning Field Asymmetric Waveform Ion Mobility Spectrometry**; James Reynolds¹; Katarzyna Szykula¹; Colin Creaser¹; ¹Loughborough University, Loughborough, United Kingdom
- WOA pm 03:30 **Development of Advanced Processing Workflow for Untargeted Volatilomics By GC×GC-TOFMS**; Pierre-Hugues Stefanuto¹; Delphine Zanella¹; Maurine Fucito¹; Florence Schleich²; Renaud Louis²; Jean-François Focant¹; ¹Liège University, Liège, Belgium; ²Liège University Hospital, Liège, Belgium
- WOA pm 03:50 **MetaboPique: A High-Throughput Computational Workflow for Validating, Annotating, and Organizing Small Molecule MS/MS Spectra Derived from Biological Samples**; Tytus D Mak¹; Concepcion A Remoroza¹; Meghan C Burke¹; Kelly H Telu¹; Stephen E Stein¹; ¹National Institute of Standards and Technology, Gaithersburg, MD
- WOA pm 04:10 **A High-Throughput Method for Obtaining Microbial Exometabolomics Data Using a 3D Printed Platform**; Caroline Birer¹; Rosalie K. Chu²; Christopher Anderton²; Erik S. Wright¹; ¹Department of Biomedical Informatics, University of Pittsburgh, Pittsburgh, PA; ²Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA

2:30 - 4:30 pm Wednesday

HYDROGEN-DEUTERIUM EXCHANGE MS: INNOVATIONS

Session Chair: Miklos Guttman (University of Washington)

B401-402

- WOB pm 02:30 **Advanced Statistical Methods for Analysis of HX-MS Data in Higher-Order Structural Comparability and Similarity Contexts Using Hybrid Significance Criteria**; Tyler S Hageman¹; David Weis¹; ¹University of Kansas, Lawrence, KS
- WOB pm 02:50 **New insights into Differences in Intrinsic HDX Rates at Different pH and Temperature**; Jun Zhang¹; Devrishi Goswami²; zhoangqi Zhang²; ¹Amgen, Inc, Thousand Oaks, CA; ²Amgen, Inc., Thousand Oaks, CA
- WOB pm 03:10 **Synergistic Structural Information about Stressed Therapeutic Antibodies from Hydrogen Deuterium Exchange and Covalent Labeling Mass Spectrometry**; Catherine Tremblay¹; Patanachai Limpikirati¹; Richard W. Vachet¹; ¹University of Massachusetts-Amherst, Amherst, MA
- WOB pm 03:30 **Hydrogen-Deuterium Exchange Mass Spectrometry Reveals the Mechanism of Multidrug Resistance in the Efflux Pump AcrB**; Argyris Politis¹; Zainab Ahdash¹; Eamonn Reading¹; Xuan Wang Kan²; Elizabeth Grimsey²; Laura J. V. Piddock²; ¹King's College London, London, United Kingdom; ²University of Birmingham, Birmingham, United Kingdom

WOB pm 03:50 **Rapid Solution-Phase HDX for Small Molecule Identification**; Sandra N Majuta¹; Chong Li¹; Kinkini Jayasundara¹; Ahmad Kiani Karanji¹; Kushani Attanayake¹; Nandhini Ranganathan¹; Peng Li¹; Stephen Valentine¹; ¹West Virginia University. C. Eugene Bennett Department of Chemistry, Morgantown, WV

WOB pm 04:10 **New Electrochemical Cell for Superior On-line Reduction of Disulfide Bonds in MS Proteomics**; Jean-Pierre Chervet¹; Pablo Sanz de la Torre¹; Hendrik Jan Brouwer¹; Martin Eysberg²; ¹Antec Scientific, Zoeterwoude, Netherlands; ²Antec Scientific, Boston, MA

2:30 - 4:30 pm Wednesday

FORENSICS: INNOVATIONS AND APPLICATIONS

Session Chair: Travis M. Falconer

(US Food & Drug Administration)

B405-407

- WOC pm 02:30 **Rapid and Sensitive Detection of Organic Explosives with PS (Paper Spray) and SAWN Surface Acoustic Wave Nebulization) Ambient Ionization Mass Spectrometry**; Lauren Pintabona¹; Alina Astefanei¹; Arian C. Van Asten¹; Garry L. Corthals¹; ¹University of Amsterdam, Amsterdam, Netherlands
- WOC pm 02:50 **Proteomic Profiling of Single Hairs Recovered after an Explosion for Protein-Based Human Identification**; Fanny Chu^{1,2}; Katelyn E. Mason¹; Deon S. Anex¹; A. Daniel Jones²; Bradley Hart¹; ¹Lawrence Livermore National Laboratory, Livermore, CA; ²Michigan State University, East Lansing, MI
- WOC pm 03:10 **Carrion Insect Species Identification From Multi-species Mixtures of Larvae Using Multi-label Classification of DART-HRMS Data for Postmortem Interval Determination**; Rabi A. Musah¹; Samira Beyramysoltan¹; Justine E. Giffen¹; Jennifer Y. Rosati²; Monica Ventura¹; ¹University at Albany-SUNY, Albany, NY; ²John Jay College of Criminal Justice, New York City, NY
- WOC pm 03:30 **Towards On-Site Drug Evidence Confirmation via Surface-Enhanced Raman Spectroscopy and Paper Spray Ionization Employed on Portable Instrumentation**; William L. Fatigante¹; Ashley R. Stelmack¹; Daniel Burr¹; John Harms¹; Jeremy D. Driskell¹; Jun-Hyun Kim¹; Jamie R Wieland¹; Christopher Mulligan²; ¹Illinois state university, Normal, IL; ²Illinois State University, Normal, IL
- WOC pm 03:50 **ASAP Mass Spectrometry for the Real-Time Identification of Psychoactive Drugs Supplied by the Public as Part of a Harm-Reduction Service**; Christopher A Whitmore^{1,2}; Guy Jones^{2,3}; Fiona Measham^{1,2}; Jackie Moseley^{1,2}; ¹Durham University, Durham, United Kingdom; ²The Loop, Manchester, United Kingdom; ³Reagent Tests, Cambridge, United Kingdom
- WOC pm 04:10 **Mass Spectrometry-Derived Information Concerning Atypical Findings Critical to Sports Drug Testing: 19-Norandrosterone and AICAR**; Mario Thevis¹; Frank Huelsemann¹; Thomas Piper¹; ¹German Sport University, Cologne, Germany





2:30 - 4:30 pm Wednesday

ENDOGENOUS PROTEIN BIOMARKERS IN DRUG DISCOVERY AND DEVELOPMENT: QUANTITATIVE ANALYSIS

 Session Chair: Naiyu Zheng (Bristol-Myers Squibb Company)
B302-305

- WOD pm 02:30 **A Sensitive LC-HRMS Method for the Quantitation of Dystrophin Protein in Human Muscle Tissue**; Keyvork Mekhssian¹; H  l  ne Montpetit¹; Romain Beauvois¹; Hironori Osaki²; Anahita Keyhani¹; ¹Altasciences, Laval, QC; ²NS Pharma, Paramus, NJ
- WOD pm 02:50 **IL2 Receptor $\alpha/\beta/\gamma$ Turnover Kinetic Measurement *In vitro* by Serial Immuno Affinity(IA) Capture and Targeted LC/MS Method**; Xiaomeng Shen¹; Kevin Cook¹; Yun Ling¹; Dan A Rock¹; Brooke Rock¹; ¹Amgen, South San Francisco, CA
- WOD pm 03:10 **Interrogation of the Tumor Microenvironment: LCMS-based Quantitation of Target, Drug, and Relevant Biomarkers for Drug Discovery**; Petia Shipkova¹; Yongxin Zhu¹; Jacob Zalaznick¹; Bogdan Slecza¹; Matthew Mazur¹; Karen Parrish¹; Zheng Yang¹; Timothy Olah¹; ¹Bristol Myers Squibb, Princeton, NJ
- WOD pm 03:30 **Proteomic Analysis Revealed Targeting Crosstalk of Histone H3K27me and H3K27ac as a Therapeutic Strategy for EZH2-Aberrant Solid Tumors**; Minjia Tan¹; Min Zhang²; Xun Huang²; Juan Yan²; Zhiwei Liu²; Linhui Zhai²; Jian Ding²; Meiyu Geng²; ¹Shanghai Institute of Materia Medica, Shanghai, China; ²Shanghai Institute of Materia Medica, Shanghai, China
- WOD pm 03:50 **Absolute Quantitation of Cellular Retinol Binding Protein, Type 1 in Cancer-Relevant Cell Lines via In-Gel Digestion**; Stephanie Zalesak¹; Wenjing Li¹; Jianshi Yu¹; Maureen Kane¹; ¹University of Maryland, Baltimore- School of Pharmacy, Baltimore, MD
- WOD pm 04:10 **Concentration Measurements of 220 Endogenous Proteins in Capillary Blood Using Dried Blood Spots, as Determined by MRM with Peptide Standards**; Azad Eshghi¹; Adam J. Pistawka²; Jun Liu³; Michael Chen⁴; Nicholas J. T. Sinclair¹; Darryl B. Hardie¹; Monica Elliott¹; Lei Chen¹; Rachael Newman¹; Christoph H. Borchers^{1, 2, 5, 6}; ¹University of Victoria-Genome BC Proteomics Centre, Victoria, BC; ²Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC; ³Department of Pathology and Laboratory Medicine, University of British Columbia, Vancouver, BC; ⁴Island Medical Program, Department of Pathology and Laboratory Medicine, University of British Columbia, Vancouver, BC; ⁵Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; ⁶Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC
- WOD pm 02:50 ***In vivo* Tissue Classification Using Surgical Robotics and Rapid Evaporative Ionisation Mass Spectrometry – towards the Chemically Aware Surgical Robot**; Eftychios Manoli¹; Burak Temelkuran¹; Julia Balog²; Steven Pringle²; Jagtar Dhanda³; Ara Darzi¹; Neil Tolley¹; Zoltan Takats¹; ¹Imperial College London, London, United Kingdom; ²Waters Corporation, Wilmslow, United Kingdom; ³Queen Victoria Hospital, East Grinstead, UK, East Grinstead, United Kingdom
- WOE pm 03:10 **Moving Forward into *in vivo* Intraoperative Diagnostic Using Water-Assisted Laser Desorption/Ionization Mass Spectrometry**; Philippe Saudemont¹; Nina Ogrinc¹; Yves-Marie Robin²; Benoit Fatou^{1, 3}; Cristian Focsa³; Michael Ziskind³; Dominique Tierny⁴; Zoltan Takats⁵; Michel Salzet¹; Isabelle Fournier¹; ¹PRISM Inserm U1192 - University of Lille, Villeneuve D'ascq Cedex, France; ²Pathology Department, Centre Oscar Lambret, Lille, France; ³University of Lille, CNRS UMR 8523 PhLAM, Villeneuve d'Ascq, France; ⁴OCR, Villeneuve d'Ascq, France; ⁵Imperial College London, Department of Surgery and Cancer, United Kingdom
- WOE pm 03:30 **Infrared Laser Based Real-Time, *in vivo* Tissue Identification in Veterinary Surgery Using Laser-Assisted Rapid Evaporative Ionization Mass Spectrometry**; Viktoria Varga¹; Steven D Pringle²; Gabriel Stefan Horkovits-Kovats³; Julia Balog³; ¹Waters Research Center Kft., Budapest, Hungary; ²Waters Corporation, Wilmslow, United Kingdom; ³Waters Research Center, Budapest, Hungary
- WOE pm 03:50 **Implementation of Ambient MS-Based Tissue Profiling for Assistance on Neurosurgery Operations of Brain Cancer**; Igor Popov¹; Anatoly Sorokin^{1, 2}; Vsevolod Shurkhay³; Vasiliy Elifirov¹; Evgeny Zhvansky¹; Stanislav Pekov^{1, 4}; Alexander Potapov³; Eugene (evgeny) Nikolaev⁵; ¹Moscow Institute of Physics and Technology (State University), Dolgoprudny, Russia; ²Institute of Cell Biophysics RAS, Pushchino, Russia; ³N. N. Burdenko Scientific Research Neurosurgery Institute, Moscow, Russia; ⁴Institute for Energy Problems of Chemical Physics RAS, Moscow, Russia; ⁵Skolkovo institute of science and technology, Moscow Region, Russian Federation
- WOE pm 04:10 **Qualitative Classification of Tissue Amyloidosis and Subtyping by Mass Spectrometry**; Srinivas V.s Chakravartula¹; Adolfo Firpo Betancourt²; Damodara Rao Mendu³; Tin Htwe Thin²; Salem Fadi³; Michael Donovan²; Carlos Cordon Cardo²; ¹Mount Sinai Hospital, New York City, New York; ²Icahn School of Medicine at Mount Sinai, New York, NY; ³Mount Sinai Hospital, New York City, NY

2:30 - 4:30 pm Wednesday

CLINICAL ANALYSIS: MS IN THE OPERATING ROOM

 Session Chair: Y. Ruben Luo (UCSF)
B308-309

- WOE pm 02:30 ***In vivo* and Intraoperative Tissue Analysis and Diagnosis Using the MasSpec Pen**; Jialing Zhang¹; Marta Sans¹; Christopher Pirko²; Rachel J. DeHoog¹; Kyana Garza¹; Clara L. Feider¹; Mary King¹; Alena Bensussan¹; John Q. Lin¹; Michael Keating¹; Timothy Hooper¹; Wendong Yu²; Chandandeep Nagi²; Sadhna Dhingra²; George Van Burren²; Stacey Carter²; William Fisher²; Omar Barakat²; Raymon Grogan²; Thomas E. Milner³; James Suliburk²; Livia S. Eberlin¹; ¹University of Texas, Department of Chemistry, Austin, TX; ²Baylor College of Medicine, Houston, TX; ³University of Texas, Austin, TX
- WOE pm 02:50 ***In vivo* Tissue Classification Using Surgical Robotics and Rapid Evaporative Ionisation Mass Spectrometry – towards the Chemically Aware Surgical Robot**; Eftychios Manoli¹; Burak Temelkuran¹; Julia Balog²; Steven Pringle²; Jagtar Dhanda³; Ara Darzi¹; Neil Tolley¹; Zoltan Takats¹; ¹Imperial College London, London, United Kingdom; ²Waters Corporation, Wilmslow, United Kingdom; ³Queen Victoria Hospital, East Grinstead, UK, East Grinstead, United Kingdom
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- WOE pm 03:50 **Implementation of Ambient MS-Based Tissue Profiling for Assistance on Neurosurgery Operations of Brain Cancer**; Igor Popov¹; Anatoly Sorokin^{1, 2}; Vsevolod Shurkhay³; Vasiliy Elifirov¹; Evgeny Zhvansky¹; Stanislav Pekov^{1, 4}; Alexander Potapov³; Eugene (evgeny) Nikolaev⁵; ¹Moscow Institute of Physics and Technology (State University), Dolgoprudny, Russia; ²Institute of Cell Biophysics RAS, Pushchino, Russia; ³N. N. Burdenko Scientific Research Neurosurgery Institute, Moscow, Russia; ⁴Institute for Energy Problems of Chemical Physics RAS, Moscow, Russia; ⁵Skolkovo institute of science and technology, Moscow Region, Russian Federation
- WOE pm 04:10 **Qualitative Classification of Tissue Amyloidosis and Subtyping by Mass Spectrometry**; Srinivas V.s Chakravartula¹; Adolfo Firpo Betancourt²; Damodara Rao Mendu³; Tin Htwe Thin²; Salem Fadi³; Michael Donovan²; Carlos Cordon Cardo²; ¹Mount Sinai Hospital, New York City, New York; ²Icahn School of Medicine at Mount Sinai, New York, NY; ³Mount Sinai Hospital, New York City, NY
- WOE pm 02:30 **Clinical Metabolomics Study Uncovers the Outcome of Radiation Therapy in Cancer Patients**; Nicholas B. Vera^{1, 2}; Evan Pannkuk³;

2:30 - 4:30 pm Wednesday

ION MOBILITY: SMALL MOLECULES, PHARMACEUTICALS, AND DMPK

 Session Chair: Erin Baker (North Carolina State University)
B312-314

- WOE pm 02:30 **Clinical Metabolomics Study Uncovers the Outcome of Radiation Therapy in Cancer Patients**; Nicholas B. Vera^{1, 2}; Evan Pannkuk³;



- WOF pm 02:50 Evagelia C Laiakis³; Albert J Fornace³; Stephen L. Coy²; Michelle Clasquin¹; Paul Vouros²; *Pfizer, Internal Medicine Research Unit, Cambridge, MA, 02139*; ²*Department of Chemistry and Chemical Biology, Northeastern University, Boston, MA 02115*; ³*Georgetown University, Washington, DC*
- WOF pm 03:10 **Characterization of Gas-Phase Structures of Drug Metabolites Using Ion Mobility-Mass Spectrometry**; Dylan H. Ross¹; Ryan P. Seguin¹; Libin Xu¹; ¹*University of Washington, Seattle, WA*
- WOF pm 03:30 **DMS Separation, IR Identification, and Quantification of Amino Acids and Related Compounds in Plasma Samples**; Francis Berthias¹; Yali Wang¹; Eskander Alhajji¹; Jean-François Benoist²; Philippe Maitre³; ¹*Université Paris-Sud, Orsay, France*; ²*Hôpital Robert Debré, Paris, France*; ³*Université Paris Sud, Orsay, France*
- WOF pm 03:50 **Rapid Detection of Fentanyl Analogs Using GC-APCI-TIMS-TOF MS**; Elisa N Shoff^{1,2}; Cesar E Ramirez¹; Francisco A. Fernandez-Lima¹; ¹*Department of Chemistry and Biochemistry, Florida International University, Miami, FL*; ²*Miami-Dade Medical Examiner Department, Miami, FL*
- WOF pm 03:50 **Development of Ion Mobility-Mass Spectrometry Methods and Collision Cross Section Database for Improved Identification of Microbiome-Derived Metabolites**; Matthew Glover¹; Omari Jones-Nelson¹; Taylor Cohen¹; Wen Yu¹; Paul Warren¹; Bret Sellman¹; Sonja Hess¹; ¹*MedImmune, Gaithersburg, MD*
- WOF pm 04:10 **Imaging Mass Spectrometry Including Ion Mobility Separation Sheds Light on Bacterial Responses to Different Cultivation Conditions**; Francesca Brescia^{1,2}; Samuele Zoratto³; Gerardo Puopolo²; Ilaria Pertot²; Martina Marchetti-deschmann³; ¹*Department of Sustainable Ecosystems & Bioresources, Research and Innovation Centre, Fondazione Edmund Mach, San Michele all'Adige, Italy*; ²*Department of Agricultural, Food, Environmental and Animal Sciences, University of Udine, Udine, Italy*; ³*Institute of Chemical Technologies and Analytics, TU Wien, Vienna, Austria*
- 2:30 - 4:30 pm Wednesday**
INSTRUMENTATION: AMBIENT IONIZATION AND APPLICATIONS
Session Chair: G. Asher Newsome (Smithsonian Institution)
Auditorium, Bldg A
- WOG pm 02:30 **First implementation of Rapid Evaporative Ionisation Mass Spectrometry (REIMS) for the At-Line Screening of Boar Carcasses in the Slaughter House**; Lieselot Y Hemeryck¹; Sara L Stead²; Anneleen Declodet¹; Steve Huysman¹; Julia balog³; Margot DeSpiegeleer¹; Steven D Pringle²; aurelien boland⁴; Lynn Vanhaecke¹; ¹*Ghent University, Ghent, Belgium*; ²*Waters Corporation, Wilmslow, United Kingdom*; ³*Waters Research Centre, Budapest, Hungary*; ⁴*Waters Benelux, Brussels, Belgium*
- WOG pm 02:50 **A Single-Cell Look at Biological Nitrogen Fixation: Rapid Determination of Metabolite Formulas from Isotopic Fine Structures in Heterogeneous Cell Populations**; Laiith Z. Samarah¹; Rikkita Khattar¹; Tina H Tran¹; Sylwia A Stopka¹; Dusan Velickovic²; Christopher R Anderton²; Jared B. Shaw²; Nikola Tolic²; David W Koppenaar²; Ljiljana Pasa-Tolic²; Beverly J Agtuca³; Gary Stacey³; Akos Vertes¹; ¹*The George Washington University, Washington, DC*; ²*Pacific Northwest National Laboratory, Richland, WA*; ³*University of Missouri, Columbia, MO*
- WOG pm 03:10 **MicroArray Droplet Ionization for Spatially Controlled Imaging of Lipids and Metabolites in Biological Samples**; Marta Sans¹; Anna Krieger¹; Bryan Wygant¹; Kyana Garza¹; C. Buddie Mullins^{1,2}; Livia S. Eberlin¹; ¹*University of Texas, Austin, TX*; ²*McKetta Department of Chemical Engineering, The University of Texas, Austin, TX*
- WOG pm 03:30 **Charge Production by Sublimation of Organic Compounds in Matrix Assisted Ionization**; Bijay Banstola¹; Kermit K. Murray¹; ¹*Louisiana State University, Baton Rouge, LA*
- WOG pm 03:50 **Understanding the Implications of Confined DART-MS: Considerations and Strategies for Optimization**; Edward Sisco¹; Thomas P. Forbes²; Matthew Staymates²; ¹*National Institute of Standards and Technology, Gaithersburg, MD*; ²*National Institute of Standards and Technology, Gaithersburg, MD*
- WOG pm 04:10 **Ion Focusing and Transport in Air Using Conductive 3D-Printed Electrodes**; Kiran Iyer¹; Brett M Marsh¹; Grace Olivia Capek¹; Shane Tichy²; Graham R. Cooks¹; ¹*Purdue University, West Lafayette, IN*; ²*Agilent Laboratories, Santa Clara, CA*
- 2:30 - 4:30 pm Wednesday**
FUNDAMENTALS: DDA AND DIA LC-MS
Session Chair: Stefan Tenzer (University Medical Center Mainz)
A411-412
- WOH pm 02:30 **diaPASEF: Toward the Ideal Mass Analyzer with Data-Independent Acquisition and Parallel Accumulation – Serial Fragmentation**; Florian Meier¹; Andreas-David Brunner¹; Max Frank²; Annie Ha²; Eugenia Voytik¹; Stephanie Kospar-Schönefeld³; Markus Lubeck³; Heiner Koch³; Scarlet Koch³; Oliver Raether³; Ben C Collins⁴; Ruedi Aebersold^{4,5}; Hannes Röst²; Matthias Mann^{1,6}; ¹*Max-Planck-Institute of Biochemistry, Martinsried, Germany*; ²*Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, ON*; ³*Bruker Daltonik GmbH, Bremen, Germany*; ⁴*ETH Zurich, Zurich, Switzerland*; ⁵*University of Zurich, Zurich, Switzerland*; ⁶*University of Copenhagen, Copenhagen, Denmark*
- WOH pm 02:50 **Combining Drift Tube Ion Mobility and Quadrupole Selectivities for Data Independent Workflows for Metabolomics**; Tim Causon¹; Max Feuerstein¹; Ruwan T. Kurulugama²; George Stafford²; John C. Fjeldsted²; Stephan Hann¹; ¹*Institute of Analytical Chemistry, Department of Chemistry, University of Natural Resources and Life Sciences (BOKU), Vienna, Austria*; ²*Agilent Technologies, Inc., Santa Clara, CA*
- WOH pm 03:10 **Improving Quantification Using MS1 and MS2 Information in Data Independent Acquisition**; Roland Bruderer¹; Ting Huang²; Jan Muntel¹; Oliver M. Bernhardt¹; Olga Vitek²; Lukas Reiter¹; ¹*Biognosys, Schlieren, Switzerland*; ²*Khoury College of Computer and Information Sciences, Boston, MA*
- WOH pm 03:30 **TKO-iQC: A Platform for Tracking Instrument Performance and Evaluating Interference in Isobaric Tag-based Workflows**; Joao A Paulo¹; Jose Navarrete-Perea¹; Steven P Gygi¹; ¹*Harvard Medical School, Boston, MA*
- WOH pm 03:50 **Using an External Reference Material to Harmonize and Calibrate Quantitative Mass Spectrometry Data at Scale**; Lindsay Pino¹; Brian C Searle²; Han-Yin Yang¹; Andrew N Hoofnagle³; William Stafford Noble¹; Michael J MacCoss¹; ¹*University of Washington, Genome Sciences, Seattle, WA*; ²*Institute for Systems Biology, Seattle, WA*; ³*University of Washington, Seattle, WA*



WOH pm 04:10 **Defying Gravity in Orbitrap Mass Spectrometry;** Jan-Peter Hauschild¹; Amelia Peterson¹; Erik Couzijn¹; Eduard Denisov¹; Denis Chernyshev¹; Christian Hock¹; Hamish Stewart¹; Ralf Hartmer¹; Christian Thoeing¹; Oliver Lange¹; Mathias Mueller¹; Arne Kreutzmann¹; Wilko Balschun¹; Aivaras Venckus¹; Alexander Kholomeev¹; Gregor Quiring¹; Frank Czemper¹; Tabiwang N. Arrey¹; Kerstin Strupat¹; Julia Kraegenbring¹; Markus Kellmann¹; Alexander Harder¹; Alexander Makarov¹; *Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

4:45-5:30 pm Wednesday
ASMS MEETING
Richard A. Yost (University of Florida), presiding
Enjoy a beverage and hear the latest ASMS news.
B302-305

5:45 - 7:00 PM WEDNESDAY WORKSHOPS

There will be light refreshments in Building A foyers. All workshops are in Building A.

01 MS-Based Interactomics: Computational Resources and Tools for Studying the Physical Interactome (Bioinformatics MS Interest Group)
Presiding: Isabell Bludau, William Noble
A402-403

The large variety of molecular functions in living systems are frequently not performed by single molecules, but are a result of the interplay between different molecular entities. Proteins, metabolites, lipids, RNA and DNA molecules interact among themselves and with each other to give rise to a large variety of functional modules inside the cell. Studying the quantity, subunit composition and topology of these modules and their dynamic change upon perturbations is therefore of fundamental interest for biology. In this workshop, we aim to introduce and discuss various strategies to analyze the physical interactome of biological molecules. We will specifically focus on available resources and software tools for (a) the in silico prediction of interactions, (b) the computational analysis of large-scale interactomics datasets (including AP-MS, cross-linking MS, protein correlation profiling, LiP-MS, etc.) and (c) the integration of data generated by multiple orthogonal strategies. We will invite leading experts in the field to present an overview of available databases and software tools as well as to provide general guidelines on their usability for different applications. Finally, we will discuss recent developments and future perspectives in the area of MS-based interactomics.

02 IMS: When Chromatography Just Won't Do (Ion Mobility MS Interest Group)
Presiding: Brian Clowers, Jakub Ujma, Ian Webb
A404-405

Fundamental measurements of gas-phase ion properties serve as the foundation describing ion mobility (IM); this property is often exploited for analytical benefits. With historical names such as Plasma Chromatography and Gaseous Electrophoresis, ion mobility techniques often have logical analogues to more traditional chromatographic techniques. Until recently, the major differentiator between IM separations and contemporary chromatographic techniques was the speed of analysis.

Advances in ion confinement and manipulation (e.g. ion funnels, T-wave, and SLIM technologies) allowed increases in the separation path lengths, thus significant enhancements in resolving power (R_p) have been achieved; often at a cost of increased separation time scales. Improvements in R_p can also be achieved by increasing the strength of the applied electric field. This, in principle offers increased R_p and reduced separation time scale, but several practicalities have to be considered. As the separating power of ion mobility techniques increases, the additional pressures are placed on the mass spectrometry systems used for detection. More specifically, as peak widths narrow in the temporal domain, minimizing peak broadening in the IM-MS transfer region (equivalent to extra-column broadening in

chromatography) becomes paramount as well as compatibility of MS analyser/detector with the high fidelity ion mobility distributions.

To provide the community with a contemporary view of ion mobility-mass spectrometry techniques this forum will highlight the emergent, fast approaches to enhance separation selectivity of gas-phase ions. This workshop will cover methods hyphenated with IM, in particular those benefiting from the speed of IM separation. Finally, this workshop aims to promote discussion about the role of ion mobility techniques in tandem with chromatographic techniques and in some cases serve as a rapid replacement for front end separations prior to mass analysis.

03 Clinical Applications: Standardization and Harmonization Efforts (Clinical Chemistry Interest Group)
Presiding: Candice Ulmer, Donald Chace
A406-407

With the advent of novel mass spectrometric reference measurement procedures and improved clinical analyzers for clinical diagnostics, standardized results have become a necessity in the clinical setting to ensure accuracy/reliability in laboratory measurements, consistent disease diagnosis, and appropriate treatment for patients. Standardization ensures that laboratory testing is accurate, reliable, and precise across methods and over time. In addition, standardization is important in the clinical setting as many clinical/public health decisions are made and evidence-based patient guidelines written using laboratory measurements. Comparable measurements are needed between multiple assays, including those performed on clinical analyzers and mass spectrometers to allow for the generation of analyte-specific reference values. As a means to harmonize immunoassays and mass spectrometric procedures, reference materials and international standards are needed for method calibration purposes and conversion values. This workshop will [1] highlight the need for harmonized results, [2] introduce ongoing standardization efforts within clinical chemistry, and [3] discuss opportunities to create and engage in commutability studies, certification programs, and clinical-based interlaboratory studies.

04 Exposomics Workshop (Exposomics Interest Group)
Presiding: Jarod Grossman, Silvia Balbo, Benedikt Warth
A408

This workshop will have a panel consisting of thought leaders in different scientific fields of the exposome space. They will discuss their work and challenges they have overcome and encountered in their research.

Global interest in the exposome is growing and this expansion can be seen in the increased number of exposome publications in peer reviewed journals since 2010. There are many funded research endeavors designed to 'explore the exposome.' In the EU, HEALS,



There will be light refreshments in Building A foyers. All workshops are in Building A.

HELIX and EXPoSOMICS are all underway. PI's represent Imperial College, London, Aristotle University of Thessaloniki and CREAL in Barcelona. The Phenome Center has been established at Imperial College, London. In the US, NIEHS has funded HERCULES at Emory University and US EPA and CDC both define the exposome as a critical entity required to better understand the non-genetic contribution to chronic disease. Moreover, major US and Canadian Universities including Harvard, University of Pennsylvania, Stanford, University of Alberta and those mentioned above are engaged in exposome research. In Japan, NIES is conducting a prospective mother / child cohort, with more than 300,000 participants, to measure the exposome and in China, several University's are moving away from measuring pollutants in air and water, and into the exposome paradigm.

**05 MS-Based Process Analytical Technology (PAT):
Testing & Control of CQAs
(Pharmaceuticals Interest Group)
Presiding: Andrew Dawdy, Richard Rogers
A410**

One major goal of biotherapeutic process development (PD) is to produce the same high quality product in every experiment regardless of scale. To achieve this goal, PD scientists need to employ process analytical technologies (PAT) that can provide data on the upstream process (e.g. temperature, pH, glucose, amino acids, cell viability, and metabolites), downstream process (e.g. process-related impurities and host-cell impurities) and product quality attributes of the final product (e.g. charge isoforms, aggregates, and glycoforms). Mass spectrometry is an extremely valuable tool for characterizing bulk drug substance to identify critical quality attributes that affect the safety and efficacy of the product. However, MS-based PAT may also be used to characterize in-process molecules and study other upstream and downstream parameters that dictate the attributes of the final product. This workshop will be an interactive discussion amongst a panel of experts and the workshop attendees on the current state of mass spectrometry-based PATs and how they are improving PD. Topics may include application of MS for real-time (on-line / at-line) analysis of in-process materials, quality by design (QbD), continuous biomanufacturing, automated sample handling / preparation, automated data processing (e.g. intact deconvolution), novel technologies for MS-based charge isoform characterization, application of proteomics or metabolomics to support process development, and others. Please join us to ask questions, share your knowledge and experience, and discuss the future of MS-based PAT for the development of biotherapeutics.

**06 Endogenous Biomarkers: Measurement to Predict
in vivo Drug-Drug Interactions
(DMPK Interest Group)**

**Presiding: Jonathan Josephs, Brian Rago, Aaron Teitelbaum
A307**

Current in vitro models at assessing drug-drug interaction (DDI) liability of a new chemical entity (NCE), though the gold standard in drug discovery, struggle with a high false-positive rate (~30%). The ability to interrogate a validated transporter biomarker, in early clinical studies, such as first-in-human (FIH) studies, would help assess DDI liability, complement the existing agency DDI risk assessment approaches, help confirm or dispute in vitro data and potentially reduce the number of dedicated DDI clinical evaluations. This could result in earlier discharging of DDI risk and lead to significant resource and time savings.

Endogenous biomarkers of CYP and transporter activity have emerged recently as a growing area of interest for biomarker research and may provide insights into the potential for clinical DDIs without the need to conduct a specific clinical trial with a probe substrate. In addition to the traditional CYP enzymes considered. Transporters include OATP1B1/1B3, OCT1, OAT2, NTCP, OCT2, MATE1 and MATE2K. Recently, publications have explored coproporphyrin isomers (CP-I and CP-III), bile acids (BAs), and N1-methylnicotinamide as potential OATP1B1/3 and renal OCT2 transporter biomarkers, respectively.

Additionally, thiamine and 6 β -hydroxycortisol have been proposed as possible endogenous probes for hepatic OCT1 and renal OAT3, respectively. Creatinine has been proposed as a biomarker for OCT2, MATE1 and MATE2K inhibition.

While using traditional triple quadrupole based assays for biomarker quantitation has been well demonstrated for a number of these biomarkers. Using UHPLC-HRMS to interrogate potential biomarkers has several advantages: targeted quantitation, multiplexing of biomarkers, and also post-acquisition data mining of novel biomarkers.

**07 The NIH and NSF Review and Funding Process
Presiding: Salvatore Sechi, Kelsey Cook, Douglas Sheeley
A309**

Many ASMS members and conference participants are supported by the National Institutes of Health or the National Science Foundation. During this workshop the general funding and review process of grant applications/proposals will be presented. Issues like identifying the best contacts, writing an effective application/proposal, 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. Tips on grant writing and insights into the review process will be presented. Substantial time will be allotted for discussion and questions. NIH and NSF staff will also be available for individual discussions with investigators during scheduled "Office Hours" in the poster exhibit hall.

**08 Why You Should Submit Your Best Manuscripts to JASMS
Presiding: Joe Loo, JASMS Editor-in-Chief
A311**

The *Journal of the American Society for Mass Spectrometry (JASMS)* was started in 1990, and it remains a premier science journal that covers all aspects of mass spectrometry, including fundamental subjects (e.g., properties of gas-phase ions, instrumentation design, etc) and applications of mass spectrometry in all fields (including chemistry, biology, physics, geology, environmental science, and life sciences). But the scientific publishing industry has undergone dramatic changes since 1990, and journals must keep pace with these changes in order to remain competitive. The Workshop will discuss the current "nuts and bolts" of the operation of JASMS, how manuscripts are handled, how the journal can grow to best serve the needs of the mass spectrometry scientific community and the members of ASMS, and why all members should consider submitting their best work to the Society's journal. Members from the JASMS Editorial Staff and the ASMS Publications Committee will spur lively discussions.

**09 Metaproteomics for the Masses: Solutions,
Opportunities and Challenges
Presiding: Pratik Jagtap, Timothy Griffin, Robert Hettich
A312**

Metaproteomics, which characterizes the protein complement of a microbiome, enables researchers to understand the network and functional roles of the expressed microbial proteins in an ecosystem, thereby opening new avenues to characterize a variety of eukaryotic (human, plant) and environmental (soil, ocean) systems. As a complement to nucleic-acid based metagenomics (which provide detailed taxonomic information about microbial composition), metaproteomics research provides information about the metabolic activities and mechanism of microbial interactions with the host or environment. However, as compared to single-organism proteomics, mass spectrometry-based metaproteomics research poses additional challenges in data acquisition, database searching, and information extraction from these very complex peptide mixtures. Moreover, advanced bioinformatics approaches are needed to properly assign peptides to appropriate proteins and functional groups, as well as handle quantitative and multi-replicate analyses.



There will be light refreshments in Building A foyers. All workshops are in Building A.

Metaproteomics research experts will discuss the current status of metaproteomics research, and highlight solutions and opportunities in the emerging field. In particular, advanced data acquisition strategies and database searching methods for peptide matching and metaprotein inference will be discussed. Experts will also participate in an informal discussion on multi-omic studies (metagenomics, metatranscriptomics, metaproteomics, and metabolomics) and quantitative and statistical analysis of multi-replicate samples.

10 Bridging the Gap between Computational Biology and Biology: Matchmaking Session
Presiding: Ewy Mathe, Corey Broeckling
A313

Nowadays, science is conducted collaboratively and most often requires experts in bench (e.g. chemistry, biology) and computational sciences. The goal of this workshop is to promote conversations between computational biology, chemistry, and biology experts and to help bridge the communication gap between the fields. While bench scientists seek help with analysis of their data, computational biologists are hungry for data to test out their solutions to data analysis problems. The aim of this workshop is thus discuss methods to bridge the language and culture gap between computational biology and biology. A secondary aim is to help researchers find each other in this large conference setting.

The session will be split into three parts: 1) brief introduction; 2) all participants share their work in 3-5 minutes; 3) informal, small group discussions (led by moderators), where tool developers/analysis experts interact with bench scientists/novice researchers to identify common interests and foster future conversations/collaborations. Topics will include broad aspects of metabolomics analysis, from data preprocessing, to statistical analyses and data interpretation.

11 Ambient Ionization: Where We Stand Now and Go from Here
Presiding: Bindesh Shrestha, Sylwia Stopka
A314

After the introduction of desorption electrospray ionization (DESI) in the mid-2000s, dozens of new ambient mass spectrometry ionization source have been introduced. These ambient ionization tools are capable of direct analysis of samples in real time, require minimal sample perturbation, and analysis is performed under native conditions. The workshop will begin with a brief introduction that addresses the current state of ambient ionization techniques, followed by brief short presentations on variations of ambient ionization methods. These brief presentations will have a maximum of four slides, consisting of introduction (slide 1), a unique or high impact application (slide 2), limitations of the technique (slide 3), and future direction and discussions (slide 4). The brief presentations will be followed by an open discussion forum focused on current challenges related to ambient ionization and its future direction. The workshop aims to encourage the participation and presentations of new investigators, postdocs, and graduate students with a balanced perspective from academia, national lab, and industry. One of the goals of the workshop will be to gather scientists interested in ambient ionization technology and start the discussion towards forming an ambient ionization interest group to address these new scientific challenges.

12 The Proteomics Standards Initiative and ProteomeXchange: Supporting Open Data Practises in Proteomics
Presiding: Juan Antonio Vizcaino, Eric Deustch, Nuno Bandeira
A315

The Proteomics Standards Initiative (PSI, <http://www.psudev.info>) and ProteomeXchange (<http://www.proteomexchange.org>) are two highly collaborative projects that are open to the contribution and ideas from everyone in the community. Since 2002, the mission of the PSI is the development and promotion of open data standards and the related software in the proteomics field. Additionally, the PSI is increasingly involved in the development of data standards for metabolomics. In a parallel effort, since 2012, the ProteomeXchange Consortium is

standardising the submission and dissemination of public proteomics data between the main proteomics data repositories, currently including the resources PRIDE, PeptideAtlas, MassIVE, jPOST, iProx and Panorama Public.

We will briefly showcase our most successful projects and highlight some of our ongoing activities, fostering discussion among participants about what future directions in both initiatives would most benefit the community. Please attend if you want your voice to be heard!

13 Fundamentals: Structural Elucidation of Proteins (Fundamentals Interest Group)
Presiding: Christian Bleiholder, Alexandre Shvartsburg
A316

Elucidation of molecular structure has been a key goal of mass spectrometry since its origins, normally achieved using tandem mass spectrometry (MS/MS) via collision-induced dissociation (CID). With the emergence of biological MS, that direction has extended to proteins and their assemblies. The major new challenges faced by structural MS in this context have been (1) critical higher-level structure (beyond primary) and connectivity of post-translational modifications not amenable to standard MS/MS approaches and (2) for primary structure, the molecular size and complexity resulting in numerous competing fragmentation pathways and thus spectral congestion. These issues have motivated the invention of novel structural tools - both expanding the MS/MS capability (via new activation and fragmentation techniques resulting in more informative products) and complementary methods based on ion mobility for overall morphology characterization and/or spectroscopy for more targeted local probes. The central path forward appears to be combining orthogonal approaches in hyphenated instrumentation to provide specific and redundant independent constraints, and developing and validating the structure-property computational models to extract the utmost information from available rich experimental data.

We will discuss the latest instrumental and methodological advances in the area across the leading approaches, highlighting their limitations that one must appreciate for successful outcomes.

Topics and tentative speakers:

- Primary structure (bottom-up and top-down): Alan Marshall
- Primary structure (top-down and complex-top-down): Neil Kelleher
- Native MS (activation methods and H/D exchange)
- Theory and ion mobility: David Russell
- Spectroscopy: Jennifer Brodbelt

14 Education: Teaching MS at the Undergraduate Level (Undergraduate Research in MS Interest Group)
Presiding: Chrisi Hughey, Jay Forsythe
A303

This workshop will provide an overview of resources available to current and/or future instructors who teach mass spectrometry at the undergraduate level. Attendees are encouraged to bring and share mass spectrometry-related materials that they have developed for lecture and/or the laboratory. We will also discuss the successes and challenges of teaching mass spectrometry at the undergraduate level. The goal of the workshop is to build a community of instructors and an online repository of instructional resources through ASMS and/or the Analytical Sciences Digital Library (ASDL). If you have materials you would like to share, please email hugheyca@jmu.edu.

15 New Ion Manipulations Prior to FT-MS (FTMS Interest Group)
Presiding: Matthew Renfrow, Lissa Anderson,
A302

The efficiency of ion trapping and transferring prior to FT-MS detection has continued to improve and the sophistication of ion manipulations and separations prior to high resolution detection continue to increase.



5:45 - 7:00 PM WEDNESDAY WORKSHOPS AND THURSDAY MORNING ORAL SESSIONS

There will be light refreshments in Building A foyers. All workshops are in Building A.

This year's FT-MS workshop will focus on new ion manipulations prior to FT-MS and what new type of FT-MS-based analysis and experimentation these developments will allow. This includes, but is not limited to, proton transfer reactions, parallel ion parking, ion mobility separations, and other novel additions to the FT-MS field. Experts from academia and industry will be available to help answer questions. The goal is to give users a preview of what future directions ions be moving as the field of FT-MS continues to expand.

16 Cannabis and Hemp Testing Requirements: How to Leverage with Mass Spectrometry Presiding: Marc Engel, Markus Roggen, Kevin Smith A301

This workshop will discuss the challenges associated with testing cannabis and cannabis concentrate (edibles, extracts, tincture etc) samples; in addition, Mass Spectrometry techniques suitable for quantifying cannabis will be presented in detail to emphasize their merit for each chemistry group (pesticides, mycotoxins, heavy metals, terpenes etc). Industry thought leaders from the US and Canada will present their latest findings on sample preparation, instrumentation configuration, and data processing specifics to quantitate cannabis and cannabis extract samples in a high throughput environment. Group discussions will also include identifying mass spectrometry topics and research opportunities within cannabis & hemp science that can support this rapidly expanding scientific landscape.

17 Getting Started with R for Mass Spectrometry Data Analysis Presiding: Ryan Benz, Jeff Jones A305

This workshop, targeted at beginner and aspiring R users, will introduce the R programming language and the ways it can be used for mass spectrometry data analysis (and data analysis in general). The

workshop will start with a gentle introduction to R and the basics of using RStudio, followed by essential data manipulation and analysis strategies using base R and tidyverse packages. Finally, analysis examples utilizing various mass spectrometry specific R packages will be presented. The goal of this workshop is to help new R users get over some of the initial roadblocks beginners often face and to kickstart their efforts toward learning how to use R effectively for data analysis tasks. Bring your laptop to follow along with the examples. Preparatory material for the workshop will be provided at:

<https://github.com/ZenBrayn/asms-2019-r-workshop>

18. Career and Collaboration Opportunities in China Presiding: Jun Qu, Andy Tao A304

Recent economic development in China has created numerous job opportunities for postdoctoral fellows and graduate students with training in mass spectrometry. The overall objective of this workshop is to provide information to those individuals with interest in seeking academic or industrial positions in China. We plan to invite 6-7 mass spectrometrists from academia, pharmaceutical companies, and instrument vendors in China as panel members for this workshop. These individuals will share with the participating graduate students and postdocs about their experiences and perspectives in finding jobs, establishing an independent research program in universities, opportunities available to mass spectrometrists, and developing international collaborations in China. We believe that the workshop will benefit young and next-generation scientists in mass spectrometry by providing a unique perspective of job and research opportunities in China and assisting with their career development. The workshop will be mixed with panelist presentations and Q/A session with the participating students and postdocs.

THURSDAY MORNING ORAL SESSIONS

From 7:00 am Thursday CORPORATE BREAKFAST SEMINARS CONVENTION CENTER ONLY

See page 16 for detailed schedule. Reservation or RSVP required.

8:30 - 10:30 am Thursday INFORMATICS: METABOLOMICS

Session Chair: **Caroline Johnson (Yale School of Public Health) Murphy Ballroom, Bldg B, Level 5**

ThOA am 08:30 **OpenSWATH Enables Automated Data Processing for Data-Independent Acquisition in Metabolomics**; [Oliver Alka](#)¹; [Michael Witting](#)^{2,3}; [Karin Kleigrew](#)⁴; [Oliver Kohlbacher](#)^{1,5,6,7}; [Hannes L. Röst](#)⁸; ¹*Applied Bioinformatics, Department of Computer Science, University of Tübingen, Tübingen, Germany*; ²*Helmholtz Zentrum München, Research Unit Analytical BioGeoChemistry (BCG), Neuherberg, Germany*; ³*School of Life Sciences Weihenstephan, Technical University of Munich, Freising, Germany*; ⁴*Bavarian Center for Biomolecular Mass Spectrometry (BayBioMS), Technical University of Munich, Freising, Afghanistan*; ⁵*Quantitative Biology Center, University of Tübingen, Tübingen, Germany*; ⁶*Biomolecular Interactions, Max Planck Institute for Developmental Biology, Tübingen, Germany*; ⁷*Institute for Translational Bioinformatics, University Hospital Tübingen, Tübingen, Germany*; ⁸*Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, ON*

ThOA am 08:50 **Development of a Unified Collision Cross Section Compendium for Compound Annotation and Chemical Class Prediction**; [Jaqueline A. Picache](#)¹; [Bailey S. Rose](#)¹; [Andrzej Balinski](#)¹; [Katrina L. Leaptrot](#)¹; [Stacy D. Sherrod](#)¹; [Jody C. May](#)¹; [John A. McLean](#)¹; ¹*Vanderbilt University, Nashville, TN*

ThOA am 09:10 **Lipid Annotator: A Rapid, Accurate, and User-Friendly Software for Comprehensive LC-HRMS/MS Lipidomics**; [Jeremy Koelmel](#)¹; [Xiangdong Li](#)²; [Sarah Stow](#)²; [Mark Sartain](#)²; [Adithya Murali](#)²; [Robin H.J. Kemperman](#)¹; [Richard A Yost](#)¹; [Timothy J. Garrett](#)¹; [Norton Kitagawa](#)¹; ¹*University of Florida, Gainesville, FL*; ²*Agilent Technologies, Santa Clara, CA*

ThOA am 09:30 **Extracting Molecular Knowledge from METASPACE, a Community Knowledge Base of Spatial Metabolomes**; [Theodore Alexandrov](#)^{1,2}; [Katja Ovchinnikova](#)¹; [Andrew Palmer](#)¹; [Vitaly Kovalev](#)¹; [Lachlan Stuart](#)¹; [Artem Tarasov](#)¹; [Renat Nigmatzianov](#)¹; [Dominik Fay](#)¹; ¹*Structural and Computational Biology Unit, European Molecular Biology Laboratory, Heidelberg, Germany*; ²*Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA*

ThOA am 09:50 **Improved Interpretation of Metabolomics Data Integrated with other Omics Data: Linear Modeling and Comprehensive Pathway Analysis Approaches**; [Jalal K. Siddiqui](#)¹; [Shunchao Wang](#)¹; [Rohith Vanam](#)¹; [Andrew Patt](#)¹; [Joseph McElroy](#)¹; [Ewy Mathe](#)²; ¹*The Ohio State University, Columbus, OH*; ²*Ohio State University Medical Center, Columbus, OH*



ThOA am 10:10 **Improving Annotation Propagation on Molecular Networks through Random Walks: Introducing ChemWalker**; [Ricardo Silva](#)^{1,2}; Pieter Dorrestein³; ¹University of California, San Diego, CA; ²NPPNS, Department of Physics and Chemistry, School of Pharmaceutical Sciences of Ribeirão Preto, University of São Paulo, Ribeirão Preto, Brazil; ³University of California San Diego, La Jolla, CA

8:30 - 10:30 am Thursday
FUNDAMENTALS: ION SPECTROSCOPY
Session Chair: Mary T. Rodgers (Wayne State University)
B401-402

ThOB am 08:30 **Integration of High-Resolution Mass Spectrometry with Cryogenic Ion Vibrational Spectroscopy**; [Evan H. Perez](#)¹; Fabian Menges¹; Sean Edington¹; Chinh Duong¹; Nan Yang¹; Mark Johnson¹; ¹Yale University, New Haven, CT

ThOB am 08:50 **Comparing Ultrahigh-Resolution Ion-Mobility Spectrometry and IR-IR Double Resonance Spectroscopy for Isomer-Resolved Spectra of Oligosaccharides**; [Robert Pellegrielli](#)¹; Stephan Warnke¹; Ahmed Ben faleh¹; Yalovenko Natalia¹; Thomas R. Rizzo¹; ¹Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

ThOB am 09:10 **Two-Color IRMPD Applied on Cryogenically Cooled Peptides: Comparisons to Traditional IRMPD and IR-UV Double Resonance Techniques**; [Christopher P. Harrilal](#)¹; Timothy S. Zwier¹; Scott A. Mcluckey¹; ¹Purdue University, West Lafayette, IN

ThOB am 09:30 **Circular Dichroism Mass Spectrometry of Biomolecular Ions**; [Steven Daly](#)¹; Frédéric Rosu²; Valérie Gabelica¹; ¹Université de Bordeaux, INSERM U1212, CNRS UMR 5320, IECB, Pessac, France; ²Université de Bordeaux, CNRS UMS3033, IECB, Pessac, France

ThOB am 09:50 **Gas-Phase Fluorescence from Trapped Biomolecular Ions: Instrumentation and Photophysical Studies**; [Prince Tiwari](#)¹; Jonas B Metternich¹; Martin F Czar¹; Renato Zenobi¹; ¹ETH Zurich, Switzerland

ThOB am 10:10 **Structures of Hydrogen-Rich DNA Tetranucleotide Cation Radicals toward Achieving Atomic-Resolution by UV/Vis Action Spectroscopy**; [Shu R. Huang](#)¹; Yue Liu¹; Yang Liu¹; Frantisek Turecek¹; ¹University of Washington, Seattle, WA

8:30 - 10:30 am Thursday
POST-TRANSLATIONAL MODIFICATIONS: QUALITATIVE & QUANTITATIVE ANALYSIS
Session Chair: Kristina Hakansson (University of Michigan)
B405-407

ThOC am 08:30 **Strategies for High Throughput MS Analysis of Acid-Labile Phosphorylation**; Gemma Hardman¹; Simon Perkins¹; Philip Brownridge¹; Andrew Jones¹; [Claire Evers](#)¹; ¹University of Liverpool, Liverpool, United Kingdom

ThOC am 08:50 **Mass Spectrometry-Based Large-Scale and Precise Identification of Citrullinated Proteins from Complex Biological Samples**; [Yatao Shi](#)¹; Zihui Li²; Xudong Shi³; Bin Wang⁴; Lingjun Li^{2,4}; ¹University of Wisconsin, Madison, WI; ²Department of Chemistry, University of Wisconsin, Madison, WI; ³Department of Surgery, School of Medicine and Public Health, University of Wisconsin, Madison, WI; ⁴School of Pharmacy, University of Wisconsin, Madison, WI

ThOC am 09:10 **ProteomeTools: Exploiting the Largest Collection of Synthetic Peptides Carrying Biologically Relevant Post-Translational Modifications for Proteome Research**; [Daniel P Zolg](#)¹; Mathias Wilhelm¹; Siegfried Gessulat^{1,2}; Tobias Schmidt¹; Michael Graber^{1,3}; Jana Zechar¹; Johannes Zerweck⁴; Tobias Knaute⁴; Hans-Christian Ehrlich²; Stephan Aiche²; Bernard Delanghe⁵; Andreas Huhmer⁶; Karsten Schnatbaum⁴; Ulf Reimer⁴; Bernhard Kuster^{1,7,8}; ¹Technical University of Munich, Freising, Germany; ²SAP SE, Potsdam, Germany; ³Ludwig-Maximilians-University Munich, Munich, Germany; ⁴JPT Peptide Technologies GmbH, Berlin, Germany; ⁵Thermo Fisher Scientific, Bremen, Germany; ⁶Thermo Fisher Scientific, San Jose, CA; ⁷Bavarian Center for Biomolecular Mass Spectrometry, Freising, Germany; ⁸Center for Integrated Protein Science Munich, Freising, Germany

ThOC am 09:30 **Critical Insight on Protein Oxidation Mapping by LC-MS/MS: Identification, Quantification, Artifacts, and Implications**; [Qian Dong](#)¹; Yuxue Liang¹; Xinjian Yan¹; Stephen E. Stein¹; ¹NIST, Gaithersburg, MD

ThOC am 09:50 **Integration of Lysine Modification Changes and Bioenergetic Phenotypes in Mouse Models of Cardiac Mitochondrial Protein Hyperacylation**; [Paul A. Grimsrud](#)¹; Michael T. Davidson¹; Kelsey H. Fisher-Wellman²; James A. Draper¹; Ling Lai³; Matthew D. Hirschev¹; Timothy R. Koves¹; Daniel P. Kelly³; Deborah M. Muoio¹; ¹Duke University School of Medicine, Durham, NC; ²East Carolina University Brody School of Medicine, Greenville, NC; ³Perelman School of Medicine - University of Pennsylvania, Philadelphia, PA

ThOC am 10:10 **Coupling Fluorescent-Activated Cell Sorting with LC-MRM-MS to Characterize Epi-Proteomic Signatures from Human Blood Cells**; [Jeannie M. Camarillo](#)¹; Suchitra Swaminathan¹; Nebiyu A Abshiru¹; Juliette A Morris¹; Madeline A Zoltek¹; Jacek W Sikora²; Paul M Thomas²; Neil L Kelleher²; ¹Northwestern University, Chicago, IL; ²Northwestern University, Evanston, IL

8:30 - 10:30 am Thursday
DRUG DISCOVERY AND DEVELOPMENT : QUANTITATIVE ANALYSIS
Session Chair: Christopher Yu (Genentech)
B302-305

ThOD am 08:30 **Utility of a Novel Acoustic Mist Ionization Front End in Early Drug Discovery: Delivery of a HTP Biochemical Screen**; [Arseniy M. Belov](#)¹; Carl A Machutta¹; Guofeng Zhang¹; Joseph Kozole¹; Jeffrey W Gross¹; Melanie V Leveridge¹; Luke Ghislain²; Sammy S Datwani²; Roland S Annan¹; ¹GlaxoSmithKline, Collegeville, PA; ²Labcyte Inc., San Jose, CA

ThOD am 08:50 **Quantitative Interactomics as a Tool for Drug Development**; [James Bruce](#)¹; Juan D. Chavez¹; Andrew Keller¹; Jared P. Mohr¹; Martin Mathay¹; ¹University of Washington, Genome Sciences, Seattle, WA

ThOD am 09:10 **Overcoming ADA Interference by Using a Hybrid LC/MS/MS Method to Quantify a Therapeutic Protein in Human Plasma**; Jia Guo¹; Dylan Sorensen²; Chad Christianson³; Tara O'Brien³; Leonor Newquist¹; Kevin Kuang¹; Ben Badillo¹; Ryan Boyer¹; Stephen Zoog¹; [Huiyu Zhou](#)¹; ¹BioMarin Pharmaceutical Inc., Novato, CA; ²Amgen, South San Francisco; ³Alturas Analytics, Moscow, ID



THURSDAY MORNING ORAL SESSIONS

- ThOD am 09:30 **Quantification of Convoluted Antibody and Antibody-Drug-Conjugate Modifications at the Intact and Middle-Down Level via ETD Fragments and Isotopically-Labeled Standards;** Joseph D Eschweiler¹; Guillaume Tremintin²; Reika Campbell¹; Julie L Heflin¹; ¹AbbVie Inc., North Chicago, IL; ²Bruker Scientific, San Jose, CA
- ThOD am 09:50 **Benchmarking of HR/AM Instruments for Monitoring and Accurately Quantifying Trace-Level Host Cell Proteins Impurities in Therapeutic Proteins;** Joanna Bons¹; Nicolas Pythoud¹; Sarah Cianféran¹; Christine Carapito¹; ¹Laboratoire de Spectrométrie de Masse BioOrganique, Université de Strasbourg, CNRS, IPHC UMR 7178, Strasbourg, France
- ThOD am 10:10 **Analysis and Characterization of Adeno Associated Virus by Charge Detection Mass Spectrometry;** Nicholas A. Lykтей¹; Zachary C. Elmore²; Eric Walton²; Aravind Asokan³; Martin F. Jarrold¹; ¹Indiana University, Bloomington, IN; ²Duke University, Durham, NC; ³Duke University School of Medicine, Durham, NC
- 8:30 - 10:30 am Thursday**
SUPRAMOLECULAR AND MACROMOLECULAR COMPLEXES
Session Chair: Stacy D. Sherrod (Vanderbilt University)
B308-309
- ThOE am 08:30 **Using Supramolecular Protein-Polymer Complexes to Probe Surface-Accessible Protein Residues;** Benqian Wei¹; Selim Gerislioglu²; Jonathan P Williams³; Chrys Wesdemiotis¹; ¹The University of Akron, Akron, OH; ²PPG, Allison Park, PA 15101; ³Waters corporation, Wilmslow, United Kingdom
- ThOE am 08:50 **Data Integration and Mass Spectrometry for Solving Structures of Intrinsically Disordered Regions of Nuclear Receptors;** Mark Chance¹; Janna Kiselar¹; Sichun Yang¹; ¹Case Western Reserve University, Cleveland, OH
- ThOE am 09:10 **Relative Stabilities of Lipoprotein Subpopulations Determined by Charge Detection Mass Spectrometry;** Corinne A. Lutomski¹; Tarick J. El-Baba¹; David E. Clemmer¹; Martin F. Jarrold¹; ¹Indiana University, Bloomington, IN
- ThOE am 09:30 **Probing Gas-Phase Unfolding Mechanism of Multimeric Protein Complexes by Native Top-Down Mass Spectrometry Using Electron Capture Dissociation and Ultraviolet Photodissociation;** Mowei Zhou¹; Weijing Liu¹; Ljiljana Pasa-Tolic¹; Jared B. Shaw¹; ¹Pacific Northwest National Laboratory, Richland, WA
- ThOE am 09:50 **Identification and Quantitation of Heterodimer Species in Co-Formulated Protein Drugs by LC-MS-Based Approaches;** Tao Xing¹; Yuetian Yan¹; Shunhai wang²; Thomas J. Daly³; Ning li¹; ¹Regeneron Pharmaceuticals Inc., Tarrytown, NY
- ThOE am 10:10 **Towards a Comprehensive Landscape of 60S Ribosomal Biogenesis;** Carolin Sailer¹; Jasmin Jansen¹; Axel Reiser²; Jan Erzberger³; Florian Stengel¹; ¹University of Konstanz, Konstanz, Germany; ²University of Stuttgart, Stuttgart, Germany; ³UT Southwestern Medical Center, Dallas, TX
- 8:30 - 10:30 am Thursday**
CLINICAL ANALYSIS USING MS
Session Chair: Yu Bai (Peking University)
B312-314
- ThOF am 08:30 **Development of Robust Spatial Metabolomics Tools for Cross-Site Analyses of Human Biopsies for Kidney Precision Medicine;** Dusan Velickovic¹; Guanshi Zhang²; Arunima Bhattacharjee¹; Jennifer Kyle¹; Ryan Sontag¹; Ljiljana Pasa-Tolic¹; Theodore Alexandrov³; Kumar Sharma²; Christopher Anderton¹; ¹Pacific Northwest National Laboratory, Richland, WA; ²University of Texas Health-San Antonio, San Antonio, TX; ³European Molecular Biology Laboratory, Heidelberg, Germany
- ThOF am 08:50 **Quantitation of Cannabinoids in Breath Samples Using a Novel Derivatization LC-MS Assay with Ultrahigh Sensitivity;** Yiqi Ruben Luo¹; Cassandra Yun¹; Kara L Lynch¹; ¹University of California, San Francisco, CA
- ThOF am 09:10 **Development of Automated, Multiplexed PI3K p110 α , PTEN, and AKT 1+2 Assays for Tumor-Tissue Samples Using Immuno-MALDI Mass Spectrometry (iMALDI);** Bjorn Frohlich¹; Robert Popp¹; Rene Zahedi²; Andre LeBlanc²; Yassene Mohammed^{1,3}; Adriana Aguilar-Mahecha⁴; Oliver Poetz⁵; Mark Basik⁶; Gerald Batist⁶; Christoph H. Borchers^{1,2,6,7}; ¹University of Victoria-Genome BC Proteomics Centre, Victoria, BC; ²Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; ³Center for Proteomics and Metabolomics, Leiden University Medical Center, Leiden, Netherlands; ⁴Segal Cancer Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; ⁵NMI Natural and Medical Sciences Institute at the University of Tuebingen, Tuebingen, Germany; ⁶Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC; ⁷Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC
- ThOF am 09:30 **Paper Spray Ionization-Mass Spectrometry (PSI-MS) for the Simultaneous Quantification of Five Tri-azole Anti-fungal Agents from Plasma Samples;** Lindsey M Kirkpatrick^{1,2}; Christine L Skaggs³; Greta J Ren³; Nicholas E Manicke⁴; ¹Indiana University School of Medicine, Pediatric Infectious Disease, Indianapolis, IN; ²James Whitcomb Riley Hospital for Children, Indianapolis, Indiana; ³Department of Chemistry and Chemical Biology, Indiana University-Purdue University Indianapolis, Indianapolis, IN; ⁴Department of Chemistry and Chemical Biology, Forensic and Investigative Sciences Program, Indiana University-Purdue University Indianapolis, Indianapolis, IN
- ThOF am 09:50 **Molecular Analysis of Endometriosis to Aid in Surgical Resection Using the Laparoscopic MasSpec Pen;** Clara Feider¹; Jialing Zhang¹; John Q. Lin¹; Marta Sans¹; Suzanne Ledet²; Katherine Sebastian²; Michael T. Breen³; Livia S. Eberlin¹; ¹The University of Texas, Austin, TX; ²Seton Medical Center, Austin, TX; ³Dell Medical School at The University of Texas, Austin, TX
- ThOF am 10:10 **Quality Control Considerations for Targeted MRM on Dried Blood Microsamples for Early Prediction of Cardiac Events;** Kelly Njine Mouapi¹; Irene Van Den Broek¹; Mitra Mastali¹; Qin Fu¹; Vidya Venkatraman¹; Noel Bairey Merz²; Brennan Spiegel³; Jennifer Van Eyk^{1,2}; ¹Advanced Clinical Biosystems Research Institute, The Smidt Heart Institute, Cedars-Sinai Medical Center, Los Angeles, CA; ²Barbra Streisand Women's Heart Center, The Smidt Heart Institute, Cedars-Sinai Medical Center, Los Angeles, CA; ³Cedars Sinai Center for Outcomes Research and Education (CS-CORE), Cedars-Sinai Medical Center, Los Angeles, CA



8:30 - 10:30 am Thursday
STABLE ISOTOPE LABELING IN MS: APPLICATIONS
 Session Chair: Chengli Zu (Corteva Agriscience)
 Auditorium, Bldg A

- ThOG am 08:30 **Probing Metabolic Pathways during Early Embryonic Development Using Stable Isotope Labeling and Single-Cell Mass Spectrometry;** Erika Portero¹; Aleena J Andrews¹; Peter Nemes¹; ¹University of Maryland, College Park, MD
- ThOG am 08:50 **A Boosting to Amplify Signal with Isobaric Labeling (BASIL) Strategy for Comprehensive Quantitative Phosphoproteomic Characterization of Small Populations of Cells;** Chia-Feng Tsai¹; Lian Yi¹; Ercument Dirice²; Adam C. Swensen¹; Jing Chen³; Marina A. Gritsenko¹; Rosalie K. Chu⁴; Paul D. Piehowski¹; Richard D. Smith^{1,4}; Karin D. Rodland¹; Clayton E. Mathews³; Rohit N. Kulkarni²; Wei-Jun Qian¹; Tao Liu¹; ¹Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA; ²Section of Islet Cell Biology and Regenerative Medicine, Joslin Diabetes Center and Harvard Medical School, Boston, MA; ³Department of Pathology, Immunology, and Laboratory Medicine, University of Florida, Gainesville, FL; ⁴Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA
- ThOG am 09:10 **Quantitative Analysis of the Fetal Tissue Translatome by Mass Spectrometry Reveals Temporal and Tissue-Specific Regulatory Networks *in utero*;** Josue Baeza¹; Coons E Barbara²; William Peranteau²; Benjamin A. Garcia¹; ¹University of Pennsylvania, Philadelphia, PA; ²Children's Hospital of Philadelphia, Philadelphia, PA
- ThOG am 09:30 **Spatial Isotope Tracer Metabolomics to Study ¹³C Labeled Metabolite Distribution in 3D Tumor Spheroid Cell Culture;** Prasad Phapale¹; Mariia Naumenko^{1,2}; Karin Mitosch^{1,3}; Theodore Alexandrov^{1,2,4}; ¹EMBL, Heidelberg, Heidelberg, Germany; ²Metabolomics Core Facility, European Molecular Biology Laboratory, Heidelberg, Germany, Heidelberg, Germany; ³Genome Biology Unit, European Molecular Biology Laboratory, Heidelberg, Germany, Heidelberg, Germany; ⁴UCSD, San Diego, CA
- ThOG am 09:50 **DIA and DDA MS for Profiling the Cancer Borealis Neuropeptidome and Peptidomic Changes Resulting from Food Intake;** Kellen DeLaney¹; Lingjun Li¹; ¹University of Wisconsin, Madison, WI
- ThOG am 10:10 **Determining the Metabolic Fate of Monosaccharides in the Glycocalyx through Stable Isotope Labeling;** Maurice Wong¹; Gege Xu¹; Mariana Barboza¹; Carlito Lebrilla¹; ¹University of California, Davis, CA

8:30 - 10:30 am Thursday
EXPOSOMICS, TOXICOLOGY, AND HUMAN HEALTH
 Session Chair: Jon R. Sobus (US EPA)
 A411-412

- ThOH am 08:30 **Wastewater Impacts on Drinking Water: Hospital and Energy-Related Wastes and the Formation of Higher-Toxicity Disinfection By-Products;** Hannah Liberatore¹; Danielle C. Westerman¹; Caroline O. Granger¹; Amy A. Cuthbertson¹; Joshua M. Allen¹; Michael J Plewa²; Elizabeth D Wagner²; Kelly D Good³; Amy McKenna⁴; Chad R. Weisbrod⁴; Jerry A. Zweigenbaum⁵; Jeanne M. VanBriesen³; Susan D. Richardson¹; ¹University of South Carolina, Columbia, SC; ²University of Illinois Urbana-

Champaign, Urbana, IL; ³Carnegie Mellon University, Pittsburgh, PA; ⁴National High Magnetic Field Laboratory, Tallahassee, FL; ⁵Agilent Technologies, Inc., Wilmington, DE

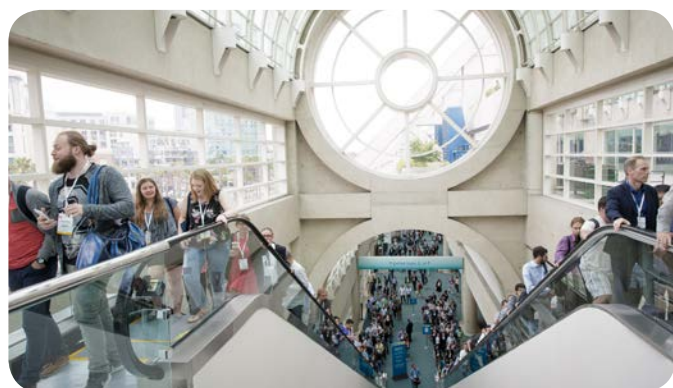
- ThOH am 08:50 ***In vitro* Hepatic Clearance of Per- and Polyfluoroalkyl Substances (PFAS);** David M. Crizer¹; Tahja M. Harris¹; Paul E. Dunlap¹; Julie R. Rice¹; Stephen S. Ferguson¹; Michael J. DeVito¹; ¹National Toxicology Program/NIEHS/NIH, Research Triangle Park, NC
- ThOH am 09:10 **HRMS-Based Metabolomics Strategy for Comprehensively Screening Biomarkers of Phthalate Exposure and their Applications;** Jing-fang Hsu¹; Chia-Lung Shih²; Pao-Chi Liao²; ¹National Health Research Institutes, Miaoli County, Taiwan; ²National Cheng Kung University, Tainan, Taiwan
- ThOH am 09:30 **An Algorithm (wSIM-CITY) for Gas Phase Fractionated (GPF) MS/MS2 Data Independent Acquisition (DIA) and Application to Neutral Loss DNA Adductomics.;** Scott J Walmsley^{1,2}; Jinshu Guo^{1,3}; Peter W. Villalta¹; Robert Turesky^{1,3}; Jinhua Wang^{1,2}; ¹Masonic Cancer Center, University of Minnesota, Minneapolis, MN; ²Institute for Health Informatics, University of Minnesota, Minneapolis, MN; ³Dept. of Medicinal Chemistry, College of Pharmacy, Minneapolis, MN
- ThOH am 09:50 **Signatures of Ambient Exposure to Benzene and Other Air Pollutants in the Human Serum Albumin Cys34 Adductome;** Joshua W Smith¹; Robert N O'Meally¹; Thomas W Kensler^{1,2}; Robert N Cole¹; John D Groopman¹; ¹Johns Hopkins University, Baltimore, MD; ²Fred Hutchinson Cancer Research Center, Seattle, WA
- ThOH am 10:10 **Multi-omics Investigation Reveals Benzalkonium Chloride Disinfectants Alter Sterol and Lipid Homeostasis in the Mouse Neonatal Brain;** Josi M. Herron¹; Kelly M. Hines¹; Hideaki Tomita¹; Ryan P. Seguin¹; Julia Y. Cui¹; Libin Xu¹; ¹University of Washington, Seattle, WA

10:30 am - 2:30 pm Thursday
THURSDAY POSTER SESSION
 Poster/Exhibit Hall ground level
 Lunch concessions are open 11:00 am - 2:00 pm

Odd-number posters present:
 10:30 am - 11:30 am **PLUS** 12:30 - 2:30 pm

Even-number posters present:
 10:30 am - 12:30 pm **PLUS** 1:30 - 2:30 pm

Poster Pick-Me-Up Snacks served at 1:30 pm





THURSDAY AFTERNOON ORAL SESSIONS

2:30 - 4:30 pm Thursday INFORMATICS: PEPTIDE AND PROTEIN IDENTIFICATION, PROTEOMICS

Session Chair: Anna Ivanova (Emory University)
Murphy Ballroom, Bldg B, Level 5

- ThOA pm 02:30 **From Single Software Tools to Fully Reproducible Workflows for the Analysis of Protein Mass Spectrometry Data**; Johannes Griss^{1,2}; Goran Vinterhalter³; Iustinian Olaru⁴; Veit Schwämmle⁴; ¹Medical University of Vienna, Vienna, Austria; ²EMBL-EBI, Hinxton, United Kingdom; ³University of Belgrade, Belgrade, Serbia; ⁴University of Southern Denmark, Odense, Denmark
- ThOA pm 02:50 **A Novel Computational Approach for Simultaneous Identification of Protein-RNA and Protein-DNA Interactions from XL-MS Data**; Timo Sachsenberg¹; Alexandra Stützer²; Aleksandar Chernev²; Eugen Netz³; Tjeerd Dijkstra⁴; Henning Urlaub^{2,5}; Oliver Kohlbacher^{1,6,7,8}; ¹University of Tübingen, Tübingen, Germany; ²Max Planck Institute for biophysical chemistry, Göttingen, Germany; ³Max Planck Institute for Developmental Biology, Tuebingen, Germany; ⁴Max Planck Institute for Developmental Biology, Tuebingen, Germany; ⁵University Medical Center Goettingen (UMG), Goettingen, Germany; ⁶Biomolecular Interactions, Max Planck Institute for Developmental Biology, Tübingen, Germany; ⁷Institute for Translational Bioinformatics, University Hospital Tübingen, Tübingen, Germany; ⁸Quantitative Biology Center, University of Tübingen, Tübingen, Germany
- ThOA pm 03:10 **PRiSM: Pattern-Based, Assumption-Free Protein Identification**; Joris Van Houtven^{1,2,3}; Kurt Boonen^{1,3}; Geert Baggerman^{1,3}; Kris Laukens^{4,5}; Jef Hooberghs^{1,6}; Dirk Valkenburg^{2,3}; ¹Flemish Institute for Technological Research (VITO), Mol, Belgium; ²University of Hasselt, Diepenbeek, Belgium; ³Centre for Proteomics, University of Antwerp, Antwerp, Belgium; ⁴biomedical informatics network Antwerpen (biomina), University of Antwerp, Antwerp, Belgium; ⁵Dept. Mathematics & Computer Science, University of Antwerp, Antwerp, Belgium; ⁶Theoretical Physics, Hasselt University, Diepenbeek, Belgium
- ThOA pm 03:30 **A “Divide and Conquer” Approach to Address Peptide-Spectrum Matching Challenges of Large Sequence Databases in Next-Generation Proteomic Applications**; Praveen Kumar^{1,2}; James E. Johnson³; Thomas McGowan³; Subina Mehta²; Ray Sajulga²; Shane Hubler⁴; Caleb Easterly²; Matthew C. Chambers⁵; Pratik Jagtap²; Timothy J. Griffin²; ¹Bioinformatics and Computational Biology, University of Minnesota-Rochester, Rochester, MN; ²Biochemistry, Molecular Biology, and Biophysics, University of Minnesota, Minneapolis, MN; ³Minnesota Supercomputing Institute, University of Minnesota, Minneapolis, MN; ⁴Rhapsody Data, LLC., Madison, WI; ⁵Vanderbilt University, Nashville, TN
- ThOA pm 03:50 **Proteomic Data Commons (PDC): A Node in the NCI Cancer Research Data Commons**; Paul A Rudnick¹; Ratna R. Thangudu²; Michael Holck²; Deepak Singhal²; Karen A. Ketchum²; Nathan J. Edwards³; Christopher R. Kinsinger⁴; Izumi Hinkson⁵; Lei Ma²; Maya Zuhl²; Yi Xin²; Padmini Chilappagari²; Anand Basu²; Michael J MacCoss⁶; ¹Spectragen Informatics, Bainbridge Island, WA; ²ESAC, Inc., Rockville, MD; ³Georgetown University Medical Center, Washington, DC; ⁴National Cancer Institute, Bethesda, MD; ⁵National Cancer

ThOA pm 04:10

Institute @ Frederick, Frederick, MD; ⁶University of Washington, Genome Sciences, Seattle, WA
Detection of Cancer Mutations in Proteomics Data with a Cloud Search Engine; Conor Jenkins¹; Megan Rigby²; Amol Prakash³; Benjamin Orsburn²; ¹Hood College Bioinformatics Program, Frederick, MD; ²National Cancer Institute @ Frederick, Frederick, MD; ³Optys Tech Corporation, Shrewsbury, MA

2:30 - 4:30 pm Thursday MICROORGANISMS AND THE MICROBIOME

Session Chair: Neha Garg (Georgia Institute of Technology)
B401-402

- ThOB pm 02:30 **Identification of Individual Bacteria in Polymicrobial Samples via Membrane Glycolipids**; David R. Goodlett¹; Alison J. Scott¹; Sung Hwan Yoon¹; So Young Ryu²; Dusan Velickovic³; Rene Boiteau⁴; Robert K. Ernst¹; Ljiljana Pasa-Tolic³; ¹University of Maryland, Baltimore, MD; ²University of Nevada, Reno, NV; ³Pacific Northwest National Laboratory, Richland, WA; ⁴Oregon State University, Crovallis, OR
- ThOB pm 02:50 **Approaches to Accurate Chemical Constitutional Analysis in Untargeted Microbial Natural Products Research**; Roger Linington; Simon Fraser University, Burnaby, BC
- ThOB pm 03:10 **Evaluation of a Biofilm Inhibitor Using Imaging Mass Spectrometry Raises Questions about Potential Therapeutic Strategies**; Alanna R Condren¹; Lisa Kahl²; Manuel Banzhaf²; Lars Dietrich²; Laura Sanchez¹; ¹University of Illinois, Chicago, IL; ²Columbia University, New York, NY; ³University of Birmingham, Birmingham, United Kingdom
- ThOB pm 03:30 **Metabolomics Activity Screening Identifies Immunomodulating Host-Microbiome Metabolites in Inflammatory Bowel Disease**; J. Rafael Montenegro-Burke¹; Bernard P. C. Kok¹; Carlos Guijas¹; Enrique Saez¹; Dennis Wolan¹; Gary Siuzdak¹; ¹The Scripps Research Institute, La Jolla
- ThOB pm 03:50 **LC-MS/MS-based Metabolomics Reveals Inhibition Effect of Gut Microbiota-Derived Metabolites on Lipid Accumulation in Hepatocytes**; Qiang Lyu¹; Hsin-Bei Tsou¹; Hsin-Yuan Chang¹; Yin-Hsuan Huang¹; Hsiao-Li Chuang²; Cheng-Chih Hsu¹; ¹National Taiwan University, Taipei, Taiwan; ²National Laboratory Animal Center, Taipei, Taiwan
- ThOB pm 04:10 **Discovering Small Molecule Products of Biosynthetic Gene Clusters by Integrating Metagenomics and Mass Spectrometry**; Liu Cao¹; Egor Shcherbin²; Hosein Mohimani¹; ¹Computational Biology Department, School of Computer Science, Carnegie Mellon University, Pittsburgh, PA; ²National Research University Higher School of Economics, St. Petersburg, Russia

2:30 - 4:30 pm Thursday QUANTITATIVE PROTEOMICS IN SYSTEMS BIOLOGY

Session Chair: Susan E. Abbatiello (Northeastern University)
B405-407

- ThOC pm 02:30 **Profiling the HSP90 Clientele in EGFR Mutant Cancer Cells**; Jason Liang¹; Trent Hinkle¹; Erik Verschueren¹; Shiva Malek²; Donald S. Kirkpatrick¹; ¹Department of Microchemistry, Proteomics and Lipidomics, Genentech Inc., South San Francisco, CA; ²Department of Discovery Oncology, Genentech Inc., South San Francisco, CA



- ThOC pm 02:50 **Investigating the Role of Histone H2A Proteolysis during Stem Cell Differentiation and Its Consequence in Nucleosome Stability**; Marie Coradin¹; Kelly R. Karch¹; Simone Sidoli¹; Benjamin A. Garcia¹; ¹University of Pennsylvania, Philadelphia, PA
- ThOC pm 03:10 **Quantitative Time-Course Profiling of Sorafenib-Treated Hepatocellular Carcinoma (HCC) Cells Through Phosphoproteome Analysis**; Emily Werth¹; Presha Rajbhandari¹; Brent R Stockwell¹; Lewis M. Brown¹; ¹Columbia University, New York, NY
- ThOC pm 03:30 **A Versatile Lentiviral Delivery Toolkit for Proximity-dependent Biotinylation in Diverse Cell Types**; Payman Samavarchi-Tehrani¹; Hala Abdouni¹; Reuben Samson¹; Cassandra Wong¹; Anne-Claude Gingras^{1,2}; ¹Lunenfeld-Tanenbaum Research Institute, Sinai Health System, Toronto, ON; ²University of Toronto, Toronto, ON
- ThOC pm 03:50 **Proteomic Analysis of Sorted Mouse Embryonic Stem Cells to Decipher Sub-populations**; Molly P. Lowndes^{1,2}; Joshua M. Brickman²; Michael L. Nielsen¹; ¹Novo Nordisk Foundation Center for Protein Research, Faculty of Health and Medical Sciences, University of Copenhagen, Copenhagen, Denmark; ²Novo Nordisk Foundation Center for Stem Cell Biology, Faculty of Health and Medical Sciences, University of Copenhagen, Copenhagen, Denmark
- ThOC pm 04:10 **Illuminating the Dark Kinome: Defining Kinase-Substrate Relationships Using Targeted Protein Degradation and Phosphoproteomics**; Rufus Hards¹; Ian LaCroix¹; Arminja N Kettenbach¹; Andrew Holland²; Scott A. Gerber¹; ¹Geisel School of Medicine at Dartmouth, Lebanon, NH; ²Johns Hopkins, Baltimore, MD
- 2:30 - 4:30 pm Thursday**
COVALENT LABELING AND CHEMICAL CROSSLINKING
Session Chair: Florian Stengel (University of Konstanz)
B302-305
- ThOD pm 02:30 **PhoX - an IMAC-enrichable Crosslinking Reagent**; Barbara A. Steigenberger^{1,2}; Roland J. Pieters³; Albert J.R. Heck^{1,2}; Richard A. Scheltema^{1,2}; ¹Biomolecular Mass Spectrometry and Proteomics, Bijvoet Center for Biomolecular Research and Utrecht Institute of Pharmaceutical Sciences, Utrecht University, Utrecht, Netherlands; ²Netherlands Proteomics Center, Utrecht, Netherlands; ³Department of Chemical Biology & Drug Discovery, Utrecht University, Utrecht, Netherlands
- ThOD pm 02:50 **Developing Cross-linking Mass Spectrometry (XL-MS) to Delineate Protein Interaction Landscapes in Living Cells**; Andrew Wheat¹; Clinton Yu¹; Xiaorong Wang¹; Lan Huang¹; ¹University of California, Irvine, CA
- ThOD pm 03:10 **Chemical Cross-Linking and Covalent Labelling Provide Insights into the Protein Organisation of Synaptic Vesicle Membranes**; Sabine Wittig¹; Marie Barth¹; Marcelo Ganzella²; Julia Preobraschenski²; Susann Kostmann¹; Angel Perez-Lara²; Reinhard Jahn²; Carla Schmidt¹; ¹HALOmern, Martin Luther University Halle-Wittenberg, Halle / Saale, Germany; ²MPI for Biophysical Chemistry, Department of Neurobiology, Göttingen, Germany
- ThOD pm 03:30 **Chemical Protein-RNA Cross-Linking Coupled with Mass Spectrometry – from Proteins to Cells**; Alexander Wulf¹; Luisa M Welp¹; Seychelle Vos¹; Sven Johansson²; Timo Sachsenberg³; Ralf Ficner²; Oliver Kohlbacher³; Patrick Cramer¹; Henning Urlaub^{1,4}; ¹Max Planck Institute for biophysical chemistry, Göttingen, Germany; ²University of Goettingen, Institute for Microbiology and Genetics, Goettingen, Germany; ³University of Tübingen, Tübingen, Germany; ⁴University Medical Center Goettingen (UMG), Goettingen, Germany
- ThOD pm 03:50 **Structure Determination of Neurodegenerative Disease-Related Misfolded Protein Aggregates by Short-Distance Crosslinking Constraint-Guided Discrete Molecular Dynamics (CL-DMD)**; Evgeniy V. Petrotchenko¹; Jason J. Serpa²; Konstantin I. Popov³; Nikolay V. Dokholyan⁴; Christoph H. Borchers^{1,2,5,6}; ¹Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; ²University of Victoria-Genome BC Proteomics Centre, Victoria, BC; ³Department of Biochemistry and Biophysics, University of North Carolina, Chapel Hill, NC; ⁴Departments of Pharmacology, and Biochemistry and Molecular Biology, Pennsylvania State College of Medicine, Hershey, PA; ⁵Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC; ⁶Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC
- ThOD pm 04:10 **Multidimensional Cross-Linking with a Tetra-Reactive Cross-Linker**; Jared P. Mohr¹; Juan D. Chavez¹; James E. Bruce¹; ¹University of Washington, Genome Sciences, Seattle, WA
- 2:30 - 4:30 pm Thursday**
PLANT "OMICS"
Session Chair: Michael R. Sussman (University of Wisconsin)
B308-309
- ThOE pm 02:30 **Elucidation of Molecular Switches Regulating Plant C3to CAM Transition Using Integrative Transcriptomics, Proteomics and Metabolomics**; Sixue Chen; University of Florida, Gainesville, FL
- ThOE pm 02:50 **Digging Deep into the Transcriptome, Proteome and Phosphoproteome of *Arabidopsis thaliana***; Julia Mergner¹; Martin Heinrich Frejno¹; Markus List¹; Maxim Messerer²; Daniel Lang²; Stefan Altmann²; Philipp Cypres³; Toby Mathieson⁴; Klaus Mayer²; Pascal Falter-Braun²; Stefanie Sprunck³; Jan Baumbach¹; Claus Schwechheimer¹; Bernhard Kuster¹; ¹Technical University of Munich, Freising, Germany; ²Helmholtz Center Munich, Neuherberg, Germany; ³University of Regensburg, Regensburg, Germany; ⁴Cellzome, a GSK company, Heidelberg, Germany
- ThOE pm 03:10 **Automated High-throughput Metabolic Analysis of Single Cells by Fiber Based Laser Ablation Electrospray Ionization Mass Spectrometry**; Sylvia Stopka¹; Ellen A Wood¹; Rikkita Khattar¹; Beverly J Agtuca²; Christopher R Anderton³; David W Koppenaar¹; Ljiljana Pasa-Tolic³; Gary Stacey²; Akos Vertes¹; ¹The George Washington University, Washington, DC; ²University of Missouri, Columbia, MO; ³Pacific Northwest National Laboratory, Richland, WA
- ThOE pm 03:30 **Establishing and Applying Mass Spectrometric Tools to Measure Levels and 13C-Labeling Kinetics of Metabolites in *Camelina sativa* Leaves and Seeds**; Yuan Xu¹; Bibin Paulose¹; Hesham Abdullah¹; Danny Schnell¹; Yair Shachar-Hill¹; ¹Michigan State University, East Lansing, MI



THURSDAY AFTERNOON ORAL SESSIONS

- ThOE pm 03:50 **Comparing Proteomic Changes during PAMP Responses and MKP1-Requiring Genetic Pathways**; [Laura A Greeley](#)¹; [Gabrielle Rupp](#)¹; [Scott C Peck](#)¹; ¹*University of Missouri, Columbia, MO*
- ThOE pm 04:10 **Novel Bioactive Cyclotide Scaffolds in *Viola inconspicua***; [Nicole C Parsley](#)¹; [Patric W Sadecki](#)¹; [Conrad J Hartmann](#)¹; [Leslie M Hicks](#)¹; ¹*UNC Chapel Hill, Durham, NC*

2:30 - 4:30 pm Thursday

ION MOBILITY: STRUCTURE

Session Chair: [Francisco Fernandez Lima](#) (Florida International University)
B312-314

- ThOF pm 02:30 **Mechanism of Amyloid Assembly: Prion-like Cross Talk between Disease Agents of Alzheimer's, Amyotrophic Lateral Sclerosis(ALS) and Type 2 Diabetes**; [Shruti Arya](#)¹; [Veronica Laos](#)¹; [Michael T. Bowers](#)¹; ¹*University of California, Santa Barbara, CA*
- ThOF pm 02:50 **Ion Mobility Spectrometry-Mass Spectrometry Reveals Subtle Differences in Structure and Stability in Wild-Type Versus Point-Mutated Variants of Chymotrypsin Inhibitor 2**; [Shannon A. Raab](#)¹; [Tarick J. El-Baba](#)¹; [Daniel W. Woodall](#)¹; [Wen Liu](#)²; [Yang Liu](#)²; [Arthur Laganowsky](#)²; [David H. Russell](#)²; [David E. Clemmer](#)¹; ¹*Indiana University, Bloomington, IN*; ²*Texas A&M University, College Station, TX*
- ThOF pm 03:10 **Combining Solution Thermal Melting with IMS-MS Analysis to Investigate the Stability Effects of Ligand Interactions in Nucleic Acid Complexes**; [Rebecca J. D'Esposito](#)^{1,2}; [Daniele Fabris](#)^{1,2}; ¹*University at Albany, Albany, NY*; ²*The RNA Institute, University at Albany, Albany, NY*
- ThOF pm 03:30 **ESI/ESI Ion/Ion Reactions in the Traveling Wave Trap of an Ion Mobility/Mass Spectrometer for Gas-Phase Structure and Sequencing**; [Veronica V. Carvalho](#)¹; [Lyndon E. L. Keeling](#)¹; [Rebecca L. Cain](#)¹; [Griffin W. Dowell](#)¹; [Prabnoor S. Nagry](#)¹; [Lindsay J. Morrison](#)²; [Jeffery M. Brown](#)³; [Ian K. Webb](#)¹; ¹*Indiana University Purdue University Indianapolis, Indianapolis, IN*; ²*Waters Corporation, Beverly, MA*; ³*Waters Corporation, Wilmslow, United Kingdom*
- ThOF pm 03:50 **Delineation of Structural Isomers by Isotopic Shifts in High-Field Ion Mobility Spectra: Element-Specific Multidimensional Fingerprints**; [Pratima Pathak](#)¹; [Matthew A. Baird](#)¹; [Gordon A. Anderson](#)²; [Alexandre A. Shvartsburg](#)¹; ¹*Wichita State University, Wichita, KS*; ²*GAA Custom Engineering, LLC, Benton City, WA*
- ThOF pm 04:10 **Towards Deciphering Tertiary Structures of Protein Glycoforms Using Tandem Trapped Ion Mobility Spectrometry-Mass Spectrometry**; [Mengqi Chai](#)¹; [Tyler C Cropley](#)¹; [Fanny C Liu](#)¹; [Christian Bleiholder](#)¹; ¹*Florida State University, Tallahassee, FL*

2:30 - 4:30 pm Thursday

INSTRUMENTATION: INNOVATIONS IN MASS ANALYZERS

Session Chair: [Lissa Anderson](#) (NHMFL-FSU)
Auditorium, Bldg A

- ThOG pm 02:30 **Initial Experimental Characterization of the New Type of FT-Mass Spectrometer Based on Multielectrode Harmonized Kingdon Traps with Different Ion Sources**; [Eugene \(evgeny\) Nikolae](#)¹; [Oleg Kharybin](#)¹; [Gleb Vladimirov](#)¹; ¹*Skolkovo Institute of*

Science and Technology, Moscow Region, Russian Federation

- ThOG pm 02:50 **A Tandem Multi-Quadrupole Ion Trap (MultiQ-IT) Electrospray Interface for an Orbitrap Mass Spectrometer**; [Andrew N. Krutchinsky](#)¹; [Kelly R. Molloy](#)¹; [Brian T. Chait](#)¹; ¹*The Rockefeller University, New York, NY*
- ThOG pm 03:10 **Implementation of Ion-Ion Proton Transfer (IIPT) Reactions on a Modified Orbitrap Tribrid Mass Spectrometer with Increased Ion-Ion Reaction Capacity**; [Christopher Mullen](#)¹; [John E.P. Syka](#)¹; [Lee Early](#)¹; [Romain Huguet](#)¹; [Jeffrey Shabanowitz](#)²; [Donald F. Hunt](#)²; ¹*Thermo Fisher Scientific, San Jose, CA*; ²*University of Virginia, Charlottesville, VA*
- ThOG pm 03:30 **Mirror Switching for Ion Isolation in a Fourier Transform Electrostatic Ion Trap Mass Spectrometer**; [Joshua Johnson](#)¹; [Gregory S. Eakins](#)¹; [Scott A McLuckey](#)¹; ¹*Purdue University, West Lafayette, IN*
- ThOG pm 03:50 **Digital Mass Filter Analysis Provides New Ways of Enhancing Sensitivity and Resolution**; [Bojana Opacic](#)¹; [Adam P. Huntley](#)¹; [Peter T. A. Reilly](#)¹; ¹*Washington State University, Pullman, WA*
- ThOG pm 04:10 **Nanomechanical Resonators based Charge Independent MS of Synthetic and Natural Nanoparticles in the 10-100 MDa Mass Range**; [Christophe Masselon](#)¹; [Shawn Fostner](#)²; [Sergio Dominguez-Medina](#)¹; [Martial Defoort](#)²; [Emeline Verhnes](#)³; [Szu-Hsueh Lai](#)¹; [Bogdan Vysotskiy](#)²; [Kavya Clement](#)¹; [Thomas Alava](#)²; [Mohammad Abdul Halim](#)¹; [Pascale Boulanger](#)³; [Sebastien Hentz](#)²; ¹*Univ. Grenoble Alpes, CEA, Inserm, BIG-BGE, 38000 Grenoble, France*; ²*Univ. Grenoble Alpes, CEA, LETI, 38000 Grenoble, France*; ³*Univ Paris Sud, Univ. Paris Saclay, CEA, CNRS, I2BC, 91198 Gif sur Yvette, France*

2:30 - 4:30 pm Thursday

FUNDAMENTALS: ION ACTIVATION AND DISSOCIATION

Session Chair: [Edwin De Pauw](#) (University of Liege)
A411-412

- ThOH pm 02:30 **Proton Transfer Reactions and Parallel Ion Parking for Intact Protein Analysis on a 21 T FT-ICR Mass Spectrometer**; [Chad R. Weisbrod](#)¹; [Lissa C. Anderson](#)¹; [Jeffrey Shabanowitz](#)²; [Donald F. Hunt](#)²; [Christopher L. Hendrickson](#)³; ¹*National High Magnetic Field Laboratory, Tallahassee, FL*; ²*University of Virginia, Charlottesville, VA*; ³*National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL*
- ThOH pm 02:50 **Combining Ion Mobility Mass Spectrometry with Photoactivation – Lighting the Way to Conformer Analysis**; [Rachelle L Black](#)¹; [Alina Theisen](#)²; [Lennart Remakers](#)¹; [Lukasz Migas](#)¹; [Jeffery M Brown](#)³; [Bruno Bellina](#)¹; [Perdita Barran](#)¹; ¹*Manchester Institute of Biotechnology, University of Manchester, United Kingdom*; ²*University of Warwick, Coventry, United Kingdom*; ³*Waters Corporation, Wilmslow, United Kingdom*
- ThOH pm 03:10 **Characterization of Native Proteins with Activation Electron Transfer Dissociation (AI-ETD)**; [Jean M Lodge](#)¹; [Dain Ryan Brademan](#)²; [Michael S Westphall](#)³; [Joshua J Coon](#)^{2,3,4,5}; ¹*University of Wisconsin, Madison, WI*; ²*Department of Chemistry, University of Wisconsin, Madison, WI*; ³*Genome Center of Wisconsin, Madison, WI*; ⁴*Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI*; ⁵*Morgridge Institute for Research, Madison, WI*



ThOH pm 03:30 **Understanding Ionization and Fragmentation within the Solution Cathode Glow Discharge Ionization Source via Thermometer Molecule Analysis;** Courtney Walton¹; Brian T. Molnar¹; Judy Wu¹; Jacob T. Shelley¹; ¹*Rensselaer Polytechnic Institute, Troy, NY*

ThOH pm 03:50 **Structures, Binding Energetics, and Dissociation Dynamics of Imidazolium-Based Ionic Liquid Clusters;** Mary T Rodgers¹; Harrison Roy²; ¹*Wayne State University, Detroit, MI*; ²*Wayne State University, Detroit, MI*

ThOH pm 04:10 **A Novel Radical Ion Dissociation Technique for MS Characterization of RNA;** Giovanni Calderisi¹; Kathrin Breuker¹; ¹*University of Innsbruck, Innsbruck, Austria*

6:30-9:30 pm Thursday
CLOSING EVENT
 Georgia Aquarium
 Advance purchase ticket is required (\$40).
 Tickets available for purchase through Monday at 12pm noon only.



4:45-5:30 pm Thursday
PLENARY LECTURE
 Presiding: Susan Richardson (University of South Carolina)
 Murphy Ballroom, Bldg B, Level Five



Chemistry of Food and Soft Drinks

Lilly D'Angelo
 Global Food & Beverage Technology Associates





POSTER OVERVIEW

Poster Presentation Schedule

Odd-numbered posters present: 10:30 am - 11:30 am PLUS 12:30 - 2:30 pm

Even-numbered posters present: 10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

MONDAY POSTERS

Set up all Monday posters
7:00 - 8:00 am

Odd-numbered posters present
10:30 - 11:30 am PLUS 12:30 - 2:30 pm

Even-numbered posters present
10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

Remove all Monday posters
7:00 - 8:00 pm

TUESDAY POSTERS

Set up all Tuesday posters
7:00 - 8:00 am

Odd-numbered posters present
10:30 - 11:30 am PLUS 12:30 - 2:30 pm

Even-numbered posters present
10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

Remove all Tuesday posters
7:00 - 8:00 pm

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Biomolecular Structure Analysis:		Art, Archaeology & Paleontology.....	023-036
Chemical Crosslinking and Covalent Labeling I.....	033-060	Biomarkers: Discovery I.....	037-068
Clinical Analysis I.....	061-083	Biomarkers: Quantitative Analysis II.....	069-099
Drug Metabolism: Qualitative & High		Clinical Analysis II.....	100-123
Throughput Analysis.....	084-098	Disease Biomarkers I.....	124-141
Drug and Metabolite Analysis: Novel Approaches for		Energy: Hydrocarbon and Petrochemical.....	142-159
Dried Biological Samples.....	099-103	Environmental: General II.....	160-191
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POSTER OVERVIEW



Poster Presentation Schedule

Odd-number posters present: 10:30 am - 11:30 am PLUS 12:30 – 2:30 pm

Even-number posters present: 10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm

WEDNESDAY POSTERS

Set up all Wednesday posters
7:00 - 8:00 am

Odd-numbered posters present
10:30 - 11:30 am PLUS 12:30 - 2:30 pm

Even-numbered posters present
10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

Remove all Wednesday posters
7:00 - 8:00 pm

THURSDAY POSTERS

Set up all Thursday posters
7:00 - 8:00 am

Odd-numbered posters present
10:30 - 11:30 am PLUS 12:30 - 2:30 pm

Even-numbered posters present
10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

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

Ambient Ionization: Applications I.....	001-031	Ambient Ionization: Applications II.....	001-032
Antibodies & Antibody Drug Conjugates II.....	032-064	Ambient Ionization: Fundamentals and Instrumentation.....	033-059
Biomarkers: Discovery II.....	065-095	Carbohydrates II.....	060-085
Biomarkers: Quantitative Analysis III.....	096-126	Data-Dependent Acquisition.....	086-092
Biomolecular Structure Analysis: Chemical Crosslinking and Covalent Labeling II.....	127-153	Data-Independent Acquisition.....	093-111
Cannabis.....	154-179	Disease Biomarkers II.....	112-130
Carbohydrates I.....	180-205	Drug Discovery/DMPK/ADME II.....	131-152
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Drug Discovery/DMPK/ADME I.....	235-254	Elemental Analysis: ICP/MS.....	160-175
Food "omics" MS Characterization of Food and Nutritional Supplements.....	255-275	Elemental Analysis: Isotope Ratio MS.....	176
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Fundamentals: Photodissociation.....	304-306	Food "omics" MS Characterization of Food and Nutritional Supplements II.....	182-203
GC/MS: Instrumentation and Applications II.....	307-329	Glycoproteins II.....	204-224
Glycoproteins I.....	330-350	Imaging MS: Disease Markers II.....	225-242
Homeland Security.....	351-360	Imaging MS: Method Development II.....	243-263
Imaging MS: Disease Markers I.....	361-379	Informatics: General, SRM, and DIA.....	264-272
Informatics: Algorithms and Statistical Advances II.....	380-402	Ion Mobility: Applications III.....	273-294
Informatics: Metabolomics.....	403-431	Ion Mobility: Fundamentals.....	295-320
Instrumentation: General.....	432-452	Isotope Labeling and Fluxomics Applications.....	321-331
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Ion Mobility: Applications II.....	479-500	LC/MS: Sample Preparation II.....	353-377
LC/MS: Chromatography and Software I.....	501-517	Lipids: ID and Structural Analysis.....	378-404
LC/MS: Sample Preparation I.....	518-542	MALDI: Applications.....	405-417
Lipids: General.....	543-564	MALDI: Fundamentals and Instrumentation.....	418-421
Metabolomics: Targeted and Quantitative Analysis.....	565-597	MALDI: Sample Preparation.....	422-430
Metabolomics: Untargeted Metabolite Profiling II.....	598-623	Metabolomics: Clinical Applications.....	431-449
Nucleic Acids and Oligonucleotides I.....	624-641	Metabolomics: General II.....	450-478
Peptides: PTM Identification.....	642-675	Metabolomics: Sample Preparation.....	479-482
Peptides: Targeted and Quantitative Analysis.....	676-703	Metabolomics: Untargeted Metabolite Profiling III.....	483-512
Proteins: Complexes/Non-covalent Interactions I.....	704-720	Microorganisms: Identification and Characterization.....	513-540
Proteomics: Quantitative III.....	721-744	Nanomaterials.....	541-548
Small Molecules: Quantitative Analysis.....	745-769	Nanoscale and Microfluidic Separations and MS.....	549-566
Toxicology.....	770-789	Natural Products.....	567-589
		Nucleic Acids and Oligonucleotides II.....	590-611
		Peptides: Fragmentation Mechanisms.....	612-617
		Proteins: Complexes/Non-covalent Interactions II.....	618-635
		Proteins: Conformation Analysis and Structural Biology.....	636-653
		Proteins: General and Membrane.....	654-673
		Proteins: PTMs II.....	674-697
		Proteomics: New Approaches II.....	698-724
		Proteomics: Quantitative IV.....	725-749
		Small Molecules: Quantitative Analysis II.....	750-777



MONDAY POSTERS

Set up all Monday posters
7:00 - 8:00 am

Odd-numbered posters present
10:30 - 11:30 am PLUS 12:30 - 2:30 pm

Even-numbered posters present
10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

Remove all Monday posters
7:00 - 8:00 pm

Biomarkers: Quantitative Analysis I.....	001-032
Biomolecular Structure Analysis:	
Chemical Crosslinking and Covalent Labeling I.....	033-060
Clinical Analysis I.....	061-083
Drug Metabolism: Qualitative & High Throughput Analysis	084-098
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Peptides: Sequence Analysis	577-584
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Proteomics: Tissue	737-768
Proteomics: Top Down Analysis I	769-787

BIOMARKERS: QUANTITATIVE ANALYSIS I 001-032

- MP 001 **Method Development and Validation of 20 Amino Acids in Human Plasma Utilizing UPLC-MS/MS Methodology;** Mackenzie Bentley¹; Dawn Dufield¹; Marsha Luna¹; Kimberly Jackson¹; Brady Roberts¹; ¹*KCAS Bioanalytical and Biomarker Services, Shawnee, KS*
- MP 002 **Determination of Vitamin A, 25-Hydroxyvitamin D2/D3 and Vitamin E in Human Serum by UPLC-MS/MS;** Liang Sun¹; Changkun Li¹; Yueqi Li¹; Taohong Huang²; ¹*Shimadzu (China) Co., LTD. Beijing Branch, Beijing, China*; ²*Shimadzu (China) Co., LTD. Shanghai Branch, Shanghai, China*
- MP 003 **Bioanalytical Approaches to Quantify "Free", "Drug-bound" and "Total" Interleukin-8 in Tissue Using Immuno-Capture Liquid Chromatography-Mass Spectrometry;** Yue Zhao¹; Huidong Gu¹; Dmitry Ostanin¹; Kezi Unsal-Kacmaz¹; Katarzyna Urbanska¹; Jianing Zeng¹; Yan Zhang¹; Renuka Pillutla¹; ¹*Bristol-Myers Squibb Co., Princeton, NJ*
- MP 004 **Quality Assessment of Oocytes for *in vitro* Fertilization Using Target Metabolomics Approach;** Ju Wang¹; Yan Ren²; Wei Zheng³; Liang Hu³; Siqi Liu²; ¹*University of Chinese Academy of Sciences, ShenZhen, China*; ²*BGI-Shenzhen, Shenzhen, China*; ³*Reproductive and Genetic Hospital of Citic-Xiangya, Changsha, China*
- MP 005 **Development of a Reference Measurement Procedure for Intact PTH and Peptides for the Improved Diagnosis, Treatment, and Prevention of CKD-MBD;** Candice Z Ulmer¹; Hubert W Vesper²; ¹*Centers for Disease Control and Prevention, Atlanta, GA*; ²*Centers for Disease Control and Prevention, Atlanta, GA*
- MP 006 **Novel Highly-Specific ID-UHPLC-MS/MS Method for the Measurement of Steroid Hormones and their Conjugates in Human Serum;** Lumi Duke¹; Paul H Kim²; Julianne Cook Botelho³; Candice Ulmer⁴; Hubert W Vesper⁴; ¹*CDC Atlanta, Atlanta, GA*; ²*Battelle Memorial Institute, Atlanta, GA*; ³*Centers for Disease Control and Prevention, Atlanta, GA*; ⁴*Centers for Disease Control and Prevention, Atlanta, GA*
- MP 007 **Systems-Wide Analysis of CD44 Knock-Down by In-Depth Quantitative Proteomics in Different Subtypes of Breast Cancer Cells;** HyeYoon Kim^{1,2}; Jung Hun Lee¹; Joseph Injae Wang¹; Han Suk Ryu²; Dohyun Han¹; ¹*Proteomics core facility, Biomedical Research Institute, Seoul National University Hospital, Seoul, South Korea*; ²*Department of Pathology, Seoul National University Hospital, Seoul National University College of Medicine, Seoul, South Korea*
- MP 008 **In-Depth Determination of Single Amino Acid Variants in CD24+ Subpopulation of Pancreatic Cancer by nano LC-MS/MS;** Jianhui Zhu¹; Zhijing Tan¹; Xinpei Yi²; Jie Zhang¹; David M. Lubman¹; ¹*University of Michigan Medical Center, Ann Arbor, MI*; ²*Academy of Mathematics and Systems Science, Chinese Academy of Sciences, Beijing, China*
- MP 009 **Rapid Quantitative Analytical Method Development and Validation for Insulin-Like Growth Factor-1 Doping Test Using UPLC-Q-Exactive Orbitrap Mass Spectrometry;** Changmin Sung¹; Minyoung Kim¹; Oh-seung Kwon¹; Hophil Min¹; ¹*Korea Institute of Science and Technology, Seoul, South Korea*
- MP 010 **Fast nano LC Separations for High Throughput Body Fluid Analysis with a TIMS Equipped QTOF and 4D Feature Alignment;** Thomas Kosinski¹; Scarlet Koch¹; Christian Meier-Credo¹; Christoph Gebhardt¹; Heiner Koch¹; ¹*Bruker Daltonik GmbH, Bremen, Germany*
- MP 011 **Quantification of Human ACTH with 25 pg/mL LLOQ in Plasma by an LC-MS/MS Method;** Baichen Zhang¹; Tian-Sheng Lu¹; Jinshui Chen¹; Guangchun Zhou¹; Elise



- Snider¹; Matthew Allen¹; Yong-Xi Li¹; ¹Medpace Bioanalytical Laboratories, Cincinnati, OH
- MP 012 **Integrative Proteomics Links CSF Biomarkers to Pathological Networks in the Alzheimer's Disease Brain;** Lenora Higginbotham¹; Lingyan Ping¹; Eric B. Dammer¹; Duc M. Duong¹; Maotian Zhou¹; Thomas S Wingo¹; Erik C.B. Johnson¹; James J. Lah¹; Allan I. Levey¹; Nicholas T. Seyfried¹; ¹Emory University, Atlanta, GA
- MP 013 **Catch them Sleeping: Quick and Routine Quantification of Melatonin in Plasma with Ultivo LC/TQ;** Mark Sartain¹; Aaron Boice¹; ¹Agilent Technologies, Santa Clara, CA
- MP 014 **High-Sensitivity and High-Resolution Top-Down LC/MS/MS Analysis of Cardiac Troponin Proteoforms;** Timothy N. Tiambeng¹; Yanlong Zhu¹; Yutong Jin¹; Ziqing Lin¹; Bifan Chen¹; Song Jin¹; Ying Ge¹; ¹University of Wisconsin Madison, Madison, WI
- MP 015 **Absolute Quantitation of Non-Human Glycan (Neu5Gc) for Gastric Cancer Screening;** Nari Seo^{1,2}; Myung Jin Oh^{1,2}; Jaekyoung Ko^{1,2}; Yoon Jin Choi³; Dong Ho Lee⁴; Hyun Joo An^{1,2}; ¹Chungnam national university, Daejeon, South Korea; ²Asia-Pacific Glycomics Reference Site, Daejeon, South Korea; ³Department of Gastroenterology, Korea University Guro Hospital, Seoul, South Korea; ⁴Department of Internal Medicine, Seoul National University Bundang Hospital, Seongnam-si, South Korea
- MP 016 **Analytical Method for Quantifying Long-Term Exposure to Acrylamide, Glycidamide, Ethylene Oxide and Acrylonitrile Using High Performance Liquid Chromatography-Tandem Mass Spectrometry;** Liquan Wang¹; Carmencita Aurora Gostilean¹; Tasia Nabors¹; Chui Y. Tse¹; Hubert W. Vesper¹; ¹Centers for Disease Control and Prevention, Atlanta, Georgia
- MP 017 **Development of a Multiplexed Quantitative Peptide Immunoaffinity LC-MS/MS Assay for the Detection of FFPE Protein Biomarkers;** Carlos A Morales Betanzos¹; Pamela Whalen²; Nagappan Mathialagan³; Eric L Powell²; Mireia Fernandez Ocana¹; ¹Pfizer, Andover, MA; ²Pfizer WRD, La Jolla, California; ³Pfizer, Groton, CT
- MP 018 **Optimization and Validation of an LC-MS/MS Method for Peripheral Serotonin as a Pharmacodynamic Biomarker of Treatment with Tryptophan Hydroxylase Inhibitors;** Katelyn Reighard Crizer¹; François Viel²; François Samson Thibault²; Michelle Palacios¹; Stephen A. Wring¹; ¹Altavant Sciences, Durham, NC; ²Syneos Health Clinique, Quebec City, PQ
- MP 019 **Development and Comparison of Two High Throughput LC-MS Methods for the Accurate Quantitation of IGF1 in Human Serum;** Pegah Jalili¹; Yue Lu¹; Judy Cao¹; Uma Sreenivasan²; Kevin Ray¹; ¹MilliporeSigma, St. Louis, MO; ²MilliporeSigma, Round Rock, TX
- MP 020 **A Systematic Evaluation of Increasing Laser Shots to Enhance the Information Content of the MALDI Analysis of Biological Fluids;** Senait G. Asmellash¹; Maxim Tsypin¹; Krista Meyer¹; Brandon Touchet¹; Heinrich Roder¹; ¹Biosesix, Boulder, CO
- MP 021 **Reducing the Need for Surrogate Matrix or Surrogate Analyte in Biomarker Assays;** Guille Metzler¹; Richard King¹; Carmen Fernandez-Metzler¹; Susan Crathern¹; ¹PharmaCadence Analytical Services, Hatfield, PA
- MP 022 **Mass Spectrometry-Based Quantification of Tau in Human Cerebrospinal Fluid Using a Complementary Tryptic Peptide Standard;** Maotian Zhou¹; Duc M Duong²; Jingting Dai²; James J. Lah²; Allan I. Levey²; Nicholas Seyfried²; ¹Emory University, Atlanta, GA; ²Emory University, Atlanta, GA
- MP 023 **Quantification of Specific Organophosphorous Pesticides, Synthetic Pyrethroids, and 2,4-Dichlorophenoxyacetic Acid by LC-MS/MS;** Dickson Wambua¹; Isuru Vidanage¹; William Roman¹; Antonia M. Calafat¹; Maria Ospina¹; ¹Centers for Disease Control and Prevention, Atlanta, Georgia
- MP 024 **Development of a High-Throughput Top-Down-Proteomic Technology to Study the Associations between Apolipoprotein A-I Proteoforms and HDL Function;** Henrique Dos Santos Seckler¹; John T Wilkins¹; Jonathan Scott Rink²; Luca Fornelli³; Richard D Leduc¹; Allan D. Sniderman⁴; Colby Shad Thaxton²; Donald Lloyd-Jones²; Philip D. Compton¹; Neil L Kelleher¹; ¹Northwestern University, Evanston, IL; ²Northwestern University, Chicago, IL; ³University of Oklahoma, Norman, OK; ⁴McGill Centre for Translational Research in Cancer, Segal Cancer Centre / Lady Davis Institute, Jewish General Hospital, Montreal, QC
- MP 025 **An Improved IonStar Proteomics Strategy Outperforms Spectronaut in Reliable Quantitative Analysis of Large Biological Cohorts;** Xue Wang¹; Jun Qu²; ¹University at Buffalo, Buffalo, NY; ²University at Buffalo, SUNY, Buffalo, NY
- MP 026 **Use of Mass Spectrometry to Evaluate the Exposure to di-2-ethylhexyl terephthalate in the U.S. General Population from the NHANES 2015–2016;** Manori Silva¹; Lee-Yang Wong¹; Ella Samandar¹; James L Preau¹; Lily T Jia¹; Antonia M. Calafat¹; ¹Centers for Disease Control and Prevention, Atlanta, Georgia
- MP 027 **Quantification of Plasma Glucosylsphingosine in Patients with Gaucher Disease Using UPLC-MS/MS;** Haoyue Zhang¹; Sarah P. Young^{1,2}; James Beasley¹; Patricia Mccaw¹; Deeksha Bali^{1,2}; Priya Kishnani²; Ashlee Stiles^{1,2}; ¹Biochemical Genetics Laboratory, Duke University Health System, Durham, NC; ²Division of Medical Genetics, Department of Pediatrics, Duke University School of Medicine, Durham, NC
- MP 028 **Fully Automated Quantitative Assessment of Methylmalonic Acid on Blood Cards Using Direct Isotope Dilution Mass Spectrometry;** Jeremiah C. Jamrom¹; Logan Miller^{1,2}; Scott Faber¹; John Kern¹; Matt Pamuku³; Skip Kingston¹; Fred D. Foster⁴; ¹Duquesne University, Pittsburgh, PA; ²Shimadzu Scientific Instruments, Inc., Columbia, Maryland; ³Applied Isotope Technologies, Pittsburgh, PA; ⁴Gerstel, Inc., Linthicum, MD
- MP 029 **Advanced Mass Spectrometry Strategies for the Discovery of New Biomarkers in Acute Myeloid Leukemia;** Sibylle Pfammatter^{1,2,3}; Eric Bonnell^{1,2}; Marie Eve Bordeleau^{1,2}; Eric Audemard^{1,2}; Louis Theret^{1,2}; Isabel Boivin^{1,2}; Sebastien Lemieux^{1,2,4}; Philippe P. Roux^{1,2,5}; Josée Hébert^{1,2,6,7}; Guy Sauvageau^{1,2,6}; Pierre Thibault^{1,2,3}; ¹The Leucegene project at Institute for Research in Immunology and Cancer, Université de Montréal, Montréal, Québec; ²Institute for Research in Immunology and Cancer, Université de Montréal, Montréal, Québec; ³Department of Chemistry, Université de Montréal, Montréal, Québec; ⁴Department of Computer Science and Operations Research, Université de Montréal, Montréal, Québec; ⁵Department of Pathology and Cell Biology, Université de Montréal, Montréal, Québec; ⁶Department of Medicine, Faculty of Medicine, Université de Montréal, Montréal, Québec; ⁷Division of Hematology-Oncology and Leukemia Cell Bank of Quebec, Maisonneuve-Rosemont Hospital, Montréal, Québec
- MP 030 **HPLC-MS/MS Method for Measuring 15 Urinary Biomarkers of Exposure to Organophosphate Flame Retardants, Plasticizers, and Pesticides;** Nayana K. Jayatilaka¹; Paula Restrepo¹; Zachary Davis¹; Meghan Vidal¹; Antonia M. Calafat¹; Maria Ospina¹; ¹Centers for Disease Control and Prevention, Atlanta, GA
- MP 031 **Selected Reaction Monitoring (SRM)-Based Rapid Measurement of GABA in Complex Clinical Samples;** Sigmund J Haidacher^{1,2}; Kathleen M Hoch^{1,2}; Qinglong Wu^{1,2}; Jasmohan S Bajaj³; Tor C Savidge^{1,2}; Anthony M Haag^{1,2};



- ¹Baylor College of Medicine, Houston, TX; ²Texas Children's Hospital, Houston, Texas; ³Virginia Commonwealth University, Richmond, VA
- MP 032 **Short Chain Fatty-Acids Analysis in brain by GC/MS to Determine Effect of Bioactive Food in Mouse Model of Alzheimer's Disease;** Eleazar Rojas Santiago¹; Tauqeerunnisa Syedaa²; Daniel Cuervo-Zanattaa²; Claudia Perez Cruz²; ¹Agilent Technologies, Mexico, Mexico; ²CINVESTAV, CDMX, Mexico
- BIOMOLECULAR STRUCTURE ANALYSIS: CHEMICAL CROSSLINKING AND COVALENT LABELING I**
033-060
- MP 033 **Protein Tertiary Structure Prediction Based on Statistical Strategies to Incorporate Cross-Linking/Mass Spectrometry Constraints;** Allan Jhonathan Ramos Ferrari¹; Guilherme Fatur Bottino¹; Leandro Martínez¹; Fabio Cesar Gozdo¹; ¹University of Campinas, Campinas, Brazil
- MP 034 **Development of a Capillary LC Method for Co-Elution of Isomeric Peptide Oxidation Products;** Niloofer Abolhasani Khaje¹; Joshua S Sharp¹; ¹University of Mississippi, University, MS
- MP 035 **Development of a Fast Photochemical Oxidation of Proteins (FPOP)-Based Protein Folding Study;** Luciano H Di Stefano¹; Danté T Johnson¹; Lisa M Jones¹; ¹University of Maryland Baltimore, Baltimore, MD
- MP 036 **Characterization of the IL-7/IL-7R α Binding Interface in Solution with Docking Guided by Mass Spectrometry-Based Cross-linking and Hydrogen Deuterium Exchange Data;** Mengru Mira Zhang¹; Guodong Chen²; Brett R Beno²; Richard Y-C Huang²; Jagat Adhikari¹; Ekaterina Deyanova²; Jing Li²; Michael Gross¹; ¹Washington University, St. Louis, MO; ²Bristol-Myers Squibb, Princeton, NJ
- MP 037 **Alpha-Synuclein Oligomers Modelled Using Crosslinking and Discrete Molecular Dynamics Simulations and Validated with Multiple Structural Proteomics Techniques;** Nicholas I Brodie^{1,2}; Venkat R. Chirasani³; Andrew G. Cairns⁴; Fredrick Almqvist⁵; Evgeniy V. Petrotchenko⁶; Nikolay V. Dokholyan³; Christoph H. Borchers^{1,2,5,6}; ¹University of Victoria-Genome BC Proteomics Centre, Victoria, BC; ²Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC; ³Departments of Pharmacology, and Biochemistry and Molecular Biology, Pennsylvania State College of Medicine, Hershey, PA; ⁴Department of Chemistry, Umeå University, Umeå, Sweden; ⁵Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; ⁶Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC
- MP 038 **Observing Gleevec's Drug Engagement in TNBC-AA and TNBC-EA Using In-Cell Fast Photochemical Oxidation of Proteins;** Emily E Chea¹; Lisa M Jones²; ¹University of Maryland, Baltimore, Baltimore; ²University of Maryland Baltimore, Baltimore, MD
- MP 039 **Normalizing Covalent Labeling Reactivity to Obtain Better Constraints for Computational Protein Structure Prediction;** Xiao Pan¹; Richard W. Vachet¹; ¹University of Massachusetts, Amherst, MA
- MP 040 **MaXLinker: An Innovative "MS3-centric" Proteome-Wide Cross-Link Search Engine with High Sensitivity and Specificity;** Kumar Yugandhar^{1,2}; Ting-Yi Wang^{1,2}; Alden King-Yung Leung^{1,2}; Michael Charles Lanz^{2,3}; Ievgen Motorykin⁴; Jin Liang^{1,2}; Elnur Elyar Shayhidin^{1,2}; Marcus Bustamante Smolka^{2,3}; Sheng Zhang⁴; Haiyuan Yu^{1,2}; ¹Department of Biological Statistics and Computational Biology, Cornell University, Ithaca, NY; ²Weill Institute for Cell and Molecular Biology, Cornell University, Ithaca, NY; ³Department of Molecular Biology and Genetics, Cornell University, Ithaca, NY; ⁴Mass Spectrometry and Proteomics Facility, Institute of Biotechnology, Cornell University, Ithaca, NY
- MP 041 **High-Resolution Hydroxyl Radical Protein Footprinting Introduction and Workflow;** John Schenkel, Jr.¹; Anna Kiselar^{1,2}; Mark Chance^{1,2}; ¹NeoProteomics, Inc., Cleveland, OH; ²Case Western Reserve University, Cleveland, OH
- MP 042 **Design, Synthesis and Application of Novel Sulfoxide-Based, Click-Chemistry Enrichable Cleavable Cross-Linkers for Protein-Protein Interaction Analysis;** Michael Stadlmeier¹; Leander Runtsch¹; Martin Wühr²; Thomas Carell¹; ¹LMU Munich, Munich, Germany; ²Princeton University, Princeton, NJ
- MP 043 **The Interactome of Mitochondria in Baker's Yeast: A Snapshot Taken by Cross-Linking Mass Spectrometry;** Andreas Linden^{1,2}; Ralf Pflanz¹; Iwan Parfentev¹; Bettina Homberg²; Markus Deckers²; Peter Rehling²; Henning Urlaub^{2,3}; ¹Max Planck Institute for Biophysical Chemistry, Goettingen, Germany; ²University Medical Center Goettingen (UMG), Goettingen, Germany; ³Max Planck Institute for Biophysical Chemistry, Goettingen, Germany
- MP 044 **Kojak 2.0: New Features for the Analysis of Cross-Linked Proteins;** Michael R. Hoopmann¹; Alex Zelter²; Michael Riffle²; Jimmy K Eng²; Trisha N Davis²; Robert L Moritz¹; ¹Institute for Systems Biology, Seattle, WA; ²University of Washington, Seattle, WA
- MP 045 **Systems Structural Biology of the Heart: Impact of Lysine Acetylation on Protein Conformations and Interactions;** Juan Chavez¹; Matthew A Walker¹; Arianne Caudal¹; Bo Zhou¹; Andrew Keller¹; Rong Tian¹; James E. Bruce¹; ¹University of Washington, Seattle, WA
- MP 046 **Structural Interrogation of Phosphorylation-Dependent Proteasome Dynamics Using a Multifaceted Cross-Linking and Targeted Quantitation-Based Approach;** Clinton Yu¹; Lan Huang¹; Xiaorong Wang¹; ¹University of California, Irvine, CA
- MP 047 **Determination of the Yield of Copper-Catalyzed Click Reaction on Individual Newly Synthesized Proteins with Azidonorleucine Inside Live Cells;** Chengzhi Cai¹; Guoting Qin¹; Rufeng Li¹; ¹University of Houston, Houston, TX
- MP 048 **Tyrosine-Specific Nitration of Influenza Hemagglutinin Proteins by Selective Covalent Labeling and Mass Spectrometry;** Carrie L. Pierce¹; Jonathan L. Bundy¹; Jakub Baudys¹; Tracie L. Williams¹; Dongxia Wang¹; Maria I. Solano¹; John R. Barr¹; ¹Centers for Disease Control and Prevention, Atlanta, Georgia 30341
- MP 049 **Acquisition Mode Characterization for the Quantitative and Qualitative Analysis of Cross-Linked Peptides by Targeted and Untargeted LC-IM-MS;** Hannah Britt¹; Suniya Khatun¹; Abubakar Hatimy¹; Jonathan P Williams²; Chris Hughes²; Tristan Cragolini¹; Nathanael Page³; Konstantinos Thalassinou¹; Johannes PC Vissers²; ¹UCL, London, United Kingdom; ²Waters Corporation, Wilmslow, United Kingdom; ³LGC Group, Teddington, United Kingdom
- MP 050 **Tools for Atomic-Resolution Protein Structure Determination in Cells: CID-Cleavable Photo-Amino Acids and Purification of Crosslinked Peptides of Any Origin;** Bjorn-Erik Wulff¹; Joshua E. Elias¹; Pehr Harbury¹; ¹Stanford University, Stanford, CA
- MP 051 **Monitoring the Aggregation-Induced Conformational Conversion of α -Synuclein Protein by Fast Photochemical Oxidation of Proteins (FPOP);** Prashant N. Jethva¹; Jing Yan¹; Eva Illes-Toth²; Michael L. Gross¹; ¹Department of Chemistry, Washington University, St. Louis, MO; ²School of Biosciences, University of Birmingham, Birmingham, United Kingdom



- MP 052 **Next Generation Dual Cleavable Cross-Linking Strategies for High Confidence Identification of Cross-Linked Peptides;** Jayanta Kishor Chakrabarty¹; Fang Zixiang¹; Abu Hena M. Kamal¹; Saiful M. Chowdhury¹; ¹University of Texas, Arlington, TX
- MP 053 **Determination of Ligand and pH-Induced Conformational Changes in the Cation-Independent Mannose-6-Phosphate Transferase by Fast Photochemical Oxidation of Proteins;** Sandeep K. Misra¹; Linda J. Olson²; Nancy M. Dahms³; Joshua S. Sharp¹; ¹University of Mississippi, University, MS; ²Medical College of Wisconsin, Milwaukee, WI; ³Medical College of Wisconsin, Milwaukee, WI
- MP 054 **Describing the Interaction XcpU and XcpW from the *Pseudomonas aeruginosa* Type II Secretion Machinery Using Cross Linking – Mass Spectrometry;** Badreddine Douzi¹; Geneviève Ball¹; Cristian A Escobar Bravo²; Edwin De Pauw³; Katrina Forest²; Romé Voulhoux¹; Loïc Quinton³; ¹CNRS, Aix-Marseille Université, IMM, Laboratoire de Chimie Bactérienne UMR7283, Marseille, France; ²Department of Bacteriology, University of Wisconsin-Madison, WI, 53706, USA, Madison, WI; ³Laboratoire de Spectrométrie de Masse - MoISys Research Unit - Liège Université, Liège, Belgium
- MP 055 **Accelerated Biomolecular Cross-Linking by Contained-Electrospray Ionization for Rapid Detection by Mass Spectrometry;** Benjamin J. Burris¹; Abraham K. Badu-Tawiah¹; ¹The Ohio State University, Columbus, OH
- MP 056 **Novel Methods for Chemical Crosslinking Based Protein Complex Analysis;** Qun Zhao¹; Yuxin An¹; Lili Zhao²; Lihua Zhang²; Yukui Zhang²; ¹Dalian Institute of Chemical Physics, Chinese Academy of Science, Dalian, China; ²Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China
- MP 057 **Application of Phenyl-based Columns in Improving the Identification of Inter-crosslinked Peptides;** Zixiang Fang¹; Yehia Z. Baghdady¹; Kevin A Schug¹; Saiful M. Chowdhury¹; ¹University of Texas Arlington, Arlington
- MP 058 **Energy Barriers to the Pre-amyloid Structural Change of β -2-microglobulin in the Presence of the Amyloidogenic Variant Δ N6 or Amyloid Inhibitors;** Blaise G. Arden¹; Richard W. Vachet¹; ¹University of Massachusetts, Amherst, MA
- MP 059 **OpenPepXL: Sensitive, Comprehensive Identification and Quantification of Protein-Protein Cross-Links;** Eugen Netz¹; Tjeerd M.H. Dijkstra¹; Timo Sachsenberg²; Oliver Kohlbacher^{1,2,3,4}; ¹Biomolecular Interactions group, Max Planck Institute for Developmental Biology, Tuebingen, Germany; ²Applied Bioinformatics group, University of Tuebingen, Tuebingen, Germany; ³Quantitative Biology Center (QBiC), University of Tuebingen, Tuebingen, Germany; ⁴Institute for Translational Bioinformatics, University Hospital Tuebingen, Tuebingen, Germany
- MP 060 **XiView: A common platform for the Downstream Analysis of Crosslinking Mass Spectrometry data;** Martin J. Graham^{1,2}; Colin Combe^{1,2}; Lars Kolbowski³; Juri Rappsilber^{1,2,3}; ¹Wellcome Centre for Cell Biology, Edinburgh, United Kingdom; ²University of Edinburgh, Edinburgh, United Kingdom; ³Technische Universität Berlin, Berlin, Germany
- MP 061 **Reducing the Global Burden of Infectious Diseases through Precision Infection Management (PIM);** Ian Lewis¹; Fiona Clement¹; Deirdre L Church²; Ashlee Earl³; Yonatan Grad⁴; Christopher Naugler²; Sergei Noskov¹; ¹University of Calgary, Calgary, AB; ²Calgary Laboratory Services, Calgary, AB; ³Broad Institute of MIT and Harvard, Cambridge, MA; ⁴Harvard T.H. Chan School of Public Health, Boston, MA
- MP 062 **Interference from Sulfonated Metabolites in the Analysis of β -Lapachone in Clinical Human-Plasma Samples Using Liquid Chromatography-Mass Spectrometry;** Seungil Cho¹; Bo Kyung Kim¹; Mi-ri Gwon¹; Young-ran Yoon¹; ¹Kyungpook National University, Daegu, South Korea
- MP 063 **Characterization of an Amphetamine Interference from Gabapentin in an LC-HRMS Confirmation Assay;** Ana Celia Grenier¹; Teresa Pekol¹; Dana Schubring¹; Charlene Johnson¹; Lawrence J Andrade¹; Robin Hyland¹; ¹Dominion Diagnostics, North Kingstown, RI
- MP 064 **Ambient Mass Spectrometry Immunoassays for the Ultra-Sensitive Biomarker Detection and Tissue Glycan Imaging;** Yu Bai¹; Shuting Xu²; Wen Ma²; Huwei Liu²; ¹College of Chemistry, Peking University, Beijing, China; ²Peking University, Beijing, China
- MP 065 **Dried Blood Spheroids for Stabilizing Acylcarnitines in Micro-liter Blood Samples Stored under Ambient Conditions;** Benji Frey¹; Deidre E. Damon¹; Abraham K. Badu-Tawiah¹; ¹The Ohio State University, Columbus, OH
- MP 066 **Quantification of 11-plex LSD Enzyme Activity Using LC-MS/MS;** Ryuichi Mashima¹; Torayuki Okuyama¹; Mari Ohira¹; ¹National Center for Child Health and Development, Setagaya-Ku, Japan
- MP 067 **A Comparison of Tenofovir Diphosphate and Emtricitabine Triphosphate Concentrations Collected in Whole Blood by a Microsampler or Dried Blood Spot;** Amanda P Schauer¹; Craig Sykes¹; Jason R Pirone¹; Nicole White¹; Hannah Bryan¹; Angela DM Kashuba¹; ¹University of North Carolina, Chapel Hill, NC
- MP 068 **A Sensitive and Robust HPLC – MS/MS (MRM) Method for the Quantitation of Hepcidin in Human Serum;** Jun Liu¹; Michael Chen²; ¹University of British Columbia, Vancouver, BC; ²Island Medical Program, Department of Pathology and Laboratory Medicine, University of British Columbia, Vancouver, BC
- MP 069 **Lipid and Apolipoprotein Changes in Response to Inflammation with Type 2 Diabetes;** Bryan Parks¹; Zsuzsanna Kuklenyik²; John R Barr²; ¹Centers for Disease Control and Prevention, Atlanta, GA; ²Centers for Disease Control and Prevention, Atlanta, Georgia
- MP 070 **Simultaneous Determination of Eight Antiepileptic Drugs and an Active Metabolite in Human Plasma by LC-MS/MS;** Tian Liu¹; Raghavendhar R Kotha¹; Stephanie Zalesak¹; Jace W Jones¹; James E Polli¹; Maureen A Kane¹; ¹Department of Pharmaceutical Sciences, University of Maryland School of Pharmacy, Baltimore, MD
- MP 071 **Fully Automated LC-MS/MS Analysis of Anticoagulants Using a Stable Isotope Labelled Internal Standards;** Toshikazu Minohata^{1,2}; Yuki Uno²; Sigrid Baumgarten³; Stéphane Moreau³; Fanny Dayot¹; Jean-François Hoeffler¹; ¹Alsachim SAS, Illkirch, France; ²Shimadzu Corporation, Kyoto, Japan; ³Shimadzu Europa GmbH, Duisburg, Germany
- MP 072 **Sensitive Cortisol Analysis Using a Single Hair with Nanoflow UPLC- MS3 Tandem Mass Spectrometry;** Chih-Wei Chang^{1,2}; Linjer Chen¹; Li-Jung Ma¹; Pin-Hsuan Wang¹; Yet-Ran Chen²; Pao-Chi Liao¹; ¹Department of Occupational and Environmental Health, Medical College, National Cheng Kung University, Tainan, Taiwan; ²Agriculture Biotechnology Research Center, Academia Sinica, Taipei, Taiwan
- MP 073 **A Two-Minute Liquid Chromatography/Ion Mobility Mass Spectrometry Method for Quantitation of 25-Hydroxyvitamin D without Interference from 3-epi-25-Hydroxyvitamin D;** Nicholas Oranji¹; Jiajun Lei¹; Timothy J. Garrett¹; Richard A Yost¹; ¹University of Florida, Gainesville, FL

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- MP 074 **A High-Performance Liquid Chromatography Tandem Mass Spectrometry Method for the Determination of Superwarfarin Rodenticides in Human Plasma;** Daniel Nosal¹; Douglas L Feinstein²; Richard B. van Breemen³; ¹Oregon State University - Linus Pauling Institute, Corvallis, OR; ²University of Illinois at Chicago, Department of Anesthesiology, Chicago, IL; ³Linus Pauling Institute, Oregon State University, Corvallis, OR
- MP 075 **Assessing Isolate-Specific Antimicrobial Resistance Patterns of *Klebsiella pneumoniae*;** Thomas D. Horvath^{1,2}; Sibel Ak^{1,2}; Sigmund J. Haidacher^{1,2}; Kathleen Hoch^{1,2}; Tor C. Savidge^{1,2}; Anthony M. Haag^{1,2}; ¹Department of Pathology and Immunology, Baylor College of Medicine, Houston, TX; ²Microbiome Center, Texas Children's Hospital, Houston, TX
- MP 076 **Mass spectrometry shows limitations of lectin-based approaches to quantify galactose-deficient IgA1 in circulation of IgA nephropathy patients and controls;** Olivier M. Lardinois¹; Patrick H. Nachman²; Jason G. Williams¹; Leesa J Deterding¹; ¹Mass Spectrometry Research and Support Group, National Institute of Environmental Health Sciences (NIEHS), Research Triangle Park, NC; ²Division of Renal Diseases and Hypertension, University of Minnesota, Minneapolis, MN
- MP 077 **Elucidating Multi-Omic Molecular Signatures of End-Term Preeclampsia and Gestational Diabetes Mellitus;** Melanie T. Odenkirk¹; Kristin E. Burnum-Johnson²; Brandie D. Taylor³; Kelly G. Stratton²; Marina A. Gritsenko²; Lisa M. Bramer²; Bobbie-Jo Webb-Robertson²; Jennifer Kyle²; Kent J. Bloodsworth²; Karl K Weitz²; Erin S Baker¹; ¹Department of Chemistry, North Carolina State University, Raleigh, NC; ²Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA; ³College of Public Health, Temple University, Philadelphia, PA 19122
- MP 078 **Development of a Quantitative Method for the Measurement of Free Oligosaccharides in Plasma and Urine from Patients with Aspartylglucosaminuria;** Beniam Berhane¹; Tim Wood¹; Laura Pollard¹; ¹Greenwood Genetic Center, Greenwood, SC
- MP 079 **Discovery of Tumor-Specific Antigens for Leukemia Immunotherapy Using a Novel Proteogenomic Approach;** Sibylle Pfammatter¹; Eric Bonneil¹; Joel Lanoix¹; Krystal Vincent¹; Chantal Durette¹; Jean-Philippe Laverdure¹; Mathieu Courcelles¹; Marie-Pierre Hardy¹; Sebastien Lemieux¹; Claude Perreault¹; Pierre Thibault¹; ¹Université de Montréal, Montréal, Québec
- MP 080 **Pharmacokinetic Interactions of a Red Clover Botanical Dietary Supplement with Drug Metabolism in Peri- and Post-menopausal Women;** Jaewoo Choi¹; Luying Chen^{2,3}; Scott W. Leonard¹; Suzanne Banuvar³; Elena Barengolts³; Marlos Viana³; Richard B. van Breemen^{2,3}; ¹Linus Pauling Institute, Oregon State University, Corvallis, Oregon; ²Linus Pauling Institute, College of Pharmacy, Oregon State University, Corvallis, OR; ³UIC/NIH Center for Botanical Dietary Supplements Research, Chicago, IL
- MP 081 **An Efficient MS Method for Screening 20 Genotypes of Human Papillomavirus;** Yun Zhao¹; Shanyun Lin¹; Panhong Liu¹; Xuehui Tang¹; Zhe Ren¹; Yan Ren¹; Siqi Liu¹; ¹BGI-Shenzhen, Shenzhen, China
- MP 082 **Development of Glycosaminoglycan Assays for Mucopolysaccharidoses Using LC-MS/MS;** Takanari Hattori¹; Tetsuo Iida¹; Jun Watanabe¹; Misa Tanaka²; Hironori Kobayashi³; Shunji Tomatsu⁴; ¹Shimadzu Corporation, Kyoto, Japan; ²MS specialite, Yokohama, Japan; ³Department of Pediatrics, Shimane University Faculty of Medicine, Izumo, Japan; ⁴Nemours/Alfred I. duPont Hospital for Children, Wilmington, Delaware
- MP 083 **A Rapid LC-MS/MS Method to Measure Simultaneously IDUA, IDS, NAGLU, GALNS and ASRB Enzymes**
- Activities in Dried Blood Spots;** Misa Tanaka¹; Jun Watanabe²; Tetsuo Iida²; Hironori Kobayashi³; ¹MS specialite, Yokohama, Japan; ²Shimadzu Corporation, Kyoto, Japan; ³Department of Pediatrics, Shimane University Faculty of Medicine, Izumo, Japan
- DRUG METABOLISM: QUALITATIVE AND HIGH THROUGHPUT ANALYSIS**
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- MP 084 **Efficient and Comprehensive Metabolite Identification by Utilizing Automatic Background Exclusion and Specific Filtering Features of Orbitrap ID-X Tribrid Mass Spectrometer;** Kai Wang¹; Sven Hackbusch²; Kate J. Comstock²; Kevin Coe¹; ¹Janssen R&D, San Diego, CA; ²Thermo Fisher Scientific, San Jose, CA
- MP 085 **A New Strategy Optimized for Metabolite Profiling on a Tribrid Mass Spectrometer Platform;** Qian Ruan¹; Kenneth P. Matuszak²; Kate J. Comstock³; ¹Bristol-Myers Squibb, Princeton, NJ; ²ThermoFisher Scientific, Bannockburn, IL; ³ThermoFisher Scientific, San Jose, CA
- MP 086 **Application of Novel Background Exclusive DDA for Automated and Sensitive MS/MS Acquisition of Unknown Herbal Medicine Components in Biological Samples;** Tingting Cai¹; Chunyan Zhu²; Ying Jin²; Jiayun Chen²; Guoqiang Liu³; Niusheng Xu³; Caisheng Wu²; Mingshe Zhu⁴; ¹WuXi AppTec, Nanjing, China; ²Xiamen University, Xiamen, China; ³Thermo Fisher Scientific, Shanghai, China; ⁴MassDefect Technologies, Princeton, NJ
- MP 087 **Highly Accurate Detection and Identification Methodology of Xenobiotic Metabolites Using Stable Isotope Labeling, LC/HRMS/MS Analysis, and Data Mining Techniques;** Masatomo Takahashi¹; Yoshihiro Izumi¹; Fukumatsu Iwahashi²; Yasumune Nakayama³; Mitsuhiro Iwakoshi²; Motono Nakao¹; Seiji Yamato²; Eiichiro Fukusaki⁴; Takeshi Bamba¹; ¹Medical Institute of Bioregulation, Kyushu University, Fukuoka, Japan; ²Sumitomo Chemical Co., Ltd., Takarazuka, Japan; ³Graduate School of Biotechnology and Life Science, Sojo University, Kumamoto, Japan; ⁴Graduate School of Engineering, Osaka University, Suita, Japan
- MP 088 **Integrating Discovery-Stage Metabolite Analysis into High-Throughput Microsomal Clearance Pipelines;** Elyse Freiburger¹; David Wagner¹; ¹AbbVie Inc., North Chicago, IL
- MP 089 **in vitro Metabolic Studies of SARMs RAD-140 and S-23 in Horse Using Ultra-High Performance Liquid Chromatography-High Resolution Mass Spectrometry;** Yat Ming So¹; Timmy Lai Sheung Choi¹; Gary Ngai Wa Leung¹; Pauly Kit Sze Chan¹; Ming Yip Lau¹; Emmie Ngai Man Ho¹; ¹Racing Laboratory, The Hong Kong Jockey Club, Hong Kong, Hong Kong
- MP 090 **Investigating Clozapine-Related Protein Binding in vitro by LC-MS/MS;** Timon Geib¹; Lekha Sleno¹; ¹UQAM, Montreal, QC
- MP 091 **Involvement of Olmutinib Reactive Metabolites on its Severe Toxic Reactions: Potential Answers by Mass Spectrometry;** Adnan A Kadi¹; Mohamed W. Attwa^{1,2}; Ali S. Abdelhameed¹; ¹College of Pharmacy, King Saud University, Riyadh, SA, Riyadh, Saudi Arabia; ²Students' University Hospital, Mansoura, Egypt
- MP 092 **Balancing Quality and Quantity in Quan/Qual LC-HRMS Analysis;** Anne-Charlotte Dubbelman¹; Filip Cuyckens²; Lieve Dillen²; Rob J. Vreeken^{1,2}; Thomas Hankemeier¹; ¹Leiden University, Leiden, Netherlands; ²Janssen R&D, Beerse, Belgium
- MP 093 **Metabolism Study of Simvastatin in Rat Tissues Using MALDI Orbitrap Mass Spectrometry;** Wencui Yin¹; Adnan A Kadi¹; Alwabli Reem¹; Rahman M A f m¹; ¹King Saud University, Riyadh, Saudi Arabia



- MP 094 **Ultraviolet Photodissociation Enables Confirmation of Site Specific Glucuronidation on Small Molecule Metabolites**; Joe R. Cannon¹; Zhoupeng Zhang¹; Joshua Nicklay²; Romain Huguet²; Scott M. Peterman²; Nichoals Duczak²; Mark Cancilla¹; ¹Merck & Co., Inc., West Point, PA; ²Thermo Fisher Scientific, San Jose, CA
- MP 095 **Quantitative Analysis of Hair Samples for Methotrexate (MTX) and Metabolite Using High-Performance Liquid Chromatography-Tandem Mass Spectrometry (LC-MS/MS) Detection**; Yeongsuk Yoo¹; Sang Kwang Lee²; Kun Cho³; ¹Korean Basic Science Institute, Cheong-ju, South Korea; ²Eulji Medi-Bio research institute, Daejeon, South Korea; ³Korea Basic Science Institute, Seoul, South Korea
- MP 096 **High Throughput Drug Accumulation Assay and Impact on Metabolome of Drug-Resistant Bacteria**; Vincent Bonifay¹; Inga V. Leus²; Brinda Chandar²; Helen I. Zgurskaya²; ¹University of Oklahoma, Norman, OK; ²University of Oklahoma, Norman, OK
- MP 097 **Improving Peptide Catabolism Interpretation Using Ion Mobility Data and Server-Based Data Review with HELM Integration**; Mark D Wrona¹; Gordon Murray²; Russell Mortishire-Smith³; Yun W Alelyunas³; Antoni Riera⁴; Tatiana Radchenko⁵; Anna Escola⁴; Ismael Zamora⁵; Jayne Kirk³; ¹Waters Corporation, Milford, MA; ²Waters Corporation, Beverly, MA; ³Waters Corporation, Wilmslow, United Kingdom; ⁴Institute for Research in Biomedicine (IRB Barcelona), The Barcelona Institute of Science and Technology, Barcelona, Spain; ⁵Lead Molecular Design, S.L., Sant Cugat Del Valles, Spain
- MP 098 **EI-MAVEN : First in Class Mass Spectrometry Data Processing Engine for Metabolomics**; Shefali Lathwal¹; Shubhra Agrawal¹; Raghav Sehgal¹; Surbhi Poddar¹; Rishabh Gupta¹; Saiful Khan¹; Sahil Kumar¹; Sabu George¹; Swetabh Pathak¹; Abhishek Jha²; ¹Elucidata, Delhi, India; ²Elucidata, Cambridge, MA
- DRUG AND METABOLITE ANALYSIS: NOVEL APPROACHES FOR DRIED BIOLOGICAL SAMPLES**
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- MP 099 **Fully Automated Forensic Screening of Dried Bloodspots with MRM Spectrum Mode**; Davor Fielitz¹; Stefan Gaugler²; Jana Rykl³; Maha Khalid Almazraoua⁴; Matthias Grill⁵; Vicente L. Cebolla⁶; Asem Quanair⁷; ¹Shimadzu Deutschland GmbH, Berlin, Germany; ²CAMAG, Muttenz, Switzerland; ³Shimadzu Switzerland, Reinach, Switzerland; ⁴The Regional Poison Control Center, Dammam, Saudi Arabia; ⁵Lipomed, Arlesheim, Switzerland; ⁶Instituto de Carboquímica, Zaragoza, Spain; ⁷Analytica One, Al-Hidd, Bahrain
- MP 100 **Probing Protein-Ligand Interactions by Native LESA Mass Spectrometry**; Eva Illes-Toth¹; Helen J. Cooper¹; ¹University of Birmingham, Birmingham, United Kingdom
- MP 101 **Incorporating Novel Synthetic DBS Substrates into a Blood Microsampling Device for Multi-Omics Analyses**; Kyle Bachus¹; Lada Staskova^{2,3}; Jeff Craig^{3,4}; Robert Shellie⁵; Ricardo Neto⁶; Dario Arrua⁶; Emily F Hilder⁶; Andrew Gooley¹; Wei Boon Hon¹; ¹Trajan Scientific and Medical, Ringwood, Australia; ²RMIT University, Melbourne, Australia; ³Centre for Molecular and Medical Research, School of Medicine, Faculty of Health Deakin University, Geelong, Australia; ⁴Murdoch Children's Research Institute, The Royal Children's Hospital, Parkville, Australia; ⁵Centre for Advanced Sensory Science (CASS), School of Exercise and Nutrition Sciences, Deakin University, Melbourne, Australia; ⁶Future Industries Institute, University of South Australia, Mawson Lakes Campus, Adelaide, Australia
- MP 102 **Organic Synthesis Reaction Monitoring of a Fentanyl Synthesis Using a Microporous Polyolefin Silica Substrate for Paper Spray Mass Spectrometry**; Thomas
D Kiselak¹; Imesha W. DeSilva²; Anika Claassen²; Guido F. Verbeck²; ¹University of North Texas, Roanoke, TX; ²University of North Texas, Denton, TX
- MP 103 **Enabling Patient Centricity in Clinical Development through at Home Sample Collection**; Melanie Anderson¹; Daniel Dreyer¹; Lingling Xue¹; Marissa Dockendorf¹; Kevin P. Bateman¹; ¹Merck & Co., West Point, PA
- ENERGY: BIOFUELS AND ALGAE**
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- MP 104 **Application of Thin-Layer Chromatography to Deep Investigation of Maltenes and Asphaltenes Compound Classes by Ultra-High Resolution Mass-Spectrometry**; Alexander Zhrebker¹; Yury kostyukevich¹; Oleg Kharybin¹; Gleb Vladimirov¹; Eugene (evgeny) Nikolaev¹; ¹Skolkovo institute of science and technology, Moscow Region, Russian Federation
- MP 105 **Comprehensive Analysis of Isoprenoid Pathway Intermediates and Associated Metabolites by HILIC-QTOF LC/MS**; Edward Baidoo¹; Yuqin Dai²; Veronica Teixeira Benites¹; ¹Joint BioEnergy Institute/LBNL, Emeryville, CA; ²Agilent Technologies, Santa Clara, CA
- MP 106 **Structure Dependent Electrospray Ionization Response of o-4 lignin Compounds**; Shardrack O. Asare¹; Bert C. Lynn¹; ¹University of Kentucky, Lexington, KY
- MP 107 **Insight into Biomass Pyrolysis from Molecular Beam Mass Spectrometry**; Steven M Rowland¹; Anne K Starace¹; Kristen Hietala¹; Daniel L Carpenter¹; ¹National Renewable Energy Lab, Golden, CO
- MP 108 **Detailed Chemical Composition of an Oak Biocrude and Its Hydrotreated Product Determined by Positive Atmospheric Pressure Photoionization FT-ICR Mass Spectrometry**; Alan G. Marshall¹; Rebecca L. Ware²; Ryan P. Rodgers²; Ofel D Mante³; David C Dayton³; Sylvain Verdier⁴; Steven M Rowland²; ¹NHMFL, Florida State Univ., Tallahassee, FL; ²National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL; ³RTI International, Research Triangle Park, NC; ⁴Haldor Topsoe A/S, Lyngby, Denmark
- MP 109 **Coupling LC-MS/MS-Based Proteomics and Targeted Metabolite Analysis Reveals Novel Enzymatic Solutions for Lignin Utilization and Valorization in *Novosphingobium aromaticivorans***; Richard J. Giannone^{1,2}; David C Garcia^{3,4}; Gerald N Presley^{2,3}; Jacob H Cecil³; Joshua K Michener^{2,3}; ¹Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN; ²Center for Bioenergy Innovation, Oak Ridge National Laboratory, Oak Ridge, TN; ³Biosciences Division, Oak Ridge National Laboratory, Oak Ridge, TN; ⁴The Bredesen Center for Interdisciplinary Research and Graduate Education, University of Tennessee, Knoxville, TN
- MP 110 **High-Resolution Mass Spectrometry (FT-ICR) Analysis of Milled Wood Lignins**; Evan Terrell¹; Vincent Carré²; Frédéric Aubriet²; Anthony Dufour³; Manuel Garcia-Perez¹; ¹Washington State University, Pullman, WA; ²Université de Lorraine, ICPM, Metz, France; ³Université de Lorraine, LRPC, CNRS, Nancy, France
- MP 111 **Application of Gas Chromatography - Mass Spectrometry for the Analysis of Structural Isomers of Lignin Dimers**; Poorva Kamali¹; Bert C. Lynn¹; ¹Department of Chemistry, University of Kentucky, Lexington, KY
- MP 112 **Using SPME-GC-MS for Chemical Profiling of Volatile Organic Compounds Emitted as Early Biomarkers of Algal Pond Crashes**; Kristen L. Reese^{1,2}; Carolyn L. Fisher³; Matthew W. Moorman⁴; A. Daniel Jones²; Matthias Frank¹; Todd W. Lane³; ¹Lawrence Livermore National Laboratory, Livermore, CA; ²Michigan State University, East Lansing, MI; ³Sandia National Laboratory, Livermore, CA; ⁴Sandia National Laboratory, Albuquerque, NM



MP 113 **Data Mining and Machine Learning Strategies for Non-Targeted Interpretation of High-Resolution Mass Spectrometry Data from Complex Biofuel Samples;** Sasa Bjelic; *Paul Scherrer Institut, Villigen PSI, Switzerland*

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MP 114 **Identification of Transformation Products and Disinfection By-Products in Wastewater Impacted Drinking Water;** Danielle C. Westerman¹; Hannah K Liberatore¹; Kristin H Cochran¹; Cassiana Montagner²; Michael J Plewa³; Leslie H Cizmas⁴; Jeanne VanBriesen⁵; Dionysios Dionysiou⁶; Ying Huang⁶; Daniel Schlenk⁷; Keith Loftin⁸; Tarun Anumol⁹; Susan D. Richardson¹; ¹*University of South Carolina, Columbia, SC*; ²*University of Campinas, Campinas, Brazil*; ³*University of Illinois Urbana-Champaign, Urbana-Champaign, IL*; ⁴*Texas A&M University, College Station, TX*; ⁵*Carnegie Mellon University, Pittsburgh, PA*; ⁶*University of Cincinnati, Cincinnati, OH*; ⁷*University of California Riverside, Riverside, CA*; ⁸*U.S. Geological Survey, Lawrence, KS*; ⁹*Agilent Technologies, Wilmington, DE*

MP 115 **Per- and Polyfluoroalkyl Substances (PFAS) Analysis in Human Serum and Plasma by Ultra-Performance Liquid Chromatography - Tandem Mass Spectrometry (UPLC-MS/MS);** M Abdul Mottaleb^{1,2}; Michael Petriello^{1,2}; Jennifer Miller³; Susan S Smyth^{1,2}; Debra K Moser³; Andrew J Morris^{1,2}; ¹*Division of Cardiovascular Medicine, University of Kentucky, Lexington, KY*; ²*Lexington Veterans Affairs Medical Center, Lexington, KY*; ³*College of Nursing, University of Kentucky, Lexington, KY*

MP 116 **Determination of Novel Dihydroxylated Polybrominated Diphenyl Ethers in Sea Fish by Gas Chromatography - Tandem Mass Spectrometry;** Mengtao Zhang¹; Jianghong Shi²; Zongwei Cai¹; ¹*Hong Kong Baptist University, Hong Kong, China*; ²*Southern University of Science and Technology, Shenzhen, China*

MP 117 **Discovery of Novel N-(4-hydroxybenzyl)valine Hemoglobin Adducts in Human Blood.;** Amanda Degner^{1,2}; Henrik Carlsson³; Isabella Karlsson³; Johan Eriksson³; Andrew Rajczewski^{1,2}; Suresh Pujari^{1,2}; Margareta Törnqvist³; Natalia Tretyakova^{1,2}; ¹*University of Minnesota, Minneapolis, MN*; ²*Masonic Cancer Center, U of MN, Minneapolis*; ³*Stockholm University, Stockholm, Sweden*

MP 118 **Quantification of Persistent Organic Pollutants in Human Blood Using Stir Bar Sorptive Extraction, GC/MS/MS, and Isotope Dilution Mass Spectrometry;** Weier Hao¹; Ashley Dillard¹; Anthony Macherone²; Jack Stuff³; Scott Faber⁴; Skip Kingston¹; Matt Pamuku⁵; ¹*Duquesne University, Pittsburgh, PA*; ²*Agilent Technologies, Inc., Wilmington, DE*; ³*Gerstel, Inc., Linthicum, MD*; ⁴*The Children's Institute of Pittsburgh, Pittsburgh, PA*; ⁵*Applied Isotope Technologies, Pittsburgh, PA*

MP 119 **GC-MS-Based Workflow for Discovery and Characterization of Biomarkers of Exposure to Greenness in Human Urine;** Zhengzhi Xie¹; Rachel Keith¹; Aruni Bhatnagar¹; Pawel Lorkiewicz¹; ¹*University of Louisville, Louisville, KY*

MP 120 **Neutral Loss and Product Ion Filtering to Screen Exposure Biomarkers to Common and Novel Phthalates: Application to a Standards Mixture ;** Syam S. Andra¹; Georgia Dolios¹; Divya Pulivarthi¹; Dhavalkumar Patel²; Emily A Spear³; Lauren Petrick¹; Manish Arora¹; Annemarie Stroustrup³; ¹*Department of Environmental Medicine and Public Health, Icahn School of Medicine at Mount Sinai, New York City, NY*; ²*School of Pharmacy, Texas Tech University Health Sciences Center, Amarillo, Texas*; ³*Department of Pediatrics, Icahn School of Medicine at Mount Sinai, New York City, NY*

MP 121 **IR-MALDESI Mass Spectrometry Imaging of Rat Placenta Tissue after Exposure to Flame Retardants;**

Crystal L Pace¹; Måns Ekelöf¹; Brian Horman²; Heather Patisaul^{2,3}; Heather Stapleton⁴; David C Muddiman^{1,3,5}; ¹*FTMS Laboratory for Human Health Research, Department of Chemistry, North Carolina State University, Raleigh, NC*; ²*Department of Biological Sciences, North Carolina State University, Raleigh, NC*; ³*Center for Human Health and the Environment, North Carolina State University, Raleigh, NC*; ⁴*Nicholas School of the Environment, Duke University, Durham, NC*; ⁵*Molecular Education, Technology, and Research Innovation Center (METRIC), North Carolina State University, Raleigh, NC*

MP 122 **A Novel Use of Isotopomers for in situ Calibration;** Anthony Qualley^{1,2}; Geoffrey Hughes^{1,2}; Thomas Malloy IV³; Ted Piatkowski³; Benjamin A Clapp²; H. Mitchell Rubenstein²; ¹*UES, Inc., Dayton, OH*; ²*USAF-AFRL, WPAFB, OH*; ³*Batelle, Columbus, OH*

MP 123 **Characterization of Arsenic Metabolites and Protein-Binding Using Chromatography Coupled to Multiple Mass Spectrometry Techniques;** Hanyong Peng¹; Bin Hu²; Qingqing Liu¹; Xiufen Lu¹; Xiaowen Yan¹; X. Chris Le³; ¹*University of Alberta, Edmonton*; ²*Wuhan University, Wuhan, China*; ³*University of Alberta, Edmonton, AB*

MP 124 **in vitro Metabolism of Bisphenol A and Five Analogs by LC-HRMS/MS;** Ons Ousji¹; Leanne Ohlund¹; Lekha Sleno¹; ¹*UQAM, Montreal, QC*

MP 125 **Extractables and Leachables Analysis Using a Quadrupole Time of Flight Mass Spectrometer Using SWATH Acquisition;** Rolf Kern¹; Patricia Sun²; Alex Liu²; ¹*SCIEX, Redwood Shores, CA*; ²*Sciex, Framingham, MA*

MP 126 **Electrochemical Simulation of Triclosan Metabolism and Toxicological Evaluation;** Hendrik Jan Brouwer¹; Jean-Pierre Chervet¹; Linyan Zhu²; Stephan Küppers³; ¹*Antec Scientific, Zoeterwoude, Netherlands*; ²*Maryland Institute for Applied Environmental Health, University of Maryland, 4200 Valley Drive, College Park, MD 20742*; ³*Research Center Jülich, Department of Analytics, Jülich, Germany*

MP 127 **Rapid Assessment of Isomeric Diversity in Perfluoroalkyl Substances (PFAS) by Ion Mobility Spectrometry-Mass Spectrometry (IMS-MS);** James Dodds¹; John C. Fjeldsted²; Erin S Baker¹; ¹*North Carolina State University, Raleigh, NC*; ²*Agilent Technologies, Inc., Santa Clara, CA*

MP 128 **Tracking Microcystin Oxidation Product Formation by Liquid Chromatography/High Resolution Mass Spectrometry (LC/HRMS) and Implications for Process Monitoring and Treatment;** Judy Westrick¹; Johnna A Birbeck¹; Nicholas Peraino¹; David C Szlag²; ¹*Wayne State University, Detroit, MI*; ²*Oakland University, Rochester, MI*

MP 129 **Detection of Endocrine Disrupting Chemicals (EDCs) and Pharmaceuticals and Personal Care Products (PPCPs) in Environmental Waters Using Online Concentration LC-MS/MS;** Johnna A Birbeck¹; Judy Westrick¹; Cassandra L Ward¹; Diana McKenzie²; ¹*Wayne State University, Detroit, MI*; ²*Bay Mills Community College, Brimley, MI*

MP 130 **Improving Non-Target Identification of Organic Contaminants by Probabilistic Ranking of Putative Structure Assignments by HR/AM MS(/MS) and Computational Mass Spectrometry;** Gordon Getzinger¹; P. Lee Ferguson¹; ¹*Duke University, Durham, NC*

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MP 131 **Polymerization in Place: Decreasing the Mobility of Halogenated Contaminants by Biotic and Abiotic Pathways;** Fan Wang¹; Shay Frankenfield¹; Thomas M. Makris¹; John L. Ferry¹; ¹*University of South Carolina, Columbia, SC*



- MP 132 **Determination of Pharmaceuticals in Wastewater Using Online Extraction by LC-MS/MS;** [Bianca Silva](#)¹; Cesar Augusto Marasco Junior²; Paulo Clairmont Feitosa de Lima Gomes²; ¹Unesp, Araraquara, Brazil; ²Unesp, Araraquara, Brazil
- MP 133 **Comprehensive Quantification of 30 Disinfection Byproducts Employing a Gas Chromatograph – Triple Quadrupole Mass Spectrometer (GC-QQQ) from Disinfected Wastewater Effluents;** Susana Y Kimura Hara¹; [Alejandro Ortega-Hernandez](#)¹; ¹University of Calgary, Calgary, AB
- MP 134 **The PFAS Conundrum: Mass Spectrometry Solutions for Addressing it;** [Ruth Marfil-Vega](#)¹; Brahm Prakash²; Gerard Byrne²; Tairo Ogura³; Yuka Fujito²; ¹Shimadzu Scientific Instruments, Columbia, MD; ²Shimadzu Scientific Instruments, Inc., Columbia, Maryland; ³Shimadzu corp., Kyoto, Japan
- MP 135 **A Comparison of Electrospray Ionization (ESI) and Paper Spray (PS) Ionization for the Analysis of Polyfluoroalkyl Substances (PFAS);** [Tavleen K. Kochar](#)¹; Megan R. Ogorchock¹; Gary L. Glish¹; ¹University of North Carolina, Chapel Hill, NC
- MP 136 **Investigating Degradation of Fluorinated Compounds in Water Using LC-Plasma Assisted Reaction Chemical Ionization-MS;** [Kunyu Zheng](#)¹; Joseph Lesniewski¹; Samuel White¹; Kaveh Jorabchi¹; ¹Georgetown University, Washington, DC
- MP 137 **The Removal of Microcystins from Water Using Treated Rice Husk;** Dilrukshika S. W. Palagama¹; Amila M. Devasurendra¹; David Baliu-Rodriguez¹; Jon R. Kirchoff¹; [Dragan Isailovic](#)¹; ¹The University of Toledo, Toledo, OH
- MP 138 **Unraveling Carbon Flow within Microbial Communities Using Stable Isotope Probing Multi-Omic Techniques;** [Mary S Lipton](#)¹; Marina A. Gritsenko¹; Samuel O. Purvine¹; Amy A. Boaro¹; Megan K. Nims¹; Alexandra Cory²; Krystin Riha¹; Thomas O. Metz¹; Young-Mo Kim¹; William C. Nelson¹; James J. Moran¹; ¹Pacific Northwest National Laboratory, Richland, WA; ²Florida State University, Tallahassee, FL
- MP 139 **Analysis of Dioxins Utilizing Time-of-Flight for Low Level Quantitation;** [Tim Conjelko](#)¹; Courtney Milner¹; Jeff Hollis¹; Matthew Curtis¹; ¹Agilent Technologies, Inc., Santa Clara, CA
- MP 140 **Standard Reference Materials for Measurements of Emerging Contaminants;** [Kevin M. Huncik](#)¹; Jessica L. Reiner²; John R. Kucklick²; ¹National Institute of Standards and Technology, Charleston, SC; ²NIST, Charleston, SC
- MP 141 **Mass Spectrometry-Based Investigations of Phytoremediation and Tertiary Water Treatment in the Sewanee Constructed Research Wetland;** [Jacqueline N. Langmo](#)¹; Anthony Wright¹; Tanisha Ghosh¹; W. Matthew Henderson²; Donovan Godbee¹; Devon Bouillion¹; Scott Torreano³; Deborah Mcgrath³; Marsha C. Black¹; Franklin E. Leach III¹; ¹University of Georgia, Athens, GA; ²Environmental Protection Agency, Athens, GA; ³The University of the South, Sewanee, TN
- MP 142 **Legacy and Emerging Perfluorinated Alkyl Substances in Water: Developing an SPE Method for LC-MS/MS Analysis;** Kari Organtini¹; Kenneth Rosnack¹; Doug Stevens¹; Euan Ross²; [Steven Lai](#)³; ¹Waters Corporation, Milford, MA; ²Waters Corporation, Wilmslow, United Kingdom; ³Waters Corporation, Beverly, MA
- MP 143 **Short Chain Chlorinated Paraffins (SCCPs) Analysis Using Negative Chemical Ionization (CI) and Low Energy EI by High-Resolution GC/Q-TOF;** Sofia Nieto¹; Matthew Curtis¹; [Nathan Eno](#)¹; Courtney Milner¹; Pierre Dumas²; ¹Agilent Technologies, Inc., Santa Clara, CA; ²Institut National de Santé Publique du Québec (INSPQ), Québec, QC
- MP 144 **Analysis of the Wastewater Effluent Samples to Identify Toxic Chemicals Using High-Resolution GC/Q-TOF;** Sofia Nieto¹; [Kai Chen](#)¹; Courtney Milner¹; Thomas Young²; ¹Agilent Technologies, Inc., Santa Clara, CA; ²University of California, Davis, Davis, CA
- MP 145 **Direct Analysis of Per- and Polyfluoroalkyl Substances (PFAS) in Ground, Surface and Waste Water by LC-MS/MS;** [Cristina C. Jacob](#)¹; Claudia P.B. Martins¹; Michael Volny¹; Alan R. Atkins²; Richard F. Jack³; ¹Thermo Fisher Scientific, San Jose, CA; ²Thermo Fisher Scientific, Hemel Hempstead, UK, Hemel Hempstead, United Kingdom; ³Thermo Fisher Scientific, Sunnyvale, California
- MP 146 **Trace Level Determination of Aniline Compounds in Water by Direct Aqueous Injection-UHPLC-MS/MS;** Mingli Zhu¹; Weifeng Zhang¹; [Lizhong Yang](#)²; Xiangdong Zhou²; Chengyuan Cai³; Feng Qin⁴; ¹Guangzhou Agricultural Products Quantity and Safety Supervisory Institute, Guangzhou, China; ²PerkinElmer Management(Shanghai) Co.,Ltd., Shanghai, China; ³PerkinElmer Management (Shanghai) Co., Ltd., Shanghai, China; ⁴PerkinElmer, Inc., Woodbridge, ON
- MP 147 **Semi-Automated Cleanup of Persistent Organic Pollutants in Environmental Samples - Complete Separation of PCDD/Fs and PCBs for Extracts in Toluene;** [Hamid Shirkhan](#)¹; Rudolf Addink¹; ¹Toxic Report, Watertown, MA
- MP 148 **How is β -Cyclocitral Formed in SPME GC/MS of a Cyanobacterium?;** Ryuji Yamashita¹; Keisuke Kanei¹; [Eri Yamauchi](#)¹; Koji Tomita²; Kiyomi Tsuji³; Ken-ichi Harada¹; ¹Meijo University, Nagoya, Japan; ²Aichi Prefectural Institute of Public Health, Nagoya, Japan; ³Kanagawa Prefectural Institute of Public Health, Chigasaki, Japan
- MP 149 **Poisoned Honey and Water: An Investigation into the Detection of Pesticides with a Novel Approach to SPE;** [Matthew Diplock](#)¹; Raquel Gonzalez de Vega¹; Andrew Minett²; Philip Doble³; ¹University of Technology Sydney, Sydney, Australia; ²Eprep Pty Ltd, Mulgrave, Australia; ³University of Technology Sydney, Sydney, Australia
- MP 150 **Analysis of Soil Extracts for Degradation Products of the Insensitive Munition DNAN via GC/MS-MS;** [Jeffrey Michael McGuire](#)¹; Mark Haley¹; Michael Simini¹; Roman Kuperman¹; ¹U.S. Army RDECOM Chemical & Biological Center, Aberdeen Proving Ground, MD
- MP 151 **Consequential Effects of Five Bisphenols Contaminated Microplastic Through Water and Simulated Intestinal Fluids: Implications for Human Health;** [Pengfei Wu](#)¹; Yuanyuan Tang²; Hangbiao Jin³; Zongwei Cai¹; ¹HongKong Baptist University, HongKong, China; ²Southern University of Science and Technology, Shenzhen, China; ³Zhejiang University of Technology, Hangzhou, China
- MP 152 **Device and Application of Real-Time VOCs Analysis in Air Based on ESI Mass Spectrometry;** [Jiancheng Yu](#)¹; Junliang Zhang¹; Keqi Tang¹; ¹Ningbo University, Ningbo, China
- MP 153 **Elucidating the Kinetics of Xanthates Decomposition in Mining Waters by Headspace Gas Chromatography-Mass Spectrometry;** [Kingsley Donkor](#)¹; Adrian Batista¹; William Primrose¹; ¹Thompson Rivers University, Kamloops, BC
- MP 154 **Aromatic Core Structure and Heteroatom Chemical Functionality Drive the Transformation of Petroleum into Water-Soluble Organic Matter;** [Sydney F Niles](#)^{1,2}; Martha L Chacón-Patiño¹; Huan Chen¹; Steven M Rowland¹; Donald F Smith¹; Christopher L. Hendrickson^{1,2}; Alan G. Marshall^{1,2}; Ryan P. Rodgers^{1,2}; ¹National High Magnetic Field Laboratory, Tallahassee, FL; ²Florida State University, Tallahassee, FL



- MP 155 **Development of Analysis and Purification Methods for Monitoring Dioxins in Sanitary Napkins**; Young Sang Kwon¹; Sung-Gil Choi¹; Seung-Min Lee¹; Dong Yeol Lee²; Sang Gon Kim²; Jong-Su Seo¹; ¹*Korea Institute of Toxicology, Munsan-eup, Jinju, South Korea*; ²*Gyeongnam Oriental Anti-aging Institute, Sancheong-gun, South Korea*
- MP 156 **Optimizing Extraction and Ionization Method for High Resolution Mass Spectrometry Analysis of Organic Compound**; Sung June Kim¹; Sunghwan Kim¹; ¹*Kyungpook National University, Daegu, South Korea*
- MP 157 **Rapid Non-Targeted Screening of Aqueous Environmental Samples Using Auto MS/MS**; Imma Ferrer¹; Daniel L. Sweeney²; E. Michael Thurman¹; Jerry A. Zweigenbaum³; ¹*University of Colorado Boulder, Boulder, CO*; ²*MathSpec, Inc., Arlington Heights, IL*; ³*Agilent Technologies, Wilmington, DE*
- MP 158 **Analysis of Perfluorinated Compounds in Drinking and Waste Water Using Sequential/Parallel Automated Solid Phase Extraction Using EPA Method 537.1**; Matthew Falkenstein¹; Tom Hall¹; ¹*Fluid Management Systems, Watertown, MA*
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- MP 160 **Electron Ionization Mass Spectrometry as Detection System for Supercritical Fluid Chromatography to Increase Identification Power of Semi-Volatile Compounds**; Francesca Rigano¹; Roberta La Tella¹; Paola Dugo^{1,2,3}; Luigi Mondello^{1,2,3}; ¹*Chromaleont SrL, Messina, Italy*; ²*University of Messina, Messina, Italy*; ³*University Campus Bio-Medico of Rome, Rome, Italy*
- MP 161 **Analysis and Quantitation of Polyfluorinated Alkyl Substances (PFAS) in EPA Method 537.1 Using High Resolution Accurate Mass Spectrometry**; Brahm Prakash¹; Christopher Gilles¹; Evelyn Wang¹; Jerry Byrne II¹; Yuka Fujito¹; William Lipps²; ¹*Shimadzu Scientific Instruments, Inc., Columbia, Maryland*; ²*Eurofins Eaton Analytical, 750 Royal Oaks Drive, Monrovia, CA*
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- MP 163 **Approaching Translational Proteomics: Accurate Quantification of >200 Histone Modifications at a Rate of 50 Samples Per Hour**; Simone Sidoli¹; Yekaterina Kori¹; Mariana Lopes²; Zuo-Fei Yuan¹; Hee Jong Kim¹; Katarzyna Kulej¹; Kevin A. Janssen¹; Laura M. Agosto¹; Julia P.C. Cunha²; Andrew J. Andrews³; Benjamin A. Garcia¹; ¹*University of Pennsylvania, Philadelphia, PA*; ²*Instituto Butantan, Sao Paulo, Brazil*; ³*Fox Chase Cancer Center, Philadelphia, PA*
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- MP 165 **Combining Bioorthogonal Chemistry and Proteomic Profiling to Study the PTM-Specific Interactome of Linker Histone H1**; Eva Hoellmueller^{1,2,3}; Martin Scheffner^{1,2}; Andreas Marx^{1,3}; Florian Stengel^{1,2}; ¹*Konstanz Research School Chemical Biology, Konstanz, Germany*; ²*Department of Biology, University of Konstanz, Konstanz, Germany*; ³*Department of Chemistry, University of Konstanz, Konstanz, Germany*
- MP 166 **Enhanced Detection of 5-methyl-2'-deoxycytidine, 5-hydroxymethyl-2'-deoxycytidine, 5-methylcytidine and 5-hydroxymethylcytidine in Human Urine Using HILIC-MS/MS**; Cheng Guo; *Zhejiang University, Hangzhou, China*
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- MP 168 **Epiroteomic Analysis of Archival Formalin-Fixed Paraffin-Embedded Tumor Tissue for Interrogating Oncogenic Mechanisms in Rare Sarcomas**; Dylan Marchione¹; Ilyana Ilieva¹; Benjamin A Garcia¹; John B Wojcik¹; ¹*The University of Pennsylvania, Philadelphia, PA*
- MP 169 **Epigenetics of Alzheimer's disease: Global Chromatin Profiling for Monitoring Histone Post-Translational Modifications in Induced Pluripotent Stem Cell Models**; James Mullahoo¹; Shawn Egri¹; Tak Ko²; Katherine C. DeRuff¹; Deborah Dele-Oni¹; Xiaodong Lu¹; Malvina Papanastasiou¹; Jennie Young²; Li-Huei Tsai²; Jacob D. Jaffe¹; ¹*Broad Institute, Cambridge, MA*; ²*Massachusetts Institute of Technology, Cambridge, MA*
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- MP 174 **Novel UHPLC-MRM-MS Approach Allows for Absolute Quantification of Histone PTMs in as Little as 20 Minutes**; Joseph Cesare¹; Zuofei Yuan¹; Steven Zhao¹; Peder Lund¹; Josue Baeza¹; Yekaterina Kori¹; Simone Sidoli¹; Hee Jong Kim¹; Hyoungjoo Lee¹; Kathryn E. Wellen¹; Benjamin A. Garcia¹; ¹*University of Pennsylvania, Philadelphia, PA*
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- MP 175 **Screening of Pesticide Residues in Food by Using High-Throughput GC-MS/MS System with Fast GC Condition**; Junkei Kou¹; Kiyotaka Konuma¹; Kouji Okuda²; Kazuaki Murayama¹; Yoshihisa Ueda¹; ¹*JEOL Ltd, Akishima, Japan*; ²*JEOL USA, Inc., Peabody, MA*
- MP 176 **Quantitation of Multi Residues Antibiotics in Milk Using LC-MS/MS**; Chandrasekar Madhappan¹; Dilip Reddy¹; Manoj G. Pillai¹; Jianru Stahl-Zeng²; ¹*SCIEX, Gurgaon, India*; ²*SCIEX, Darmstadt, Germany*
- MP 177 **Screening of Multiclass Illegal Adulterants in Supplements and Spices via Extracted Common Ion Chromatograms and Neutral Loss Scan by UHPLC-Q/TOF-MS**; Jisu Hur¹; Beom-Hee Kim¹; Ki Jung Paeng²; Jongki Hong¹; ¹*Kyung Hee University, Seoul, South Korea*; ²*Yonsei university, wonju, South Korea*



- MP 178 **Fast and Simultaneous LC/MS/MS Analysis for Veterinary Drugs in Meat Combined with STQ method;** Natsuyo Asano¹; Eishi Imoto¹; Mami Okamoto¹; Mikie Shima²; Jun Watanabe¹; ¹Shimadzu corp., Kyoto, Japan; ²AiSTI Science Co., Ltd., Wakayama, Japan
- MP 179 **Rapid Authentication of Fish Species Using Peptide Probes Isolated in the ProTrap XG;** Alan A. Doucette¹; Jessica L. Nickerson¹; Katie Halliday¹; Joshua Turner¹; ¹Department of Chemistry, Dalhousie University, Halifax, NS
- MP 180 **Supercritical Fluid Chromatography Coupled to Tandem Mass Spectrometry for the Analysis of Pesticide Residues in Dried Spices;** Víctor Cutillas¹; María Murcia-Morales¹; María del Mar Gómez-Ramos¹; Ann-Christin Niehoff²; Stéphane Moreau²; Amadeo R. Fernández-Alba¹; ¹European Union Reference Laboratory for Pesticide Residues in Fruits & Vegetables. University of Almería, Agrifood Campus of International Excellence (ceiA3) Department of Hydrogeology and Analytical Chemistry, Almería, Spain; ²Shimadzu Europa GmbH, Duisburg, Germany
- MP 181 **EU Compliant Routine Quantitative Dioxin, Dioxin-Like PCB and Marker PCB Analysis by GC-MS/MS Using an Advanced Electron Ionisation Source;** Dominic Roberts¹; Alexander Schachtele²; Richard Law³; Tim Anderson⁴; Adam Ladak⁴; Cristian Cojocariu³; ¹Thermo Fisher Scientific, Runcorn, United Kingdom; ²European Union Reference Laboratory for Halogenated POPs in feed and food, Freiburg, Germany; ³Thermo Fisher Scientific, Tudor Road, United Kingdom; ⁴Thermo Fisher Scientific, Austin, TX
- MP 182 **Comprehensive Identification of Migrating Compounds from Plastic Food Packaging Materials Using High Resolution Accurate Mass Spectrometry;** María José Gómez Ramos¹; Anna Bauer²; Ana Lozano²; Amadeo R. Fernández-Alba²; ¹University of Almería, Almería, Spain; ²University of Almería, Almería, Spain
- MP 183 **Developing a Robust LC-MS/MS Method for the Determination of Anionic Polar Pesticides in a Range of Food Stuffs without Derivatization;** Dimple Shah¹; Benjamine Wuyts²; Euan Ross²; Simon Hird²; Keil Brinster¹; Kenneth Rosnack¹; Tammy Hicks¹; ¹Waters Corporation, Milford, MA; ²Waters Corporation, Wilmslow, United Kingdom
- MP 184 **A New Automated Approach for the Determination of Mycotoxins in Cereals Using Online SPE-LC-MS/MS;** Peter Ringeling¹; Boris Bartolec¹; Cornelis Tump¹; Gertjan Merjenburgh¹; Florian Van der Hoeven¹; Jamie Foss²; ¹Spark Holland, Emmen, Netherlands; ²PerkinElmer, Shelton, Connecticut
- MP 185 **Multiresidue Analysis of Pesticides in Turmeric (Curcuma longa) Powder by GCMS/MS Using QuEChERS' Extraction Method;** Sunil Singh¹; Durvesh Sawant^{2,3}; Sanket Anand Chiplunkar²; Nitish Suryawanshi²; Satyendra Thakur¹; Prashant Hase²; Aseem Wagle²; Dheeraj Handique²; Jitendra Kelkar²; Pratap Rasam²; Ajit Datar²; ¹Shimadzu Analytical (India) Pvt. Ltd., New Delhi, India; ²Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India; ³Ramnarain Ruia College, Mumbai, India
- MP 186 **Determination of Coumarin in Electronic Cigarette Liquids by UHPLC Coupled with Isotope Dilution Tandem Mass Spectrometry;** Jingcun Wu¹; Erasmus Cudjoe¹; Xia Geng²; Joshua Ye³; Feng Qin¹; ¹PerkinElmer Inc., Woodbridge, ON; ²PerkinElmer Management(Shanghai)Co.,Ltd., Shanghai, China; ³Perkin Elmer Canada, Woodbridge, ON
- MP 187 **Application of a Novel Background Exclusion Data-Dependent Acquisition Method to Retrospective Analysis of Target Pesticides and Unknown Xenobiotics in Food;** Chunyan Zhu¹; Guo-yin Lai²; Ying Jin¹; Guoqiang Liu³; Niusheng Xu³; Caisheng Wu¹; Mingshe Zhu⁴; ¹Xiamen University, Xiamen, China; ²Xiamen Customs, Xiamen, China; ³Thermo Fisher Scientific, Shanghai, China; ⁴MassDefect Technologies, Princeton, NJ
- MP 188 **High Throughput Target and Suspect Pesticide Analysis Using a New LC/Q-TOF Screener Software;** Karen E. Yannell¹; Kai Chen²; ¹Agilent Technologies, Santa Clara, CA; ²Agilent Technologies, Inc., Santa Clara, CA
- MP 189 **Up in Vape: What is in my E-Juice Other than Nicotine, Propylene Glycol, and Glycerin;** Ron Honnold¹; Matthew Curtis¹; ¹Agilent Technologies, Inc., Santa Clara, CA
- MP 190 **Analysis of Patulin in Fruit Juices and Extracts Using Liquid Chromatography Triple Quadrupole Mass Spectrometry;** Claudia P.B. Martins¹; Cristina C. Jacob¹; Michael Volny¹; Mary L. Blackburn¹; ¹Thermo Fisher Scientific, San Jose, CA
- MP 191 **A Fast, Sensitive and Comprehensive Assay to Quantify Pesticide Residues in Dietary Supplements Using GC/MS/MS Coupled with QuEChERS Extraction Method;** Aihua Liu¹; Abhijit Ghosh¹; Spencer Carter¹; ¹Dyad Labs, Salt Lake City, UT
- MP 192 **Quantitative Analysis of Aminoglycoside Veterinary Drugs in Solid Milk Products by LC-MS/MS;** Benjamin L. Oyler¹; James B. Wittenberg²; Christine H. Parker¹; ¹FDA, College Park, MD; ²Alcohol and Tobacco Tax and Trade Bureau, Beltsville, MD
- MP 193 **Decomposition and Species Identification in Salmon by High-Resolution Mass Spectrometry with Multivariate Analysis;** Randy Self¹; Michael McLendon¹; Christopher Lock¹; ¹U.S. FDA, Bothell, WA
- MP 194 **High Throughput Determination of Multi-Class Toxic Alkaloids in Food by High Performance Liquid Chromatography-Tandem Mass Spectrometry;** Guoying Lai¹; Lijian Wu¹; Dunming Xu¹; Zhigang Zhang¹; Meiling Lu²; ¹Technique Center of Xiamen Customs, Xiamen, China; ²Agilent Technologies (China) Limited, Beijing, China
- MP 195 **Development and Validation of a New Sensitive and Rapid UPLC-MS-MS Method to Determine Acrylamide in Coffee;** Yilong Zheng¹; Zhitian Zhang¹; Jillian O'connell¹; Junsuo Li¹; ¹Intertek, Champaign, IL
- MP 196 **Characterization of Farmer's Cheese with LC-MS/(MS) for Authenticity Purposes;** Henk W. Gerritsen¹; Robert Jan A.N. Lamers²; Martin Alewijn¹; Marco H. Blokland¹; Monique G.E.G. Bremer¹; Ioana M. Barbu¹; ¹RIKILT Wageningen UR, Wageningen, Netherlands; ²Abundnz B.V., Woerden, Netherlands
- MP 197 **Analysis of Odor Components in Fish by Shimadzu Off-Flavor System;** yong wang¹; Jun Fan²; ¹Shimadzu (China) Co.,Ltd. Beijing Branch, Beijing, China; ²Shimadzu (China) Co., Ltd. Shanghai Branch, Shanghai, China
- MP 198 **Off-Flavor System of Shimadzu Analyzes the Odor Components in Edible Oil;** Liu Xiaohua; ¹Shimadzu (China) Co., Ltd., Guangzhou, China
- MP 199 **Discrimination of Soybean Oil and Olive Oil by Benchtop Linear MALDI-TOF;** Dun Junling; ¹Shimadzu (China) Co., Ltd., Shanghai, China
- MP 200 **Toxin Profiling in Fish Samples from the Indian Ocean Implicated in Ciguatera-Like Poisoning;** Ann Abraham¹; Katherine Baltzer¹; Kathleen El Said¹; Kyle Andrews¹; ¹Division of Seafood Science and Technology, FDA, Dauphin Island, AL
- MP 201 **A High Profile: Detection and Identification of Synthetically-derived Psychoactive Material through Sorbent-Facilitated Headspace Mass Spectral Analysis and Chemometrics;** Meghan G. Fogerty¹; Rabi A. Musah¹; ¹University at Albany-SUNY, Albany, NY

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- MP 201 **A High Profile: Detection and Identification of Synthetically-derived Psychoactive Material through Sorbent-Facilitated Headspace Mass Spectral Analysis and Chemometrics;** Meghan G. Fogerty¹; Rabi A. Musah¹; ¹University at Albany-SUNY, Albany, NY



- MP 202 **Investigation of Early Death-Induced Changes in Rat Brain by SPME-HPLC-HRMS: *in vivo* Versus Post Mortem Comparative Study**; Sofia Lendor¹; Mariola Olkowicz¹; Ezel Boyaci¹; Miao Yu¹; Mustansir Diwan²; Nathaly Reyes-Garcés¹; German Augusto Gómez Ríos¹; Clement Hamani²; Janusz Pawliszyn¹; ¹Department of Chemistry, University of Waterloo, Waterloo, ON; ²Neuroimaging Research Section, Centre for Addiction and Mental Health, Toronto, ON
- MP 203 **Fast Screening of Explosives by Direct Analysis in Real Time Mass Spectrometry**; Mengliang Zhang¹; Virginia L Benefield¹; Jared Frazier¹; ¹Middle Tennessee State University, Murfreesboro, TN
- MP 204 **Assessing Peptide Profiling Reproducibility of Single Source Human Head Hair**; Maria Lawas¹; Katherine F. Jones¹; Katelyn E. Mason²; Deon S. Anex²; Traci L. Carlson¹; Luisa V. Forger¹; Brian A. Eckenrode³; Bradley Hart²; Joseph Donfack³; ¹Counterterrorism and Forensic Science Research Unit, Visiting Scientist Program, Federal Bureau of Investigation Laboratory Division, Quantico, VA; ²Forensic Science Center, Lawrence Livermore National Laboratory, Livermore, CA; ³Counterterrorism and Forensic Science Research Unit, Federal Bureau of Investigation Laboratory Division, Quantico, VA
- MP 205 **Analytical Separation of Isomeric U-Series Compounds Using Liquid Chromatography Tandem Mass Spectrometry**; Melissa F. Fogarty¹; Amanda L.A. Mohr²; Francis X. Diamond³; Barry K Logan^{2,3}; ¹Center for Forensic Science Research and Education, Willow Grove, PA; ²CFSRE, Willow Grove, PA; ³NMS Labs, Willow Grove, PA
- MP 206 **Liquid Chromatography-High-Resolution Mass Spectrometry for the Determination of Cannabinoids, Cannabinoid-Metabolites, and Amphetamine-Type Stimulants in Human Hair**; Sunjoo Kim¹; Yongho Shin¹; Won-gu Choi¹; Hye Suk Lee¹; ¹The Catholic University of Korea, Buchen, South Korea
- MP 207 **Comparing the Efficiencies of Common Extraction Methods For Explosive Residues Off Various Surfaces Using Gas Chromatography/Mass Spectrometry**; Shannon Lamy¹; Alyssa Marsico¹; ¹University of New Haven, West Haven, CT
- MP 208 **On-Site Identification of Forensic Evidence by Novel Coiled Micro-Extraction Sampling Device for Portable GC/MS Instrumentation**; Zachary E Lawton¹; Leah Rynearson²; Marisa San Antonio²; Sara M Davis²; Sarah Goda²; Meghann McMahon³; Pauline Leary⁴; Koby Kizzire²; Brooke Kammrath²; ¹PerkinElmer, Shelton, CT; ²University of New Haven, West Haven, CT; ³Wisconsin State Police, Milwaukee, WI; ⁴Federal Resources, Stevensville, MD
- MP 209 **High Resolution Designer Drug Screening Using a High-Sensitivity Q-TOF Mass Spectrometer and an Extended Tandem Mass Spectrum Library**; Jeff Dahl¹; Rachel Lieberman²; Joseph Kahl³; Alex Giachetti³; ¹Shimadzu, Columbia, MD; ²Shimadzu Scientific Instruments, Inc., Columbia, MD; ³Miami-Dade Medical Examiner Department, Miami, FL
- MP 210 **Identification of Human Haemoglobin Variants through Advanced Forensic Mass Spectrometry of Blood**; Cameron Heaton¹; Laura Cole¹; Richard R McCole²; Jason Eyre³; Simona Francese¹; ¹BMRC, Sheffield Hallam University, Sheffield, United Kingdom; ²DSTL, Porton Down, Salisbury, United Kingdom; ³BMS Haemolysis Lab, Haematology Department, Sheffield Teaching Hospital, Sheffield, United Kingdom
- MP 211 **An Automated Ignitable Liquid Analysis Workflow for Forensic Laboratories**; Troy J Ernst¹; Scott J Campbell²; John H Moncur²; ¹Michigan State Police - Grand Rapids Laboratory, Grand Rapids, MI; ²SpectralWorks Limited, Runcorn, United Kingdom
- MP 212 **Peptide Spectral Libraries for Purified Ricin and Forensically Relevant Castor Seed Extracts**; Isabelle G. O'Bryon¹; Abigail E. Tucker¹; Brooke L.D. Kaiser¹; Eric Merkley¹; Karen L. Wahl¹; ¹Pacific Northwest National Laboratory, Richland, WA
- MP 213 **A method for Simultaneous Targeted and Non-Targeted LC-HRMS/MS Drug Screening in Forensic Toxicology**; Jason E Schaff¹; Preston C Lowe¹; Madeline A Montgomery¹; Cynthia L Morris-Kukoski¹; ¹FBI Laboratory Chem Unit, Quantico, VA
- MP 214 **Use of Image Quality Scores to Determine Fingerprint Age in MALDI imaging**; Madison L Thomas¹; Paige Hinners¹; Young Jin Lee¹; ¹Iowa State University, Ames, IA
- MP 215 **Thread Spray Mass Spectrometry for Direct Analysis of Hemoglobin in Whole Blood**; Sierra Jackson¹; Abraham K. Badu-Tawiah¹; ¹The Ohio State University, Columbus, OH
- MP 216 **Rapid and Quantifiable Screening Method for 64 Drugs in Human Blood by Direct Probe Ionization/Tandem Mass Spectrometry (DPiMS)**; Tasuku Murata¹; Shinji Funatsu¹; Koretsugu Ogata¹; Hitoshi Tsuchihashi²; Yumi Hayashi^{3,4}; Kei Zaitzu^{2,4}; ¹Shimadzu Corporation, Kyoto, Japan; ²Department of Legal Medicine and Bioethics, Nagoya University Graduate School of Medicine, Nagoya, Japan; ³In Vivo Real-Time Omics Laboratory, Institute for Advanced Research, Nagoya University, Nagoya, Japan; ⁴Pathophysiological Laboratory Sciences, Department of Radiological and Medical Laboratory Sciences, Nagoya University Graduate School of Medicine, Nagoya, Japan
- MP 217 **Automated immunoaffinity purification of large peptides followed by LC-MS(/MS) analysis**; Monica Mazzarino¹; Filippo Martinelli¹; Marta Senofonte¹; Xavier de la Torre¹; Francesco Botrè^{1,2}; ¹Antidoping laboratory, Rome, Italy; ²Department of Experimental Medicine, "Sapienza" University of Rome, Rome, Italy
- MP 218 **Use of IRMPD Spectroscopy to Characterize Derivatives of Aldehydes Considered Emerging Explosive Threat Compounds**; Connor J Graca¹; Luke Metzler¹; Theodore Corcovilos¹; Giel Berden²; Jonathan Martens²; Jos Oomens^{2,3}; Michael Van Stipdonk¹; ¹Duquesne University, Pittsburgh, PA; ²Radboud University Nijmegen, Institute for Molecules and Materials, FELIX Facility, Nijmegen, Netherlands; ³University of Amsterdam, Amsterdam, Netherlands
- MP 219 **Q-Exactive Parameter Optimization for Maximum Signal Intensity when Using LDTD**; Sarah Demers¹; Serge Auger¹; Jean Lacoursière¹; Pierre Picard¹; ¹Phytronix Technologies, Quebec, QC
- MP 220 **Evaluation of Micro Volume Sample Preparation Technology Newly Designed for Forensic Toxicology with High Resolution Accurate Mass Spectrometry**; Eishi Imoto¹; Yujin Natori²; Jun Watanabe¹; Hitoshi Tsuchihashi²; Kei Zaitzu²; Ichiro Hirano¹; ¹Shimadzu corp., Kyoto, Japan; ²Department of Legal Medicine & Bioethics, Nagoya University Graduate School of Medicine, Nagoya, Japan
- MP 221 **Counterfeit Medicines Identification: A Comparison of Simplified APCI and EI Based MS Methods**; Sangeeta Tanna¹; Rachel Armitage¹; John Ogwu¹; Graham Lawson¹; ¹De Montfort University, Leicester, United Kingdom
- MP 222 **Analysis of Cosmetic Products for Evidentiary Value via Paper Spray and Paper Cone Spray Ionization-Mass Spectrometry**; Abigail M. Poehls¹; Shahnaz Mukta¹; Christopher C. Mulligan¹; ¹Illinois State University, Normal, IL
- MP 223 **Rapid Profiling of Authentic Forensic Evidence via Paper Cone Spray Ionization Employed on Portable MS Instrumentation**; Ashley R. Stelmack¹; William L. Fatigante¹; Shahnaz Mukta¹; Christopher C. Mulligan²; ¹Illinois state university, Normal, IL; ²Illinois State University, Normal, IL



- MP 224 **The Performance of Nanoparticle-Modified Paper Substrates Employed as Surface Transfer Swabs for Combined SERS and PSI-MS Investigation;** Trevor J. McDaniel¹; Noah W. McClurg¹; William L. Fatigante¹; Jun-Hyun Kim¹; Jeremy D. Driskell¹; Christopher Mulligan²; ¹Illinois state university, Normal, IL; ²Illinois State University, Normal, IL
- MP 225 **Electron Ionization (EI) Fragmentation Studies of Reduced Bipyridyl Herbicides: Towards a Reliable Quantitative Approach for Postmortem Samples;** Carlos González¹; Marielos Arias¹; Diego Arias¹; ¹Sección de Toxicología, Departamento de Ciencias Forenses, San Joaquín de Flores, Costa Rica
- MP 226 **Chemical Differentiation of CITES-Protected Dalbergia Timber Using DART/QToF and TSP/GC/MS;** Dayue Shang¹; Pamela Brunswick¹; Jeffrey Yan¹; Joy Bruno¹; Philip Evans²; Graham Van Aggelen¹; Marcus Kim³; ¹Environment and Climate Change Canada, North Vancouver, BC; ²University of British Columbia, Vancouver, BC; ³Agilent Technologies, Inc., Wilmington, DE
- MP 227 **Simultaneous Analysis of 260 Pesticides in Human Urine Using Scaled-Down QuEChERS Approach and Tandem Mass Spectrometry;** Yongho Shin¹; Sunjoo Kim¹; Won-gu Choi¹; Hye Suk Lee¹; ¹The catholic university of korea, Bucheun, South Korea
- MP 228 **Application for Forensic Analysis: Discrimination of Fibers Using Trace Organic Additive and Pyrolyzate Marker;** Chikako Takei¹; Kenichi Yoshizawa¹; Shinji Azuma²; ¹BioChromato, Inc., Fujisawa, Japan; ²BioChromato USA, San Diego, California
- MP 229 **Fragmentation Pathways of α -pyrrolidinophenone Derivative Synthetic Cathinones;** Jay Tyler Davidson¹; Zachary J. Sasiene²; Younis Abiedalla³; C. Randall Clark³; Glen P. Jackson^{1,2}; ¹Department of Forensic and Investigative Science, West Virginia University, Morgantown, WV; ²C. Eugene Bennett Department of Chemistry, West Virginia University, Morgantown, West Virginia; ³Department of Drug Discovery and Development, Harrison School of Pharmacy, Auburn University, Auburn, AL
- FUNDAMENTALS: ION ACTIVATION/DISSOCIATION**
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- MP 230 **Peptide Sequence Influence on the Differentiation of Valine and Norvaline by Hot Electron Capture Dissociation;** Wendy Zhong¹; Zhidan Liang²; Xiang Yu³; ¹Merck, Rahway, NJ; ²Amgen Inc., Boston, MA; ³Merck & Co., West Point, PA
- MP 231 **Analysis of Phenetole in its First Excited State and Ionic Ground State: Effects of the Side Chain;** Niklas Helle¹; Tassilo Muskat¹; Jurgen Grotemeyer¹; ¹Christian-Albrechts-Univ, Kiel, Germany
- MP 232 **Surface-Induced Dissociation of Protein Complexes in an FT-ICR Mass Spectrometer: Experimental and Simulated Performance;** Dalton Snyder^{1,2}; Jing Yan³; Vicki Wysocki^{1,2}; ¹The Ohio State University, Columbus, OH; ²Resource for Native Mass Spectrometry Guided Structural Biology, Columbus, OH; ³Washington University, St. Louis
- MP 233 **Gas-Phase Dissociation of Imidazolium and Benzimidazolium Cations: Effects of Substituent Identity;** Maleesha De Silva¹; Amanda Patrick¹; ¹Mississippi State University, Starkville, MS
- MP 234 **High Energy Collision-Induced Dissociation of Biological Peptides;** Xinyao Jing¹; Carolyn J Cassady¹; ¹The University of Alabama, Tuscaloosa, AL
- MP 235 **Comparison of Reagent Gas for Charge Transfer Dissociation (CTD) Mass Spectrometry of Peptides and Oligosaccharides;** Zachary J. Sasiene¹; Praneeth M. Mendis¹; Glen P. Jackson^{1,2}; ¹C. Eugene Bennett Department of Chemistry, West Virginia University, Morgantown, WV; ²Department of Forensic and Investigative Science, West Virginia University, Morgantown, WV
- MP 236 **Gas Phase Reactions of Heptamethine Cyanine Dyes Using Femtosecond-Laser-Pulse Induced Photodissociation and Collision-Induced Dissociation;** Elena Mitrofanov¹; Tassilo Muskat¹; Jurgen Grotemeyer¹; ¹Christian-Albrechts-Univ, Kiel, Germany
- MP 237 **Structural Characterization of Intact Proteins Using Electron Capture Dissociation within an Ion Mobility Enabled TOF;** Jonathan P. Williams¹; Lindsay J. Morrison²; Chris Hughes³; Jeffery M. Brown³; Joseph S. Beckman⁴; Valery G. Voinov⁴; ¹Waters Corporation, Wilmslow, United Kingdom; ²Waters Corporation, Beverly, MA; ³Waters Corporation, Wilmslow, United Kingdom; ⁴e-Msion Inc., Corvallis, OR
- MP 238 **A Comparison of Negative Ion Radical-Driven Dissociation and Collision-Induced Dissociation on Acidic Peptides;** Can Cui¹; Chelsea L. Mcmillen¹; Carolyn J. Cassady¹; ¹The University of Alabama, Tuscaloosa, AL
- MP 239 **Multiple-Stage Tandem Mass Spectrometry of Peptide Radical Ions in the Omnitrap Platform;** Mariangela Kosmopoulou¹; Dimitris Papanastasiou¹; Roman Zubarev²; ¹Fasmatech, Athens, Greece; ²Karolinska Institutet, Stockholm, Sweden
- MP 240 **Oligosaccharides – Suppression of Metal-Salt Induced Adducts Using Electrospray-Ionization and SORI-CID Fragmentation;** Volker Iwan¹; Tassilo Muskat¹; Jurgen Grotemeyer¹; ¹Christian-Albrechts-Univ, Kiel, Germany
- MP 241 **Formation of Non-Zwitterionic π -Centered Glycylglycyltryptophan Radical Cations during the Gas-Phase Dissociation of Zwitterionic Copper(II)-GXW Complexes: Structural, Mechanistic, and Photodissociation Spectroscopic Inves;** Yinan Li¹; mengzhu li¹; Chi Kit Andy Siu²; Jonathan Martens³; Jos Oomens³; Keung Ivan Chu¹; ¹Department of Chemistry, The University of Hong Kong, Hong Kong, Hong Kong; ²Department of Chemistry, City University of Hong Kong, Hong Kong, Hong Kong; ³FELIX Laboratory, Institute for Molecules and Materials, Nijmegen, Netherlands
- MP 242 **Isomeric α -Carbon- and π -Centered Glycylglycyltryptophan Radical Cations and their Dissociation Product Ions: Structural, Energetic, Mechanistic, and Spectroscopic Investigations;** Mengzhu Li¹; Yinan Li¹; Chi Kit Andy Siu²; Jonathan Martens³; Jos Oomens³; Keung Ivan Chu²; ¹Department of Chemistry, The University of Hong Kong, Hong Kong, Hong Kong; ²Department of Chemistry, City University of Hong Kong, Hong Kong, Hong Kong; ³FELIX Laboratory, Institute for Molecules and Materials, Nijmegen, Netherlands
- MP 243 **Understanding the Perplexing and Interesting Pathways of Peptoid Fragmentation;** Yadwinder Singh Mann¹; Yuntao Zhang¹; Jianhua Ren¹; ¹University of the Pacific, Stockton, CA
- MP 244 **Accelerating Ion-Molecule Reactions Using Supplemental RF-Activation in a Linear Ion Trap;** Berwyck L. J. Poad¹; Reuben S. Young¹; David L. Marshall¹; Stephen J Blanksby¹; ¹Queensland University of Technology, Brisbane, Australia
- MP 245 **The HDX Approach to Evidence the Stepwise Character of Controlled Enantioselective Reduction of Copper (II) Complexes with Polar Amino-Acids, Application;** Ekaterina Darij¹; Annelaure Damont²; Denis Lesage³; Sandra Alves³; Alain Perret¹; Yves Gimbert⁴; François Fenaille²; Jean-Claude Tabet^{2,3}; ¹Génomique métabolique, Genoscope, Institut François Jacob, CEA, CNRS, Univ Evry, Université Paris-Saclay, Evry, France; ²SPI, LEMM, CEA, INRA, Université Paris Saclay, Gif-sur-Yvette, France;



- ³CNRS, Institut Parisien de Chimie Moléculaire, Sorbonne Université, IPCM, Paris, France; ⁴Université Grenoble Alpes and CNRS, DCM (UMR 5250), Grenoble, France
- MP 246 **Novel C α -C β Cleavage of N-terminal Phenylalanine Residues of Tyrosine-Containing Peptide Radical Cations: Structural, Mechanistic, and Photodissociation Spectroscopic Investigations;** Wai Kit Tang¹; Xiaoyan Mu²; Naiping Dong²; Jonathan Martens³; Daniel Michael Spencer²; Mengzhu Li²; Jos Oomens³; Chi Kit Andy Siu¹; Ivan K. Chu⁴; ¹Department of Chemistry, City University of Hong Kong, Hong Kong, Hong Kong; ²Department of Chemistry, University of Hong Kong, Hong Kong, Hong Kong; ³FELIX Laboratory, Institute for Molecules and Materials, Nijmegen, Netherlands; ⁴University of Hong Kong, Hong Kong, Hong Kong
- MP 247 **Hydrogen Atom Attachment to the Histidine and Tryptophan Containing Peptides in Gas-Phase;** Daiki Asakawa¹; Hidenori Takahashi²; Shinichi Iwamoto²; Koichi Tanaka²; ¹AIST, Tsukuba, Japan; ²Shimadzu corp., Kyoto, Japan
- MP 248 **Trends from >10,000 Assigned Fragment Ions in Native Top-Down Mass Spectrometry;** Ashley Ives¹; Henrique Seckler¹; Ryan T Fellers¹; Luis F. Schachner²; Steven Matthew Patrie¹; Neil L Kelleher¹; ¹Northwestern University, Evanston, IL; ²Northwestern University, Evanston, IL
- MP 249 **Charge Carrier and Charge State Effects in Free Radical Initiated Peptide Sequencing (FRIPS);** Eunju Jang¹; Gabriela Grigorean¹; Nicholas B. Borotto¹; Kristina Hakansson¹; ¹University of Michigan, Ann Arbor, MI
- MP 250 **Implementation and Characterization of an RF Ion Funnel-Based Surface-Induced Dissociation (SID) Device on a Q-IM-TOF Platform;** Benjamin J Jones^{1,2}; Alyssa Q. Stiving^{1,2}; Joshua D. Gilbert¹; Zachary L. VanAernum^{1,2}; Sophie R. Harvey^{1,2}; ¹The Ohio State University, Columbus, OH; ²Resource for Native Mass Spectrometry Guided Structural Biology, The Ohio State University, Columbus, OH
- MP 251 **Evidence for Reversible Internal Hydride/Deuteride Transfers from Sodiated Deprotonated Fructose-6-Phosphate and Arginine Complex with Solvated Salt Structure;** Ekaterina Daryi¹; Sandra Alves²; Yves Gimbert³; Alain Perret¹; François Fenaille⁴; Jean-Claude Tabet^{2,4}; ¹Génomique métabolique, Genoscope, Institut François Jacob, CEA, CNRS, Univ Evry, Université Paris-Saclay, Evry, France; ²CNRS, Institut Parisien de Chimie Moléculaire, Sorbonne Université, IPCM, Paris, France; ³Université Grenoble Alpes and CNRS, DCM (UMR 5250), Grenoble, France; ⁴SPI, LEMM, CEA, INRA, Université Paris Saclay, Gif-sur-Yvette, France
- MP 252 **An Orthoester Derivatization Strategy for the Structure Elucidation of Vicinal Diols;** Renzo A Samame¹; Chengli Zu¹; Daniel Knueppel¹; Jeffery Gilbert¹; ¹Corteva Agriscience, Indianapolis, IN
- MP 253 **Collision-Induced Dissociation of Proton-Bound Base Pairs of 1-Methylcytosine with N-Methylguanines;** Sang Yun Han¹; Jeong Ju Park¹; ¹Gachon University, Seongnam, South Korea
- MP 254 **Dissociation Studies of Astrobiologically Relevant Nucleobase Anions;** Alexandra A Dobbs¹; Bryan E Metz¹; Diego T Novoa¹; Aaron R Wegener²; Callie A Cole¹; ¹Fort Lewis College, Durango, CO; ²Texas A&M University, College Station, TX
- MP 255 **Fragmentation of Deprotonated 7- & 9-Methylguanine in an Astrochemical Context;** Diego T. Novoa¹; Aaron R. Wegener^{1,2}; Alexandra A. Dobbs¹; Callie A. Cole¹; ¹Fort Lewis College, Durango, CO; ²Texas A&M University, College Station, TX
- FUNDAMENTALS: ION MOLECULE, ION/ION, ION/ELECTRON INTERACTIONS**
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- MP 256 **An In-Vitro Study of Aromatic Stacking of Drug Molecules;** Ludovic Muller¹; Shelley N. Jackson¹; Amina S. Woods¹; ¹NIH/NIDA-IRP, Baltimore, MD
- MP 257 **A Gas-phase Reactivity Study of Distonic Phenylcarbenes;** Erlu Feng¹; Zaikuan Yu¹; Jacob Milton¹; Tinh Hoang¹; Hilkka Kenttämää¹; ¹Purdue University, West Lafayette, IN
- MP 258 **Surface Interaction of Selected Transition Metals and Semiconductors with H2 Plasma Generated Species;** Joshua Rieger¹; Kai Kroll¹; Hendrik Kersten¹; Thorsten Benter¹; ¹University of Wuppertal, Wuppertal, Germany
- MP 259 **Charge Inversion of Protein Cations via Gas-Phase Ion/Ion Reactions with Hyaluronic Acid Anions;** Hsi-Chun Chao¹; Mack Shih¹; Abdirahman M. Abdillahi¹; Scott A McLuckey¹; ¹Purdue University, West Lafayette, IN
- MP 260 **Extracting Mass Information from Large Biomolecules via Ion-Ion Reaction Chemistry;** Abdirahman M Abdillahi¹; Nan Wang¹; David J. Foreman¹; Hsi-Chun Chao¹; Kenneth W Lee¹; Scott A McLuckey¹; ¹Purdue University, West Lafayette, IN
- MP 261 **Characterization of Activated Ion-Electron Transfer Dissociation (AI-ETD) Reaction Kinetics;** Trenton M Peters-clarke¹; Benton J Anderson¹; Jean M Lodge²; Dain R Brademan¹; Kevin L Schauer^{2,3}; Michael S Westphall²; Joshua J Coon^{1,2,4,5}; ¹Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706; ²Genome Center of Wisconsin, Madison, WI; ³Thermo Fisher Scientific, West Palm Beach, FL; ⁴Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI; ⁵Morgridge Institute for Research, Madison, WI
- MP 262 **Gas-phase Photodissociative Crosslinking of Diazirine-Modified Adrenaline with the Binding Motif of beta-2 Adrenergic Receptor;** Yang Liu¹; Shu R. Huang¹; Frantisek Turecek¹; ¹University of Washington, Seattle, WA
- MP 263 **The thermochemistry of the Ion-Molecule Reactions of Uranium Fluoride Species by Guided Ion Beam Tandem Mass Spectrometry;** Amanda Bubas¹; Cameron J. Owen¹; Peter B. Armentrout¹; ¹University of Utah, Salt Lake City, UT
- FUNDAMENTALS: ION SPECTROSCOPY**
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- MP 264 **Investigating Conformational Effects of DNA-drug Interactions by Gas-phase Förster Resonance Energy Transfer;** JoAnn C Chen¹; Stephen V Sciuto¹; Rebecca A Jockusch¹; ¹University of Toronto, Toronto, ON
- MP 265 **Utility of Infrared Photodissociation Spectroscopy on Identifying Post-Translational Modifications;** Laura Bailey¹; Larry F. Tesler¹; Nicolas C. Polfer¹; ¹University of Florida, Gainesville, FL
- MP 266 **Nucleophilic Substitution in the Gas Phase by an Unlikely Nucleophile, Cl-, following Anion Attachment;** Gabriel GaiFFE^{1,2}; Maxime C. Bridoux²; Jane S. Murray³; Peter Politzer³; Philippe Maître⁴; Richard B. Cole¹; ¹Sorbonne Université, Faculté des Sciences et Ingénierie, Paris, France; ²Commissariat à l'Energie Atomique - DAM, Bruyères-le-Châtel, France; ³University of New Orleans, Department of Chemistry, New Orleans, Louisiana; ⁴Université Paris-Sud, Laboratoire de Chimie Physique, Orsay, France
- MP 267 **Combining Ultrahigh-Resolution Ion-Mobility Spectrometry with Cryogenic IR Spectroscopy for the Analysis of Glycan Mixtures;** Ahmed Faleh¹; Stephan Warnke¹; Thomas R. Rizzo¹; ¹EPFL, Lausanne, Switzerland
- MP 268 **An IRMPD Spectroscopic and Computational Study of Gaseous Protonated and Metal Cationized Guanine-Cytosine Base Pairs and Guanine-Containing Mismatches;** Ruodi Cheng¹; Jonathan Martens²;



- Estelle Loire³; Travis Fridgen⁴; ¹Memorial University of Newfoundland, ST JOHN'S, NL; ²Radboud University Nijmegen, Institute for Molecules and Materials, FELIX Facility, Nijmegen, Netherlands; ³Universite Paris Sud, Orsay, France; ⁴Memorial University of Newfoundland, St. John's, NL
- MP 269 **Shining Light on Gas-Phase Ions to Study Solvent Effects: Spectral Switching in a Model Dye;** Iden Djavani-Tabrizi¹; Rebecca A Jockusch¹; ¹Department of Chemistry, University of Toronto, Toronto, ON
- MP 270 **Automated UV Action Spectroscopy on a Modified 3D Ion Trap MS for Structural Analysis of DNA Cation-Radicals;** Andy Dang¹; James Gladden¹; Yue Liu¹; Brandon Mozzone¹; Frantisek Turecek¹; ¹University of Washington, Seattle, WA
- MP 271 **Proton and Radical Transfers in Hydrogen-Rich DNA Tetranucleotide Cation Radicals: An Experimental and Computational Study;** Yue Liu¹; Shu R Huang¹; Yang Liu¹; Frantisek Turecek¹; ¹University of Washington, Seattle, WA
- MP 272 **Measurement of the Asymmetric UO₂²⁺ Stretching Frequency for [UVIO₂(X)₃] (X = F, Cl, Br and I) Species Using IRMPD Spectroscopy;** Irena Tatosian¹; Luke Metzler¹; Connor J Graca¹; Theodore Corcovilos¹; Jonathan Martens²; Giel Berden²; Jos Oomens²; Michael Van Stipdonk¹; ¹Duquesne University, Pittsburgh, PA; ²Radboud University Nijmegen, Institute for Molecules and Materials, FELIX Facility, Nijmegen, Netherlands
- MP 273 **Raman Spectroscopy of Solutes in Nano-electrospray Ionization (nESI) Spray Plumes and Neutral Droplets;** Brett Michael Marsh¹; Denilson de Oliveira¹; Kiran Iyer¹; Grace Olivia Capek¹; Dor Ben-Amotz¹; R. Graham Cooks¹; ¹Purdue University, West Lafayette, IN
- MP 274 **The Insecticide Imidacloprid and some its Fragmentation Products: An IRMPD Spectroscopic and Computational Study;** Kelsey J Menard¹; Jonathan Martens²; Travis Fridgen¹; ¹Memorial University of Newfoundland, St. John's, NL; ²FELIX Laboratory, Institute for Molecules and Materials, Nijmegen, Netherlands
- MP 275 **Characterizing Single-Turn Alpha Helices via Cold Ion Spectroscopy of Model Compounds;** John Lawler¹; Tim Hill²; David Fairlie²; Scott A McLuckey¹; Timothy S. Zwier¹; ¹Purdue University, West Lafayette, IN; ²University of Queensland, St. Lucia, Australia
- FUNDAMENTALS: METAL ION CATIONIZATION, METAL-LIGAND INTERACTIONS, CATALYSIS**
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- MP 276 **Detection of Key Reaction Intermediates in Cobalt-Catalyzed Electrochemical CO₂ Reduction Using Electrochemical Mass Spectrometry;** Hetong Qi^{1,2}; Katherine Walker³; Qi Wang⁴; Brian Hivick²; Yi Cai²; Richard N Zare³; Hao Chen⁴; ¹Xi'an Jiaotong University, Xi'an, China; ²Ohio University, Athens, OH; ³Stanford University, Stanford, CA; ⁴New Jersey Institute of Technology, Newark, NJ
- MP 277 **Investigation of the C-H Activation Reactivity of Graphene-Supported Single-Atom Catalyst Models in the Gas Phase;** Michael Borrome¹; Scott Gronert^{1,2}; ¹Virginia Commonwealth University, Richmond, VA; ²University of Wisconsin-Milwaukee, Milwaukee, WI 53211
- MP 278 **Mechanistic Study of C-H Activation of Alcohols and Ethers by a Cationic Iridium(III) Dichloride Phenanthroline Complex;** Rozalie Corea¹; Scott Gronert^{1,2}; ¹Virginia Commonwealth University, Richmond, VA; ²University of Wisconsin-Milwaukee, Milwaukee, WI
- MP 279 **Using the Phenanthroline as the Chelator to Develop a Method for Fast-Screening of Metal Ions by ESI Mass Spectrometry;** Pai-Chi Syue¹; Kuok-Fai Li¹; Bo-Yi Zhang¹; Hui-Ling Chiang¹; Ching-yi Lien¹; Kuo-Lung Ku¹; ¹National Chiayi University, Chiayi City, Taiwan
- MP 280 **Utilization of Gas-Phase Transition Metal Oxide Complexes LMO⁺ in Oxidation of Organic Compounds;** Nikko Sideris¹; Richard a. j. O'hair²; Victor Ryzhov¹; ¹Northern Illinois University, Dekalb, IL; ²University of Melbourne, Melbourne, Australia
- MP 281 **Decarboxylative Coupling Reactions Catalyzed by First-Row Transition Metal Complexes with Crown Ether;** Elettra L. Piacentino¹; Fotis Pappas Pappas²; Kostantinos Pappas²; Michael Lesslie²; Thomas M. Gilbert²; Richard A. J. O'hair³; Victor Ryzhov²; ¹Northern Illinois University, Dekalb; ²Northern Illinois University, Dekalb, IL; ³University of Melbourne, Melbourne, Australia
- MP 282 **Gas-Phase Study of C-N Coupling Reactions Catalyzed by Transition Metal Complexes;** Kevin E Parker¹; Victor Ryzhov²; ¹Northern Illinois University, DeKalb, IL; ²Northern Illinois University, Dekalb, IL
- FUNDAMENTALS: MOLECULAR MODELING/QUANTUM MECHANICAL CALCULATIONS**
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- MP 283 **Comparing Theoretical and Experimental Collisional Cross Sections of Carbohydrates to Determine Density Functional Theory Calculation Accuracy;** Emily D. Ziperman¹; Emvia I. Calixte¹; Meg E. McCutcheon¹; Srinivas Pulipaka¹; Elyssia S. Gallagher¹; ¹Baylor University, Waco, TX
- MP 284 **Quasi-Harmonic Approximation for the Thermochemical Stability of Small Proton Bound Clusters – A Theoretical Study;** Alexander Haack¹; Walter Wissdorf¹; Hendrik Kersten¹; Thorsten Benter¹; ¹University of Wuppertal, Wuppertal, Germany
- MP 285 **A Novel Concept of Ionisation Site Induced Fragmentation in Positive Ion ESI of C-O Bonds of Ether or Ester Groups;** Maria Ashe¹; Mansoor Saeed²; Peter Howe²; Chris K. Skylaris¹; G. John Langley¹; ¹The University of Southampton, Southampton, United Kingdom; ²Syngenta Jealott's Hill International Research Centre, Bracknell, United Kingdom
- MP 286 **Transfer of FeIII from Catechol to Enterobactin Complexes: an Empirical and Theoretical Study;** Daryl Giblin¹; Lindsey Steinberg²; Jan R Crowley²; Michael L. Gross³; Jeffrey P Henderson²; ¹Washington University, St. Louis, MO; ²Washington University, School of Medicine, St. Louis, MO; ³Washington University, St. Louis, MO
- MP 287 **Enhanced Protonation of Amino Acids and Dipeptides Using Cr(III): Developing the Basis for Proteomics Studies;** Rudradatt Persaud¹; Carolyn J Cassidy¹; David A. Dixon¹; ¹The University of Alabama, Tuscaloosa, AL
- MP 288 **Computational Prediction of Gas-Phase Acidities for Small Acidic Peptides and their Amides;** Ashley S McNeill¹; Can Cui¹; Justin M Adam¹; William C Jackson¹; Michael A Raddatz¹; Carolyn J Cassidy¹; David A Dixon¹; ¹The University of Alabama, Tuscaloosa, AL
- MP 289 **M06-2X and G3(MP2) Proton Affinity Estimation for Organo-Phosphorus Compounds;** Howard G Mayes¹; Jordan M Rabus¹; Benjamin J Bythell¹; ¹University of Missouri, St. Louis, MO
- MP 290 **MD Simulations on Gaseous Protein Ions Using Solution Force Fields: Is there a Problem?;** Justin H Lee¹; Lars Konermann²; ¹University of Western Ontario, London, ON; ²University of Western Ontario, London, ON
- MP 291 **Supercharging Mechanism for Unfolded Proteins: Insights from MD Simulations and IMS/MS;** Insa Peters¹; Haidy Metwally¹; Lars Konermann²; ¹University of Western Ontario, London, ON; ²Univ. of Western Ontario, London, ON

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- MP 292 **Thin Film Dialysis HX-MS Reveals Protein Interfaces during Reversible Self-Association of Monoclonal Antibodies at High Concentration;** Mihiri Weerasinghe¹; Yangjie Wei²; Reza Esfandiary³; C. Russell Middaugh²; David D Weis^{1,4}; ¹Department of Chemistry, University of Kansas, Lawrence, Kansas (KS); ²Department of Pharmaceutical Chemistry, University of Kansas, Lawrence, KS; ³Department of Formulation Sciences, MedImmune LLC, Gaithersburg, MD; ⁴Department of Pharmaceutical Chemistry, University of Kansas, Lawrence, KS
- MP 293 **Which Spectra Should We Pick? Limitations of the Extracted Ion Chromatogram in HDX-LC-MS Analysis;** Jeff Morrow; Sierra Analytics, Modesto, CA
- MP 294 **A Comparison between Two Automated HDXMS Systems, as Applied to Epitope Mapping;** Aik Roy Heng¹; Deepa Balasubramaniam¹; Jonathan Fitchett¹; Ruben Haro²; Michael J. Chalmers³; ¹Lilly Biotechnology Center, San Diego, CA; ²Discovery Automation, Centro de Investigación, Alcobendas, Spain; ³Lilly Research Laboratories, Eli Lilly and Company, Indianapolis, IN
- MP 295 **An Algorithm for Calculation of the Protein Fraction Synthetic Rate Using 2 Time Points;** Sergei Ilchenko¹; Andrew Haddad¹; Kwangwon Lee¹; Probodh Sadana¹; Rovshan Sadygov²; Takhar Kasumov¹; ¹Northeast Ohio Medical University, Rootstown, OH; ²University of Texas Medical branch, Galveston, TX
- MP 296 **Single-Residue Resolution of HX-MS Obtained Using ExD in a Q-ToF;** Joseph C. Meeuwse^{1,2}; Yury V. Vasil'ev^{1,2}; Valery G. Voinov^{1,2}; Nathan I. Lopez^{1,2}; Joseph S. Beckman^{1,2}; ¹e-MSion, Inc., Corvallis, OR; ²Oregon State University, Corvallis, OR
- MP 297 **Sparse Representation for Hydrogen Exchange Mass Spectrometry (HX-MS) Data Using LASSO Optimization;** Yuqi Shi¹; Jarod Hart¹; David D Weis¹; ¹University of Kansas, Lawrence, KS
- MP 298 **HDX-MS as a Tool for Probing Conformational Stability in Industrial Applications;** Daniel W Pedersen^{1,2}; Jeppe C Mouritsen¹; Christian I Jørgensen¹; Thomas J D Jørgensen²; ¹Novozymes A/S, Bagsværd, Denmark; ²University of Southern Denmark, Odense, Denmark
- MP 299 **Optimization of a Low-temperature LC-MS system for Hydrogen/Deuterium Exchange Mass Spectrometry;** Mulin Fang¹; Zhe Wang¹; Jiwon Kang¹; Kellye A Cupp-Sutton¹; Christina Bourne¹; Si Wu¹; ¹University of Oklahoma, Norman
- MP 300 **Integrated Software Platform for Analyzing Hydrogen-Deuterium Exchange and Oxidative Footprinting Data for Solvent Accessibility;** Wilfred Tang¹; Marshall Bern¹; Rose D Lawler¹; Yong J. Kil¹; Eric Carlson¹; Saketh Chemuru²; Nicole D Wagner²; Liuqing Shi²; Henry Rohrs²; Daisy W. Leung²; Michael L Gross²; ¹Protein Metrics Inc., Cupertino, CA; ²Washington University, St. Louis, MO
- MP 301 **An Integrated, Dual-Proteolysis, -30 oC HPLC Platform for Hydrogen-Deuterium Exchange Mass Spectrometry with Minimized H for D Back-exchange;** Jeffrey W Hudgens^{1,2}; Kyle W. Anderson^{1,2}; Ioannis Karageorgos^{1,2}; ¹National Institute of Standards and Technology, Rockville, MD; ²Institute for Bioscience and Biotechnology Research, Rockville, MD
- MP 302 **Refinement of an Algorithm for High-Resolution HDX-MS Data Analysis Combined with HaDeX;** Dominik Cysewski¹; Weronika Puchala¹; Aleksandra Badaczewska-Dawid¹; Katarzyna Dabrowska¹; Michal Kistowski¹; Michal Burdukiewicz²; Michal Dadlez¹; ¹Institute of Biochemistry and Biophysics, Polish Academy of Sciences, Warsaw, Poland; ²Warsaw University of Technology, Warsaw, Poland

- MP 303 **deMix: Automated HDX-MS Data Analysis Reveals Conformational Isomer Proteins;** Seungjin Na¹; Jae-Jin Lee²; Jong Wha J. Joo³; Kong-Joo Lee²; Eunok Paek¹; ¹Hanyang University, Seoul, South Korea; ²Ewha Womans University, Seoul, South Korea; ³Dongguk University-Seoul, Seoul, South Korea
- MP 304 **Characterization of Conformational Differences between Coexisting Protein States Using Differential Hydrogen/Deuterium Exchange during Proteoform Separation;** Yue Shen¹; Xiuxiu Zhao¹; Guanbo Wang¹; David D. Y. Chen²; ¹Nanjing Normal University, Nanjing, China; ²University of British Columbia, Vancouver, BC
- MP 305 **SeleXION® Differential Mobility Hardware Enables Facile, Tunable Gas-Phase Hydrogen-Deuterium Exchange for Small Molecules and Proteins;** Brendon Seale^{1,2}; Yves Le blanc²; ¹York University, Toronto, ON; ²SCIEX, Concord, ON
- MP 306 **Can Spray Solvent Conductivity Modify the Exchange Time for In-Electrospray H/D Exchange of Carbohydrate-Metal Adducts?;** Tara Liyanage¹; Alexis N. Edwards¹; Elyssia S. Gallagher¹; ¹Baylor University, Waco, TX
- MP 307 **Characterization of Intra-Column Processes in Cross-Path Reactive Chromatography (XP-RC) Using Hydrogen/Deuterium Exchange and MS Detection;** Miaowei Xu¹; Cedric E. Bobst¹; Igor A. Kaltashov¹; ¹University of Massachusetts, Amherst, MA
- MP 308 **Hydrogen/Deuterium Exchange Coupled to MS/MS to Elucidate Site-Specific Labeling of Carbohydrates;** H. Jamie Kim¹; Elyssia S. Gallagher²; ¹Baylor University, Waco, TX; ²Baylor University, Waco, TX
- MP 309 **20S Proteasome Complex Structure Conformation and Dynamics Study by Hydrogen Deuterium Exchange Mass Spectrometry;** Shaunak Paval¹; Terry Zhang²; Rosa Viner³; Albert Konijnenberg⁴; David C Schriemer¹; Andreas Huhmer³; ¹University of Calgary, Calgary, AB; ²ThermoFisher, San Jose, CA; ³Thermo Fisher Scientific, San Jose, CA; ⁴Thermo Fisher Scientific, Eindhoven, Netherlands

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- MP 310 **New Developments in the Modeling of Ion Fragmentation by MS Interpreter Software;** Alexey V. Mayorov¹; Yuri A. Mirokhin¹; Dmitrii V. Tchekhovskoi¹; Stephen E. Stein¹; ¹NIST, Gaithersburg, MD
- MP 311 **LC/GC Technical Replicates Data Multiplexing Leverages FTMS Applications;** Konstantin O. Nagornov¹; Anton N. Kozhinov¹; Florian Albrieux²; Carole Reymond²; Markus Zennegg³; Davide Bleiner³; Natalia Gasilova⁴; Laure Menin⁵; Yury O. Tsybin¹; ¹Spectroswiss, Lausanne, Switzerland; ²IFP Energies nouvelles, Solaise, France; ³Swiss Federal Laboratories for Materials & Technology (EMPA), Dübendorf, Switzerland; ⁴Ecole Polytechnique Fédérale de Lausanne, Sion, Switzerland; ⁵Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland
- MP 312 **High Accuracy Self-Calibration Method for High Resolution Mass Spectra;** Boris Kozlov¹; Vasily Makarov²; Jeffery M. Brown¹; Keith Richardson¹; ¹Waters Corporation, Wilmslow, United Kingdom; ²MS Consulting, Bar, Montenegro
- MP 313 **Investigation of Human Embryo Culture Media Using a Quadrupole Time-Of-Flight (Q-TOF) Mass Spectrometer;** Helen Hao¹; Evelyn H Wang²; Jerry Byrne II²; Jennifer Davis²; Katie Pryor²; Christopher Gilles²; ¹Shimadzu Scientific Instruments, Inc., Columbia, MD; ²Shimadzu Scientific Instruments, Inc., Columbia, Maryland



- MP 314 **A Chroma Change Study of Acid-Blue 9 Dye with PA12 Powder by UPLC-PDA-HRMSn**; [Stone Ouyang](#)¹; Mark Kowalski¹; Ali Emamjomeh¹; Jesiska Tandy¹; ¹*Hewlett-Packard Company, San Diego, CA*
- MP 315 **Qualitative Characterization and Quantitative Assessment of Monoclonal Antibodies Using Protein Metrics and nSMOLTM coupled with the Shimadzu LC-MS 9030 Q-ToF**; [Vikki Johnson](#)¹; Stephen Kurzyneic²; ¹*Shimadzu Scientific Instruments, Carlsbad, CA*; ²*Shimadzu Scientific Instruments, Inc., Columbia, Maryland*
- MP 316 **Quantitation of 4,4'-Methylenedianiline and Characterization of Unknown Leachables in Simulated Sweat Migrations Using Liquid Chromatography Quadrupole-TOF Mass Spectrometry**; [Noelle Elliott](#)¹; Marshall Henry¹; Kate Willis¹; ¹*Intertek, Allentown, PA*
- MP 317 **FTMS Isotopic Simulator: a Like-for-Like Comparison of Experimental and Theoretical Mass Spectra**; Natalia Gasilova¹; Konstantin O. Nagornov²; Anton N. Kozhinov²; Laure Menin³; [Yury Tsybin](#)²; ¹*EPFL Valais, Sion, Switzerland*; ²*Spectroswiss Sàrl, Lausanne, Switzerland*; ³*EPFL, Lausanne, Switzerland*
- MP 318 **High Resolution Quadrupole Mass Spectrometry Analysis for Fusion Reactor and Plasma Facing Materials**; [Gregory Thier](#)¹; Luke Kephart¹; Jian Wei¹; ¹*Extrel CMS, Pittsburgh, PA*
- MP 319 **Evaluation of Orbitrap and Time-of-Flight Mass Analyzers for High-Throughput Metabolomics**; [Michelle Reid](#)¹; Tobias Fuhner¹; Nicola Zamboni¹; ¹*ETH Zurich, Zurich, Switzerland*
- MP 320 **Extractables & Leachables Analysis Using the Hi-Resolution Accurate Mass GC/QTOF**; [Thomas S Talwar](#)¹; Matthew Curtis²; ¹*Agilent Technologies, Inc., Wilmington, DE*; ²*Agilent Technologies, Inc., Santa Clara, CA*
- MP 321 **Molecular Structure Study of Polyether Polyols by UPLC-QTOF MS**; [Junyan Liu](#); *Sinopec Shanghai Research Institute of Petrochemical Technology, Shanghai, China*
- MP 322 **Simultaneous Profile and Determination of Statin Composition in Various Media and Biological Matrices by Accurate Mass and High Resolution LC-QTOF-MS**; Wei Chen¹; Patrick Lin¹; Bih Hsu¹; [Zicheng Yang](#)²; Xuejun Peng²; Guillaume Tremintin²; ¹*Pharmout Laboratory, Fremont, CA*; ²*Bruker Daltonics, San Jose, CA*
- MP 323 **Critical Comparison of Fourier Transform Mass Spectrometry Platforms for Metabolite Elemental Formula Elucidation Purposes**; [Danning Huang](#)¹; Marcos Bouza Areces¹; David Gauli¹; Arthur S. Edison²; Facundo M. Fernandez¹; ¹*Georgia Institute of Technology, Atlanta, GA*; ²*University of Georgia, Athens, GA*
- MP 324 **Sensitive Perfluoroalkyl Substance (PFAS) Screening Using High Resolution Accurate Mass Spectral Library**; [Gerard Byrne](#)¹; Brahm Prakash¹; Evelyn Wang¹; Christopher Gilles¹; ¹*Shimadzu Scientific Instruments, Inc., Columbia, MD*
- MP 325 **Untargeted Metabolomics and 13C-Labeling in Tissue Culture for Identifying Unknown Human Biotransformation Products of Xenobiotics**; [Mira Flasch](#)¹; Christoph Bueschl²; Lydia Woelfingseder¹; Rainer Schuhmacher²; Doris Marko¹; Benedikt Warth^{1,3,4}; ¹*University of Vienna, Faculty of Chemistry, Department of Food Chemistry and Toxicology, Vienna, Austria*; ²*University of Natural Resources and Life Sciences, Department of Agrobiotechnology, Center for Analytical Chemistry, IFA-Tulln, Vienna, Austria*; ³*Research Network Chemistry Meets Microbiology, University of Vienna, Vienna, Austria*; ⁴*Vienna Metabolomics Center (VIME), Vienna, Austria*
- MP 326 **Facile Generation of Absorption-Mode Mass Spectra on FT-ICR MS Instruments**; [Anton N. Kozhinov](#)¹; Konstantin O. Nagornov¹; Yury O. Tsybin¹; ¹*Spectroswiss, Lausanne, Switzerland*
- MP 327 **Using TOF-MS to Improve Quality in High Throughput Laboratories**; [Lucas Marshall](#), MS¹; Jason Hull, MS¹; Rebecca Heltsley, PhD¹; ¹*Aegis Sciences Corporation, Nashville, TN*
- MP 328 **Developments in Orbitrap Mass Spectrometry on a Modified Tribrid Mass Spectrometer**; [Jesse D. Canterbury](#)¹; Graeme McAlister¹; Michael W. Senko¹; Romain Huguet¹; Aaron Robitaille¹; Arne Kreuzmann²; Daniel Mourad²; Konstantin Aizikov²; Dmitry Grinfeld²; Alexander Makarov²; ¹*Thermo Fisher Scientific, San Jose, CA*; ²*Thermo Fisher Scientific, Bremen, Germany*
- MP 329 **Targeted Screening of Coumarins and Furanocoumarins in Essential Oils Utilizing Accurate Mass on a High-Resolution Quadrupole Time-of-Flight Mass Spectrometer**; [Jennifer C Davis](#)¹; Evelyn H Wang¹; Katie Pryor¹; Gerard Byrne¹; Helen Hao¹; Christopher Gilles¹; ¹*Shimadzu Scientific Instruments, Inc., Columbia, Maryland*
- MP 330 **Suspect Screening for Antimicrobials and Other Micropollutants in Wastewater and Surface Waters from Asia using High Resolution Mass Spectrometry**; [Diana Aga](#)¹; Luisa Angeles¹; ¹*University at Buffalo, Buffalo, NY*
- MP 331 **Advanced Proteomics Quality Control Samples for Assessing Reversed-Phase Liquid Chromatography Tandem Mass Spectrometry Performance Metrics**; [Jaclyn Gowen Kalmar](#)¹; Michael S. Bereman¹; David C Muddiman¹; ¹*North Carolina State University, Raleigh, NC*
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- MP 332 **Co-registration and Analysis of MALDI and Confocal Fluorescence Images of Stem Cell Colonies via Multivariate Regression**; [Arina A Nikitina](#)¹; Danning Huang²; Sarah Seals³; Li Li²; Melissa Kemp³; Facundo M Fernandez²; ¹*School of Biological Sciences, Georgia Institute of Technology, Atlanta, GA*; ²*School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA*; ³*The Wallace H. Coulter Department of Biomedical Engineering, Georgia Institute of Technology and Emory University, Atlanta, GA*
- MP 333 **Dissimilarity Metrics Mapping Algorithm for Assist Region Detection in Mass Spectrometry Imaging**; Evgeny Zhvansky¹; Anatoly Sorokin^{1,2}; Daniil Ivanov¹; Vasilii Eliferov¹; Anna Bugrova³; [Stanislav Pekov](#)^{1,4}; Igor Popov^{1,4}; Eugene (evgeny) Nikolaev⁵; ¹*Moscow Institute of Physics and Technology (State University), Dolgoprudny, Russia*; ²*Institute of Cell Biophysics RAS, Pushchino, Russia*; ³*Institute of Biochemical Physics RAS, Moscow, Russia*; ⁴*Institute for Energy Problems of Chemical Physics RAS, Moscow, Russia*; ⁵*Skolkovo institute of science and technology, Moscow Region, Russian Federation*
- MP 334 **Automatic Identification of Suborgan Regions in MS Imaging**; [Laura Castellanos-García](#)¹; Richard W. Vachet¹; ¹*University of Massachusetts, Amherst, MA*
- MP 335 **Development and Benchmarking of Automated, Computational Registration of Microscopy and MALDI Imaging Mass Spectrometry Datasets**; [Heath Patterson](#)¹; Michael D. Tuck²; Martin Dufresne^{2,3}; Richard M. Caprioli^{2,3,4}; ¹*Vanderbilt University, Nashville, TN*; ²*Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN*; ³*Department of Biochemistry, Vanderbilt University, Nashville, TN*; ⁴*Department of Chemistry, Vanderbilt University, Nashville, TN*
- MP 336 **Automated MS Imaging Data Processing Pipeline for Routine and Creative Data Explorations: from Data Acquisition to Archiving**; [Teresa Murta](#)¹; Spencer A. Thomas¹; Alex Dexter¹; Ala Al-Afeef¹; Adam J. Taylor¹; Bin Yan¹; Chelsea J. Nikula¹; Efstathios Elia¹; Kenneth N. Robinson¹; Rory T. Steven¹; Tingting Fu¹; Weiwei Zhou¹;



- Xavier Loizeau¹; Josephine Bunch^{1,2}; ¹National Physical Laboratory, London, United Kingdom; ²Imperial College, London, United Kingdom
- MP 337 **Fully Automated Mass Alignment and Recalibration of MALDI TOF Imaging Data from N-Linked Glycans;** Tobias Boskamp^{1,2}; Alyson Black³; Anand Mehta³; Richard Drake³; Yujin Hoshida⁴; Dennis Trede¹; Peter Maass^{1,2}; ¹SCiLS, Bremen, Germany; ²University of Bremen, Bremen, Germany; ³Medical University of South Carolina, Charleston, SC; ⁴University of Texas Southwestern Medical Center, Dallas, TX
- MP 338 **An Ion Mobility Quadrupole Time of Flight Mass Spectrometry Imaging Workflow;** Daniela Mesa Sanchez¹; Stephen Creger¹; Ruwan T Kurulugama²; John C. Fjeldsted²; Julia Laskin¹; ¹Purdue University, West Lafayette, IN; ²Agilent Technologies, Inc., Santa Clara, CA
- MP 339 **Co-Registered Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry and Time-of-Flight Secondary Ion Mass Spectrometry Data for Visualizing Sub-cellular Brain Signaling Pathways;** Steven T King¹; Matthias Lorenz¹; Nikolay Borodinov¹; Junghoon Chae¹; Chad A Steed¹; Anton V. Ilevlev¹; Olga S Ovchinnikova¹; ¹Oak Ridge National Laboratory, Oak Ridge, TN
- MP 340 **Optimized Data Analysis Pipeline for MALDI Imaging Based Tumor Typing from FFPE Tissue Samples Evaluated on Six Benchmark Classification Tasks;** Delf Lachmund¹; Jonathan von Schroeder¹; Tobias Boskamp^{1,2}; Lena Hauberg-Lotte¹; Jan H. Kobarg²; Sören-Oliver Deininger³; Katharina Kriegsmann⁴; Mark Kriegsmann⁴; Rita Casadonte⁵; Jörg Kriegsmann⁵; Peter Maass^{1,2}; ¹University of Bremen, Bremen, Germany; ²SCiLS, Bremen, Germany; ³Bruker Daltonik GmbH, Bremen, Germany; ⁴University of Heidelberg, Heidelberg, Germany; ⁵Proteopath, Trier, Germany
- MP 341 **Co-Registered MALDI and ToF-SIMS Data for Visualizing Sub-cellular Signaling Pathways in the Brain;** Matthias Lorenz¹; Stephen T. King¹; Chad A. Steed¹; Junghoon Chae¹; Anton V. Ilevlev¹; Olga S. Ovchinnikova¹; ¹Oak Ridge National Laboratory, Oak Ridge, TN
- MP 342 **Unsupervised Segmentation of Mass Spectrometric Ion Images Characterizes Morphology of Tissues;** Dan Guo¹; Kylie Bemis¹; Catherine Rawlins¹; Jeffery Agar¹; Olga Vitek¹; ¹Northeastern University, Boston, MA
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- MP 343 **High Efficiency Miniature Imaging Mass Spectrometer;** Xiangyu Guo¹; Wenbo Cao¹; Xiaoxiao Ma¹; Xinwei Liu¹; Zheng Ouyang^{1,2}; ¹State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instrument, Tsinghua University, Beijing, China; ²Weldon School of Biomedical Engineering and Department of Chemistry, Purdue University, West Lafayette, IN
- MP 344 **21 T MALDI FT-ICR Mass Spectrometry for High Performance Molecular Imaging;** Donald F. Smith¹; Andrew P. Bowman²; Shane R. Ellis²; Greg T. Blakney¹; Ron M. A. Heeren²; Christopher L. Hendrickson^{1,3}; ¹National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL; ²Maastricht Multimodal Molecular Imaging (M4I) Institute, Division of Imaging Mass Spectrometry, Maastricht, Netherlands; ³Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL
- MP 345 **Observation on Regeneration Behavior of Zebrafish Caudal Fin Using High-Spatial Resolution Mass Spectrometric Imaging;** Jae Young Kim¹; Sun Young Lee¹; Ji-Won Park²; Dong-Kwon Lim³; Dae Won Moon¹; ¹Daegu Gyeongbuk Institute of Science and Technology, Daegu, South Korea; ²Chungnam National University, Daejeon, South Korea; ³Korea University, Seoul, South Korea
- MP 346 **Optimized Rapid Matrix Sublimation Device for MALDI Mass Spectrometry Imaging;** Vasily Eliferov¹; Daniil Ivanov¹; Andrey Shivalin¹; Igor Popov^{1,2}; Eugene (Evgeny) Nikolaev³; ¹Moscow Institute of Physics and Technology (State University), Dolgoprudny, Russia; ²Institute of Biochemical Physics RAS, Moscow, Russia; ³Skolkovo institute of science and technology, Moscow Region, Russian Federation
- MP 347 **Upgrade of an LTQ-Orbitrap XL MALDI Source for High Spatial Resolution in Image Experiments;** Raul Montero¹; Lucía Martín-Saiz¹; Jone Garate¹; Beatriz Abad-García¹; Jose A Fernandez²; ¹University of the Basque Country, Leioa, Spain; ²Universidad del País Vasco, Leioa, Spain
- MP 348 **Characteristics of MALDI-Imaging on a New Dual Ion Source QTOF with TIMS Separation;** Arne Fuetterer¹; Juergen Suetering¹; Janina Oetjen¹; Niels Goedecke¹; Stephanie Kaspar-Schoenefeld¹; Scarlet Koch¹; Shannonn Cornett²; Alice Ly¹; Jens Fuchser¹; Lucy Woods¹; Oliver Raether¹; Jens Hoehndorf¹; ¹Bruker Daltonik GmbH, Bremen, Germany; ²Bruker Daltonics Inc., Billerica, MA
- MP 349 **Atmospheric Pressure Mass Spectrometry Imaging with Post-Ionisation;** Rory Thomas Steven¹; Kenneth N. Robinson¹; Alex Dexter¹; Michael Shaw¹; Teresa Murta¹; Bin Yan¹; Weiwei Zhou¹; Ian S Gilmore¹; Zoltan Takats²; Josephine Bunch^{1,2}; ¹National Physical Laboratory, London, United Kingdom; ²Imperial College London, London, United Kingdom
- MP 350 **High-Resolution Ion Microscope Imaging over Broad Mass Ranges Using a Reflectron;** Michael Burt¹; Robert Burleigh¹; Ang Guo¹; Fei Gao¹; Natasha Smith¹; Mark Brouard¹; ¹University of Oxford, Oxford, United Kingdom
- MP 351 **Gas-Phase Charge Inversion Ion/Ion Reactions on an FT-ICR Mass Spectrometer for Fatty Acids Identification in Imaging Mass Spectrometry;** Julia R Bonney¹; Xizheng Diao¹; Steve L. Van Orden²; Boone M. Prentice¹; ¹University of Florida Department of Chemistry, Gainesville, FL; ²Bruker Daltonics Inc., Billerica, MA
- MP 352 **Co-Registered, Cellular-Resolution Mass Spectrometry and Fluorescence Imaging for the Multi-Omic Targeting of Rare Cell Types;** Eric C. Spivey^{1,2}; Josiah C. McMillen^{1,3}; David M. Anderson¹; Daniel J. Ryan^{1,3}; Jeffrey M. Spraggins^{1,3,4}; John P. Wiksw^{2,5,6}; Richard M. Caprioli^{1,3,4}; Jeremy L. Norris^{1,4}; ¹Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; ²Vanderbilt University Department of Biomedical Engineering, Nashville, TN; ³Vanderbilt University Department of Chemistry, Nashville, TN; ⁴Vanderbilt University Department of Biochemistry, Nashville, TN; ⁵Vanderbilt Institute for Integrative Biosystems Research and Education, Nashville, TN; ⁶Vanderbilt University Department of Physics, Nashville, TN
- MP 353 **MALDI Spatial Resolution Improvement Using MALDI-2 Post-Ionization;** Josiah C. McMillen^{1,2}; Eric C. Spivey^{2,3}; Daniel J. Ryan^{1,2}; Jeffrey M. Spraggins^{1,2,4}; Richard M. Caprioli^{1,2,4,5,6}; ¹Department of Chemistry, Vanderbilt University, Nashville, TN; ²Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; ³Department of Biomedical Engineering, Vanderbilt University, Nashville, TN; ⁴Department of Biochemistry, Vanderbilt University, Nashville, TN; ⁵Department of Pharmacology, Vanderbilt University, Nashville, TN; ⁶Department of Medicine, Vanderbilt University, Nashville, TN
- MP 354 **Sub-Cellular Chemical and Functionals Imaging AFM-MS and Analysis of Biological Tissues;** Ryan Wagner¹; Matthias Lorenz²; Olga S Ovchinnikova³; Roger Proksch¹; ¹Oxford Instruments, Santa Barbara, CA; ²University of Tennessee / Oak Ridge National Laboratory, Oak Ridge, TN; ³Oak Ridge National Laboratory, Oak Ridge, TN
- MP 355 **Characterization of a Prototype MALDI timsTOF Pro for High-Performance Imaging Mass Spectrometry;** Katerina V Djambazova^{1,2}; Lukasz Migas³; Nathan Heath Patterson²



- ⁴; Raf Van de Plas³; Richard M. Caprioli^{1,2,4,5,6}; Jeffrey M. Spraggins^{1,2,4}; ¹Department of Chemistry, Vanderbilt University, Nashville, TN; ²Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; ³Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; ⁴Department of Biochemistry, Vanderbilt University, Nashville, TN; ⁵Department of Medicine, Vanderbilt University, Nashville, TN; ⁶Department of Pharmacology, Vanderbilt University, Nashville, TN
- MP 356 **Development of High Spatial Resolution and High Speed Projection-type Imaging Mass Spectrometer;** Jun Aoki¹; Michisato Toyoda¹; ¹Osaka University, Toyonaka, Japan
- MP 357 **Coupling IR-MALDESI and Ion Mobility-Mass Spectrometry for Rapid Isomer Distinction in Imaging Experiments;** Måns Ekelöf¹; James N. Dodds¹; Jeffrey G. Mann²; Kenneth P. Garrard¹; Sitora Khodjanizyazova¹; Erin S Baker¹; David C. Muddiman¹; ¹North Carolina State University, Raleigh, NC; ²JGM Associates, Burlington, MA
- MP 358 **Understanding the Role of Electrospray Solvent Composition on the Ionization of Diverse Chemical Classes by IR-MALDESI MSI;** Måns Ekelöf¹; David C. Muddiman^{1,2}; Michael C. Bagley¹; Liana Gouveia¹; ¹North Carolina State University, Raleigh, NC; ²Molecular Education, Technology, and Research Innovation Center (METRIC), North Carolina State University, Raleigh, NC
- MP 359 **RastirX: A Versatile Platform for Imaging Arbitrary Spatial Patterns;** Kenneth P. Garrard^{1,2}; Måns Ekelöf¹; Sitora Khodjanizyazova¹; Michael C. Bagley¹; David C. Muddiman^{1,3}; Elias P. Rosen⁴; William M. Gilliland, Jr.⁴; Angela D. M. Kashuba⁴; ¹FTMS Laboratory for Human Health Research, Department of Chemistry, North Carolina State University, Raleigh, NC; ²Precision Engineering Consortium, North Carolina State University, Raleigh, NC; ³Molecular Education, Technology, and Research Innovation Center (METRIC), North Carolina State University, Raleigh, NC; ⁴Division of Pharmacotherapy and Experimental Therapeutics, University of North Carolina at Chapel Hill, Chapel Hill, NC
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- MP 360 **A Quantitative Evaluation of Ion Chromatogram Extraction Algorithms;** Annika Tostengard¹; Robert Smith²; ¹The University of Montana, Missoula, MT; ²University of Montana Missoula, Missoula, MT
- MP 361 **LipidAnalyst: A Deep Neural Network Approach for Standardized and Comprehensive Lipidomic Analysis;** Naren Gajenthra Kumar¹; Aliakbar Panahi²; Joseph J Nalluri³; Dayanjan S Wijesinghe²; ¹Department of Microbiology and Immunology, Virginia Commonwealth University, Richmond, VA; ²Department of Pharmacotherapy and Outcomes Sciences, Virginia Commonwealth University, Richmond, VA; ³Department of Radiation Oncology, Virginia Commonwealth University, Richmond, VA
- MP 362 **AP3: An Advanced Proteotypic Peptide Predictor for Targeted Proteomics by Integrating Peptide Digestion Probability;** Zhiqiang Gao¹; Cheng Chang^{2,3}; Yan Fu¹; ¹NCMIS, RCSDS, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, Beijing, China; ²Beijing Institute of Lifeomics, Beijing, China; ³Beijing Proteome Research Center, Beijing, China
- MP 363 **Focus on the Spectra that Matter by Clustering of Quantification Data in Shotgun Proteomics;** Matthew The¹; Lukas Kall¹; ¹Royal Institute of Technology, Stockholm, Sweden
- MP 364 **Predicting Optimal Values of Parameters for Peak Deconvolution Using a Convolutional Neural Network;** Yuichiro Fujita¹; Akira Noda¹; Yohei Yamada¹; Katsuyuki Taneda¹; Junko Iida^{1,2}; Shigeki Kajihara¹; ¹Shimadzu Corporation, Kyoto, Japan; ²Osaka University Shimadzu Analytical Innovation Research Laboratory, Suita, Japan
- MP 365 **Simulated Impacts of Mass Resolving Power on the Resulting Mass Error Distribution in Mass Spectrometry Analysis;** Melaine O Couch¹; Martha L. Chacón-Patiño¹; Christopher L. Hendrickson^{1,2}; Yuri E. Corilo¹; ¹National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL; ²Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL
- MP 366 **Predicting Ion Mobility Collision Cross Sections by Combining Conventional and Data Driven Modelling;** Robbin Bouwmeester^{1,2}; Lennart Martens^{1,2}; Sven Degroeve^{1,2}; Keith Richardson³; Johannes PC Vissers³; ¹VIB-UGent Center for Medical Biotechnology, Ghent, Belgium; ²Department of Biochemistry, Ghent University, Ghent, Belgium; ³Waters Corporation, Wilmslow, United Kingdom
- MP 367 **A New Spectral Baseline Subtraction Algorithm for Reducing Artefacts in Protein Deconvolution;** Lyle Burton¹; Xu Guo¹; Gordana Ivosev¹; Ron Bonner²; ¹SCIEX, Concord, ON; ²Ron Bonner Consulting, Newmarket, ON
- MP 368 **Toffee: A Highly Compressed, Efficient, File Format for DIA-MS;** David Clarke¹; Akila Seneviratne¹; Brett Tully¹; ¹ProCan, Children's Medical Research Institute, The University of Sydney, Westmead, Australia
- MP 369 **Increased Peptide Detection Accuracy in DIA-MS via Chemical and Random Additive Noise Elimination (Crane);** Akila J Seneviratne¹; Brett Tully¹; ¹ProCan, Children's Medical Research Institute, The University of Sydney, Westmead, Australia
- MP 370 **Exploring DIA Proteomics Spectra with Tensor-based Deconvolution;** Filip Buric¹; Aleksej Zelezniak^{1,2}; ¹Chalmers University of Technology, Gothenburg, Sweden; ²Science for Life Laboratory, KTH - Royal Institute of Technology, Stockholm, Sweden
- MP 371 **Repeat-Preserving Decoy Database for False Discovery Rate Estimation in Peptide Identification;** Johra Muhammad Moosa¹; Shenheng Guan^{1,2}; Michael F. Moran^{2,3}; Bin Ma¹; ¹David R. Cheriton School of Computer Science, University of Waterloo, Waterloo, ON; ²Program in Cell Biology and SPARC BioCentre, Hospital for Sick Children, Toronto, ON; ³Department of Molecular Genetics, University of Toronto, Toronto, ON
- MP 372 **MS-PROTINI: A Protein-Protein Interaction-Assisted Algorithm for the Confidence Assessment of Peptide and Protein Identifications in Mass Spectrometry-Based Proteomics;** Francesca A. Barry¹; Zhibin Ning¹; Daniel Figeys¹; Mathieu Lavallée-adam¹; ¹University of Ottawa, Ottawa, ON
- MP 373 **Peptide Migration Time Prediction in Capillary Zone Electrophoresis Mass Spectrometry Using a Convolutional Neural Network Model;** Wenrong Chen¹; Liangliang Sun²; Xiaowen Liu^{1,3}; ¹Department of BioHealth Informatics, Indiana University-Purdue University Indianapolis, Indianapolis, Indiana; ²Department of Chemistry, Michigan State University, East Lansing, 48824; ³Center for Computational Biology and Bioinformatics, Indiana University School of Medicine, Indianapolis, IN
- MP 374 **A Novel Algorithm for Automating Fragment Ion Structure Assignment Using High Mass Accuracy MS/MS data;** Neil Loftus¹; Kirsten Hobby¹; Alan Barnes¹; ¹Shimadzu Corporation, Manchester, United Kingdom
- MP 375 **Factor Analysis Identifies Biologically Meaningful Proteoform Families of Human ApoA-I;** Richard LeDuc¹; Henrique Seckler²; John T Wilkins²; Ryan T Fellers²; Joseph B Greer²; Paul M Thomas²; Neil L Kelleher²; ¹Northwestern



- University, Bloomington, IN; ²Proteomics Center of Excellence, Northwestern University, Chicago, IL
- MP 376 **GPU-Based Signal Processing Optimization for 1&2D FT-ICR Mass Spectrometer Data**; Marc Haegelin¹; Fabrice Bray¹; Anne Jeannin-Girardon²; Pierre Collet²; Christian Rolando¹; ¹Université de Lille, Villeneuve d'Ascq, France; ²Université de Strasbourg, Strasbourg, France
- MP 377 **Massodon: A Tool for in Depth Analysis of your Mass Spectrum**; Mateusz Krzysztof Lacki¹; Frederik Lermyte^{2,3,4}; Błażej Miasojedow⁵; Michał Piotr Startek⁵; Stefan Tenzer¹; Frank Sobott^{2,6,7}; Dirk Valkenborg^{3,8,9}; Anna Gambin⁵; ¹University Medical Center Mainz, Mainz, Germany; ²Biomolecular and Analytical Mass Spectrometry group, University of Antwerp, Belgium; ³Centre for Proteomics (University of Antwerp/VITO (Belgium)), Antwerpen, Belgium; ⁴School of Engineering, University of Warwick, Coventry, United Kingdom; ⁵University of Warsaw, Warsaw, Poland; ⁶Astbury Centre for Structural Molecular Biology, University of Leeds, United Kingdom; ⁷School of Molecular and Cellular Biology, University of Leeds, United Kingdom; ⁸Flemish Institute for Technological Research (VITO), Mol, Belgium; ⁹Interuniversity Institute for Biostatistics and Statistical Bioinformatics, Hasselt, Belgium
- MP 378 **Using Isotopic Cluster, Neutral Loss and Adduct Analyses to Improve Component Detection in LC HRAM MS Experiment**; Juraj Lutisan¹; Michal Gramblička¹; Zofia Lutišanová¹; Robert Mistrik¹; Xiaojie C. Ding²; Vladimír Pátoprský³; ¹HighChem, Bratislava, Slovakia; ²Thermo Fisher Scientific, San Jose, CA; ³Slovak Academy of Sciences, Bratislava, Slovakia
- MP 379 **Automated Predicting Fragmentation Scheme for Molecules during Collision-Induced Dissociation**; Grzegorz Skoraczynski¹; Michal Ciach^{1,2}; Michal Startek¹; Anna Gambin¹; ¹Faculty of Mathematics, Informatics and Mechanics, University of Warsaw, Warsaw, Poland; ²Centrum voor Statistiek, Hasselt University, Diepenbeek, Belgium
- MP 380 **An Efficient Method for Cosine Similarity Threshold Search Using a Peak Indexing Strategy**; Jonghun Park¹; Yuliang Li¹; Jianguo Wang¹; Benjamin Pullman¹; Yannis Papakonstantinou¹; Nuno Bandeira¹; ¹UC San Diego, La Jolla, CA
- MP 381 **Bioinformatics Optimization Approaches for the Label-Free Quantitation of Ubiquitinated Peptides in Bottom-Up MS-Based Proteomics**; Arzu Tugce Guler¹; Karen A. Sap¹; Aleksandra Bury¹; Karel Bezstarosti²; Jeroen A.A. Demmers²; Eric A. Reits¹; ¹Amsterdam UMC, Amsterdam, Netherlands; ²Erasmus MC, Rotterdam, Netherlands
- MP 382 **Using Generalized Chemical Artificial Intelligence to Calculate Molecular Properties, Including GC Retention Indices**; Lewis Geer¹; Stephen E. Stein¹; William E. Wallace¹; ¹NIST, Gaithersburg, MD
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- MP 383 **Prosit: Investigating Vast and Complex Peptide Spaces by Boosting Identification Confidence through Highly-Accurate Fragment Intensity Predictions**; Siegfried Gessulat^{1,2}; Tobias Schmidt¹; Daniel P Zolig¹; Julia Rechenberger¹; Patroklos Samaras¹; Steven Verbruggen^{3,4}; Bernard Delanghe⁵; Andreas Huhmer⁶; Karsten Schnatbaum⁷; Ulf Reimer⁷; Hans-Christian Ehrlich²; Stephan Aiche²; Gerben Menschaert^{3,4}; Bernhard Kuster^{1,8,9}; Mathias Wilhelm¹; ¹Technical University of Munich, Freising, Germany; ²SAP SE, Potsdam, Germany; ³Ghent University, Ghent, Belgium; ⁴BioBix Lab, Ghent, Belgium; ⁵Thermo Fisher Scientific, Bremen, Germany; ⁶Thermo Fisher Scientific, San Jose, CA; ⁷JPT Peptide Technologies GmbH, Berlin, Germany; ⁸Bavarian Center for Biomolecular Mass Spectrometry, Freising, Germany; ⁹Center for Integrated Protein Science Munich, Freising, Germany
- MP 384 **Improved Algorithms for Identifying Phosphopeptides in Peptide Tandem Mass Spectral Libraries**; Sergey Sheetlin¹; Dmitrii V. Tchekhovskoi¹; Zheng Zhang¹; Stephen E. Stein¹; ¹NIST, Gaithersburg, MD
- MP 385 **The Mouse Quantitative Proteomics Knowledge Base: CPTAC-Validated Quantitative Targeted Proteomics Assays for Discovery in Mouse Models**; Yassene Mohammed^{1,2}; Pallab Bhowmick¹; Sarah A. Michaud¹; Helena Pětrošová¹; Christoph H. Borchers^{1,3,4,5}; ¹University of Victoria-Genome BC Proteomics Centre, Victoria, BC; ²Center for Proteomics and Metabolomics, Leiden University Medical Center, Leiden, Netherlands; ³Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC; ⁴Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; ⁵Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC
- MP 386 **Targeted Proteomics Assays for FDA-Approved Protein Biomarkers**; Yassene Mohammed^{1,2}; Simon Roope¹; Pallab Bhowmick¹; Christoph H. Borchers^{1,3,4,5}; ¹University of Victoria-Genome BC Proteomics Centre, Victoria, BC; ²Center for Proteomics and Metabolomics, Leiden University Medical Center, Leiden, Netherlands; ³Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC; ⁴Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; ⁵Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC
- MP 387 **Peak Finding and Quantification Improvements in Skyline**; Nicholas Shulman¹; Brian C Searle^{2,3}; Micheal J MacCoss¹; Brendan X MacLean¹; ¹University of Washington, Seattle, WA; ²Systems Biology, Seattle, WA; ³Proteome Software, Portland, OR
- MP 388 **Bonfire Search Engine for Precursor-Independent Identification of Peptides with Exact or Open Modification to Uncover the "Dark Proteome"**; Wen Yu¹; Raghothama Chaerkady¹; Xiaotao Qu¹; Sonja Hess¹; David A Fenstermacher¹; ¹MedImmune, Gaithersburg, MD
- MP 389 **ImmuNOVO: A Software Tool for Constrained de novo Sequencing of Neo-Epitope Peptides from Immunopeptidomics**; Sujun Li¹; Haixu Tang²; ¹Indiana University, Bloomington, IN; ²Indiana University Bloomington, Bloomington, IN
- MP 390 **Extremely Efficient Open Modification Spectral Library Searching Using Spectrum Hashing and GPUs Allows Large-Scale PTM Profiling**; Wout Bittremieux^{1,2}; Kris Laukens²; William Stafford Noble¹; ¹University of Washington, Seattle, WA; ²University Of Antwerp, Antwerp, Belgium
- MP 391 **Improving Peptide Identification by Library Search from Chimeric Spectra**; Wenju Zhang¹; Zhewei Liang¹; Xin Chen¹; Lei Xin¹; Baozhen Shan¹; ¹Bioinformatics Solutions Inc., Waterloo, ON
- MP 392 **A New Feature-Based Workflow Unifies DDA and DIA Data Analysis**; Wen Zhang¹; Weiping Sun¹; Ziaur Rahman¹; Yi Liu¹; Lei Xin¹; ¹Bioinformatics Solutions Inc., Waterloo, ON
- MP 393 **Identification of Inconsistent Peptide Recovery and Aberrant Peptide Termini as Sources of Sample Variability in Patient-derived Tumor Samples**; Meghan Burke¹; Zheng Zhang¹; Yuri A. Mirokhin¹; Dmitrii V. Tchekhovskoi¹; Stephen E. Stein¹; ¹National Institute of Standards and Technology, Gaithersburg, MD



- MP 394 **Robust Cross-Linked Peptide Detection Using Pretrained Neural Networks**; William E Fondrie¹; William Stafford Noble¹; ¹The University of Washington, Seattle, WA
- MP 395 **Validation of Peptide Identification Using Housekeeping Genes as Positives in Supervised Learning**; Honglan Li¹; Seungjin Na¹; Kyu-Baek Hwang²; Eunok Paek¹; ¹Hanyang University, Seoul, South Korea; ²Soongsil University, Seoul, South Korea
- MP 396 **Ion Mobility Enhanced Matching between LC-MS Runs and Collisional Cross Section Prediction Improve Identification and Quantification in MaxQuant**; Nikita Prianchnikov¹; Favio Salinas Soto¹; Heiner Koch²; Scarlet Koch²; Markus Lubeck²; Sven Brehmer²; Juergen Cox¹; ¹Max Planck Institute of Biochemistry, Martinsried, Germany; ²Bruker Daltonik GmbH, Bremen, Germany
- MP 397 **phosMS-GF+: Database Dependent Search Engine for Improved Phosphopeptide Identifications**; Daniela M Schlatter¹; Sean Maxwell²; Mark R. Chance¹; ¹Center for Proteomics and Bioinformatics, CWRU, Cleveland, Ohio; ²Case Western Reserve University, Cleveland, OH
- MP 398 **Automating Distributed Analysis of Large MS/MS Datasets**; Julie S Wertz¹; Jeremy Carver¹; Nuno Bandeira¹; ¹University of California San Diego, La Jolla, CA
- MP 399 **Indexed Retention Time (IRT) Prediction of Peptides by Deep Learning**; Shenheng Guan^{1,2}; Jia Rong Wu¹; Michael F. Moran^{2,3}; Bin Ma¹; ¹University of Waterloo, Waterloo, ON; ²SPARC BioCentre, Hospital for Sick Children, Toronto, Ontario; ³University of Toronto, Toronto, Ontario
- MP 400 **Improved Label-Free Quantification with MaxQuant through more Robust Feature Alignment**; Mai Sun¹; Xuemei Zeng¹; Nathan A. Yates^{1,2}; ¹Biomedical Mass Spectrometry Center, University of Pittsburgh Schools of the Health Sciences, Pittsburgh, PA; ²Department of Cell Biology, University of Pittsburgh School of Medicine, Pittsburgh, PA
- MP 401 **Bolt: A New Age Peptide Search Engine for Comprehensive MS/MS Sequencing through Vast Protein Databases in Minutes**; Amol Prakash¹; Swetaketu Majumder¹; Shadab Ahmad¹; Conor Jenkins²; Benjamin Orsburn³; ¹Optys Tech Corporation, Shrewsbury, MA; ²Hood College Bioinformatics Program, Frederick, MD; ³National Cancer Institute @ Frederick, Frederick, MD
- MP 402 **Comparison of Open-Search Tools**; Fengchao Yu¹; Guo-Ci Teo¹; Andy T. Kong¹; Felipe V. Leprevost¹; Hui-Yin Chang¹; Alexey I. Nesvizhskii¹; ¹University of Michigan, Ann Arbor, MI
- MP 403 **METATRYP 2.0: Improvements in METATRYP Software for Metaproteomic Least Common Ancestor Analyses within the Ocean Protein Portal**; David Gaylord¹; Jaclyn Saunders¹; Noelle Held¹; Nick Symmonds¹; Adam Shepherd¹; Michael Chagnon²; Danie Kinkade¹; Tom Delmont³; A. Murat Eren³; Chris Dupont⁴; Mak Saito¹; ¹Woods Hole Oceanographic Institution, Wood Hole, MA; ²RPS Ocean Science, South Kingston, RI; ³University of Chicago, Chicago, IL; ⁴J. Craig Venter Institute, La Jolla, CA
- MP 404 **Exploring Phosphopeptide Variability across Search Engines and Parameters**; Bhoomi Bhatt¹; Alexander Saltzman¹; Mei Leng¹; Antrix Jain¹; Anna Malovannaya¹; ¹Baylor College of Medicine, Houston, Texas
- MP 405 **Shifted Ions Searching and Other Improvements in the MSFragger Database Search Engine**; Guo Ci Teo¹; Andy T. Kong¹; Hui-Yin Chang¹; Felipe Da Veiga Leprevost¹; Dmitry Avtonomov¹; Alexey I. Nesvizhskii¹; ¹University of Michigan, Ann Arbor, MI
- MP 406 **Prediction of z+1 Hydrogen Rearrangement in ETD Spectra**; Jia R Wu¹; Bin ma¹; Shenheng Guan¹; ¹University of Waterloo, Waterloo, ON
- MP 407 **Open Modification Analysis of Keratin Proteins in Hair and Skin Samples**; Brett S Phinney¹; Michelle R Salemi¹; Glendon J Parker²; Zachary C Goecker²; Robert H Rice²; ¹Proteomics Core Facility, UC Davis Genome Center, University of California, Davis, Davis, CA; ²Department of Environmental Toxicology, University of California, Davis, CA, Davis, CA
- MP 408 **The Sushi Proteome Project towards Unveiling Dietary Metaproteomes without Genomic Information**; Hiroshi Nishida¹; Akiyasu C. Yoshizawa¹; Tsuyoshi Tabata¹; Naoyuki Sugiyama¹; Shujiro Okuda²; Yasushi Ishihama¹; ¹Graduate School of Pharmaceutical Sciences Kyoto University, Kyoto, Japan; ²Niigata University Graduate School of Medical and Dental Sciences, Niigata, Japan
- MP 409 **Development of Custom Peptide MS/MS Analysis Software for Use in a Regulated Environment**; Roger E Moore¹; Denise A Keen¹; Gabriel B Gugiu¹; ¹City of Hope, Duarte, CA
- MP 410 **The Curation of Transcriptomic Data for Use as a Proxy Protein Database for Unsequenced Tree Nuts**; Cary Pirone-davies¹; Melinda A. McFarland¹; Christine H. Parker¹; Timothy R. Croley¹; ¹U.S. Food and Drug Administration, College Park, MD
- MP 411 **Parametric Model Selection Methods for Estimating Target and Decoy Distributions Using Mass Spectrum Characteristics**; Benjamin A. Stark¹; Robert Smith¹; ¹University of Montana, Missoula, MT
- MP 412 **MetaMorpheus Multi-Protease Parsimony Significantly Improves Protein Inference in Bottom-Up Proteomics**; Rachel M. Miller¹; Robert J. Millikin¹; Connor V. Hoffmann¹; Stefan K. Solntsev¹; Gloria M. Sheynkman²; Michael R. Shortreed¹; Lloyd M. Smith¹; ¹University of Wisconsin, Madison, WI; ²Dana-Farber Cancer Institute, Boston, MA
- MP 413 **A Novel LC-MS Deep Learning Based Cancer Detection Program and Improvements with Retention Time Correction**; Yuichi Kokabu¹; Yukihiko Fukamachi¹; Yoriko Takahashi¹; Yasuto Yokoi¹; Masaya Ono²; ¹MITSUI KNOWLEDGE INDUSTRY CO., LTD., Minato-ku, Japan; ²National Cancer Center Research Institute, Chuo-ku, Japan
- MP 414 **Optimizing the Isolation Width in Orbitrap Instruments to Maximize the Number of Label-Free Quantified Peptides and Protein**; Carmen Paschke¹; Waqas Nasir¹; Kai Fritzscheier¹; Rosa Rakownikow Jersie-Christensen¹; Tabiwang N. Arrey¹; David Horn²; Martin Zeller¹; Romain Huguet²; Bernard Delanghe³; ¹Thermo Fisher Scientific, Bremen, Germany; ²ThermoFisher, San Jose, CA; ³Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany
- MP 415 **An Automated Data Analysis Workflow for Intact and Sub-Unit Mass Analysis of Protein Reagents Using Different Mass Spectrometry Platforms**; Dylan Sorensen¹; Han-Yin Yang¹; St. John Skilton²; Eric Carlson²; Dhanashri Bagal¹; ¹Amgen, South San Francisco, CA; ²Protein Metrics Inc., Cupertino, CA
- MP 416 **FragPipe: A Fast Proteomics Pipeline with MSFragger Search Engine at Heart**; Dmitry Avtonomov¹; Andy T. Kong¹; Felipe V. Leprevost¹; Guo-Ci Teo¹; Hui-Yin Chang¹; Alexey I. Nesvizhskii¹; ¹University of Michigan, Ann Arbor, MI
- MP 417 **End-to-End Integration of Known Variants and Modifications from PEFF into the Trans-Proteomic Pipeline for Enriched MS/MS Sequence Determination**; Luis Mendoza¹; Eric W Deutsch¹; Jimmy K Eng²; Robert L Moritz¹; ¹Institute for Systems Biology, Seattle, WA; ²University of Washington, Seattle, WA
- MP 418 **TOMAHTO - An API-enhanced, TMT-based, Targeted Protein Assay with Real-time Instrument Control**; Qing Yu¹; Devin K Schweppe¹; Jose Navarrete-Perea¹; Christopher M. Rose²; Bhavin Patel³; John C Rogers³; Steven P Gygi¹; ¹Harvard Medical School, Boston, MA; ²Genentech, South San Francisco, CA; ³ThermoFisher Scientific, Rockford, IL



- MP 419 **Model-Free SILAC Quantitation Yields Robust Reproducible Results**; [David Chiang](#)¹; Patrick Chu¹; ¹Sage-N Research, Inc., Milpitas, CA
- MP 420 **gpGrouper: A Gene-Centric Peptide Grouping Procedure Accurately Distributes Shared Peptides Across Gene Products and Species**; [Alexander Saltzman](#)¹; Bhoomi Bhatt¹; Mei Leng¹; Anna Malovannaya¹; ¹Baylor College of Medicine, Houston, TX
- MP 421 **Assessing the validity of protein inference on a large environmental metaproteomic dataset - ProteOMZ Expedition of the Central Pacific Ocean**; [Jaclyn K. Saunders](#)¹; Matthew McIlvin¹; Dawn Moran¹; Noelle Held¹; Chris Dupont²; Alyson Santoro³; Mak Saito¹; ¹Woods Hole Oceanographic Institution, Woods Hole, MA; ²J. Craig Venter Institute, La Jolla, CA; ³University of California, Santa Barbara, Santa Barbara, CA
- MP 422 **Propagating Uncertainty in Protein-Level Quantifications is Key to Robust Downstream Analysis of Bottom-Up Proteomics Data**; Alexander Phillips¹; Ranjeet S Bhamber²; Anna Tierney³; Martin Rusilowicz³; Simon Maskell¹; Simon Hubbard³; Andrew R Jones¹; Richard Unwin³; [Andrew W Dowsey](#)²; ¹University of Liverpool, Liverpool, United Kingdom; ²University of Bristol, Bristol, United Kingdom; ³University of Manchester, Manchester, United Kingdom
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- MP 423 **Automated Software for Enhanced Ion Mobility-Mass Spectrometry Analyses with Structures for Lossless Ion Manipulations**; [Aivett Bilbao](#)¹; Joon-Yong Lee¹; Bryson C. Gibbons¹; Gabe Nagy¹; Matthew E. Monroe¹; Thomas O. Metz¹; John C. Fjeldsted²; Yehia M. Ibrahim¹; Richard D. Smith¹; ¹Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA; ²Agilent Technologies, Santa Clara, CA
- MP 424 **New Data Container Construct for Automated Processing of LC/UV/MS Data to Support High Throughput Chemistry**; [Richard Lee](#)¹; Andrey Paramonov¹; ¹ACD/Labs, Toronto, ON
- MP 425 **The Web-Based Application for Exploring Isoform Specific Protein Expression Patterns in Mass Spectrometry Proteomics Data Repositories**; [Han-Yin Yang](#)¹; Bradford W. Gibson¹; ¹Amgen Inc., South San Francisco, CA
- MP 426 **Systematic Evaluation of Cross-linked Peptide Search Engines**; [Zhen-lin Chen](#)¹; Jia-Ming Meng¹; Yong Cao²; Ji-Li Yin¹; Run-Qian Fang¹; Sheng-Bo Fan¹; Chao Liu¹; Wen-Feng Zeng¹; Yue-He Ding²; Dan Tan²; Long Wu¹; Wen-Jing Zhou¹; Hao Chi¹; Rui-Xiang Sun²; Meng-Qiu Dong²; Si-Min He¹; ¹Institute of Computing Technology, Chinese Academy of Sciences, Beijing, China; ²National Institute of Biological Sciences, Beijing, China
- MP 427 **Populating a Vacuum Ultraviolet Spectroscopy Library Using Tandem GC/UV-MS and Chemometric Deconvolution of Real-World Sample Data**; [Shubhneet Warar](#)¹; Ian G. M. Anthony²; Christina A. Gaw²; Touradj Solouki²; ¹Baylor University, Waco, TX; ²Baylor University, Waco, TX
- MP 428 **triMS5 – A Novel Data Format for LC-IMS-MS Data Sets Providing Scalable Representation for Sparse Profile Data**; Jennifer Leclair¹; Thomas Kemmer¹; Andreas Hildebrandt¹; [Stefan Tenzer](#)²; ¹University of Mainz, Mainz, Germany; ²University Medical Center Mainz, Mainz, Germany
- MP 429 **A Platform Approach to Managing Developability and Manufacturability Assessments of Biotherapeutics**; [Albert Van Wyk](#)¹; Joe Shambaugh²; John McCarter²; Aude Tartiere³; Christopher Smith²; Amanda Fitzgerald²; Cassandra Wigmore⁴; Peter Haber⁵; ¹Genedata Ltd, Cambridge, United Kingdom; ²Genedata, Inc., Lexington, MA; ³Genedata, Inc., San Francisco, CA; ⁴Genedata AG, Basel, Switzerland; ⁵Genedata GmbH, Munich, Germany
- MP 430 **Customizable Quality Control Metrics and Notifications with Panorama, AutoQC, and Skyline**; [Josh Eckels](#)¹; Vagisha Sharma²; Marty Pradere¹; Ankur Juneja¹; Angelica Omayei¹; Cory Nathe¹; Sweta Jewargikar¹; Michael J MacCoss²; Brendan X MacLean²; ¹LabKey, San Diego, CA; ²University of Washington, Seattle, WA
- MP 431 **ASMS 2019 Abstract - Audit Logs to Enforce Document Integrity in Skyline and Panorama**; Tobias Rohde¹; [Rita Chupalov](#)¹; Nicholas Shulman¹; Josh Eckels²; Brian S Pratt¹; Michael J MacCoss¹; Brendan X MacLean¹; ¹University of Washington, Seattle, WA; ²LabKey, San Diego, CA
- MP 432 **MZView: Web-based Free Software for LC-MS Data Visualization**; [Lin Wu](#)¹; Bin Ma¹; ¹University of Waterloo, Waterloo, ON
- MP 433 **On-Demand Construction of HRAM MSn Spectral Libraries: Where Acquisition Meets Curation**; Jakub Mezey¹; Samuel Benkovič¹; Melissa Montoya²; Tim Stratton²; Robert Mistrik¹; [Michal Raab](#)¹; ¹HighChem, Bratislava, Slovakia; ²Thermo Fisher Scientific, Austin, Texas
- MP 434 **Implementing a Generic Scripting Node to a Standard Proteomics Workflow Processing Software**; [Frank Berg](#)¹; Kai Fritzscheier¹; Carmen Paschke¹; Torsten Ueckert¹; David Horn²; Bernard Delanghe¹; ¹Thermo Fisher Scientific, Bremen, Germany; ²ThermoFisher, San Jose, CA
- MP 435 **Simple Interface Web Application for Biomaker Validation**; [Jaenyeon Kim](#)¹; Hyunsoo Kim²; Injoon Yeo³; Areum Sohn²; Youngsoo Kim^{2,3,4}; ¹Seoul National University, Seoul, South Korea; ²Seoul National University College of Medicine, Seoul, South Korea; ³Seoul national university, Seoul, South Korea; ⁴Seoul National University Hospital, Seoul, South Korea
- MP 436 **mzMLb: A PSI Standards Compatible Binary Mass Spectrometry Data Format for Efficient Read/Write Speed and Storage Space Requirements**; [Ranjeet S Bhamber](#)¹; Andris Jankevics²; Andy Jones³; Andrew Dowsey¹; ¹University of Bristol, Bristol, United Kingdom; ²University of Birmingham, Birmingham, United Kingdom; ³University of Liverpool, Liverpool, United Kingdom
- MP 437 **The implementation of MSFragger and Philosopher/PeptideProphet nodes in Proteome Discoverer**; [Hui-Yin Chang](#)¹; Andy T. Kong¹; Felipe V. Leprevost¹; Guo Ci Teo¹; Venkatesha Basrur¹; Alexey I. Nesvizhskii¹; ¹University of Michigan, Ann Arbor, MI
- MP 438 **Proteomics Standards Initiative Extended FASTA Format (PEFF)**; [Pierre-Alain Binz](#)¹; Jim Shofstahl²; Juan Antonio Vizcaino³; Harald Barsnes⁴; Robert Chalkley⁵; Gerben Menschaert⁶; Emanuele Alpi⁷; Karl Clauser⁷; Jimmy K Eng⁸; Lydie Lane⁹; Sean seymour¹⁰; Gerhard Mayer¹¹; Martin Eisenacher¹¹; Yasset Perez-Riverol³; Eugene Kapp¹²; Luis Mendoza¹³; Peter R. Baker⁵; Eric Deutsch¹³; ¹CHUV Centre Hospitalier Universitaire Vaudois, Lausanne, Switzerland; ²Thermo Fisher Scientific, San Jose, California; ³EMBL-EBI, Hinxton, United Kingdom; ⁴University of Bergen, Bergen, Norway; ⁵UCSF, San Francisco, CA; ⁶Ghent University, Gent, Belgium; ⁷Broad Institute of MIT and Harvard, Cambridge; ⁸University of Washington, Seattle, WA; ⁹SIB Swiss Institute of Bioinformatics, Geneva, Switzerland; ¹⁰Seymour Data Science, San Francisco, California; ¹¹Ruhr University Bochum, Bochum, Germany; ¹²University of Melbourne, Melbourne, Australia; ¹³Institute for Systems Biology, Seattle, WA



- MP 439 **Proteomics Standards Initiative (PSI) Universal Spectrum Identifier (USI)**; [Eric Deutsch](#)¹; Juan Antonio Vizcaino²; Yasset Perez-Riverol²; Jeremy Carver³; Benjamin Pullman³; Shin Kawano⁴; Zhi Sun¹; Luis Mendoza¹; Pierre-Alain Binz⁵; Gerben Menschaert⁶; Nuno Bandeira³; ¹Institute for Systems Biology, Seattle, WA; ²EMBL-EBI, Hinxton, United Kingdom; ³UCSD, La Jolla, CA; ⁴Database Center for Life Science, Kashiwa, Japan; ⁵CHUV Centre Hospitalier Universitaire Vaudois, Lausanne, Switzerland; ⁶Ghent University, Gent, Belgium
- MP 440 **Repository Scale MS1 Data Processing and Analysis Across Different LC-MS Methods**; [Christine M Aceves](#)¹; Alan K Jarmusch¹; Mingxun Wang¹; Fernando Vargas¹; Pieter Dorrestein¹; ¹Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA
- MP 441 **Panorama Public: ProteomeXchange and Cloud Storage Integration**; [Vagisha Sharma](#)¹; Brian Connolly¹; Josh Eckels²; Dave Bradlee²; Angelica Omaiye²; Trey Chadick²; Michael J MacCoss¹; Brendan X MacLean¹; ¹University of Washington, Seattle, WA; ²LabKey, San Diego, CA
- MP 442 **ProteinExplorer: A Repository-Scale Resource for Exploration of Protein Detection in Public Mass Spectrometry Data Sets**; [Benjamin Pullman](#)¹; Julie S Wertz¹; Jeremy Carver¹; Nuno Bandeira¹; ¹UC San Diego, La Jolla, CA
- MP 443 **proteoQ: An R Package for Versatile Integration of Bioinformatics with Multiplex, High-precision Proteomics**; [Qiang Zhang](#)¹; R Reid Townsend²; ¹Washington University School of Medicine, St. Louis, MO; ²Washington University, School of Medicine, St. Louis, MO
- MP 444 **LipidXplorer Web: An Online Tool for Simplified and Streamlined Lipid Identification by Shotgun Lipidomics**; [Eduardo Jacobo Miranda Ackerman](#)¹; Nils Hoffmann²; Oskar Knittelfelder¹; Kai Schuhmann¹; Robert Ahrends²; Andrej Shevchenko¹; ¹Max Plank Institute for Molecular Cell Biology and Genetics, Dresden, Germany; ²Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Dortmund, Germany
- MP 445 **MassIVE: Converting Terabytes of Raw Public Data into Reusable Community Knowledge**; [Jeremy Carver](#)¹; Mingxun Wang¹; Benjamin Pullman¹; Julie S Wertz¹; Nuno Bandeira¹; ¹UCSD, La Jolla, CA
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- MP 446 **Small Molecule Detection from Biofluids using an Automated Plate-Based Paper Spray System**; [Nicholas Manicke](#)¹; Greta J. Ren¹; Cornelia Boeser²; Neloni Wijeratne²; ¹IUPUI Department of Chemistry & Chemical Biology, Indianapolis, IN; ²ThermoFisher, San Jose, CA
- MP 447 **Analysis of PFASs in Environmental Waters by DART-MS with Coated Dip-it Sampling in Minutes**; [Robert Cody](#)¹; Simin D. Maleknia²; ¹JEOL USA, Inc., Peabody, MA; ²University of Technology Sydney, Sydney, Australia
- MP 448 **Vapor Assisted Ionization Enhancement in An Enclosed Nano-ESI Source**; Yixin Zhu¹; Georgia Dolios²; Fangjun Wang³; Rong Wang²; [Kai Tang](#)¹; ¹Zhejiang Haochuang Biotech Co. Ltd., Hangzhou, China; ²Icahn School of Medicine at Mount Sinai, New York, NY; ³Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China
- MP 449 **Enhancement of Molecular Coverage by Solvent Gradient Electrospray Ionization Using Theta-Glass Capillary Emitters with Laser Ablation Mass Spectrometry**; [Sara K Mattson](#)¹; Sylwia A Stopka¹; Akos Vertes¹; ¹George Washington University, Washington, DC
- MP 450 **Modelling and Experimental Progress towards the Fabrication of Robust Constant-Bore Emitters and their Evaluation on a Novel Electrospray Test Device**; [Kyle Bachus](#)¹; Joe Giddings²; Herbert Foo¹; Heike Ebendorff-Heidepriem^{2,3}; Yvonne Stokes²; Andrew A Gooley¹; ¹Trajan Scientific and Medical, Ringwood, Australia; ²University of Adelaide, Adelaide, Australia; ³Institute for Photonics and Advanced Sensing, Adelaide, Australia
- MP 451 **Evaluation of Bare and Modified Copper Surfaces as Spray Initiators for Ambient Ionization**; [Michael C. Godwin](#)¹; William D. Hoffmann¹; ¹Texas State University, San Marcos, TX
- MP 452 **Intra-well Imaging of Fluid Meniscus and Mass Spectra via Acoustic Mist Ionization Mass Spectrometry**; [Eric Hall](#)¹; Lucien Ghislain¹; Yi-wen Huang¹; Sammy S Datwani¹; ¹Labcyte Inc., San Jose, CA
- MP 453 **Development of Novel Ion Source in a Portable Mass Spectrometer**; Yi-Shin Chen¹; [I-Chung Lu](#)¹; ¹Department of Chemistry, National Chung Hsing University, Taichung City, Taiwan
- MP 454 **Acoustic-Droplet-Ejection to the Open-Port Probe Sampling Interface of MS (ADE-OPP-MS) - the Automated High-Throughput Bioanalysis Platform for Drug Discovery**; [Chang Liu](#)¹; Hui Zhang²; Wenyi Hua²; Jianhua Liu²; David M Cox¹; Thomas R. Covey¹; ¹SCIEX, Concord, ON; ²Pfizer Inc., Groton, CT
- MP 455 **Direct Coupling of Magnetic Nanoparticles and Enhancement of Blade Spray Ionization Mass Spectrometry for Quantitation of Analytes in Complex Matrices**; [Varoon Singh](#)¹; German Augusto Gomez Rios^{1,2}; Milaan Thirukumar¹; Daniel Rickert¹; Janusz Pawliszyn³; ¹University of Waterloo, Waterloo, ON; ²Restek Corporation, Bellefonte, PA; ³University of Waterloo, Waterloo, ON
- MP 456 **Comparison of Electrospray and Impactor Ionization (Unispray) Tandem Mass Spectrometry for the Analysis of Newborn Screening Biomarkers**; [Gylian M Pena](#)¹; Timothy Lim¹; Joanne Mei¹; Konstantinos Petritis¹; ¹CDC, Atlanta, GA
- MP 457 **Establishing Better Laboratory Protocols for Desorption Ionization Using through Hole Alumina Membrane (DIUTHAME)**; [Yasuhide Naito](#)¹; Masahiro Kotani²; Miui Takimoto²; Takayuki Ohmura²; ¹GPI, Hamamatsu, Japan; ²Hamamatsu Photonics K.K., Iwata, Japan
- MP 458 **Large-Area Triboelectric Nanogenerator Nano-electrospray Ionization**; [Marcos Bouza Areces](#)^{1,2}; Yafeng Li¹; Changsheng Wu¹; Zhong Lin Wang^{1,3}; Facundo M. Fernandez^{1,2}; ¹Georgia Institute of Technology, Atlanta, GA; ²Center for Chemical Evolution, Atlanta, GA; ³Beijing Institute of Nanoenergy and Nanosystems, Chinese Academy of Sciences, Beijing, China
- MP 459 **Routine Absorption Mode FTMS Data Display with an Ethoxylated Anionic Detergent as a Dual-Role (Mass and Phase) Calibrant**; [Daniel Cole](#)¹; Peifeng Hu¹; ¹Baxter Healthcare, Round Lake, IL
- MP 460 **Surface Effects in Droplet Chemistry Revealed by Transmission-Mode Liquid Desorption Electrospray Ionization**; [Taghi Sahraei](#)¹; Dmytro Kulyk¹; Abraham K. Badu-Tawiah¹; ¹The Ohio State University, Columbus, OH
- MP 461 **Liquid Injection Field Desorption Ionization in a Host EI/CI Source of a Time-of-Flight Mass Spectrometer**; [Mathias Linden](#)¹; H. Bernhard Linden¹; Jürgen H. Gross²; ¹Linden CMS GmbH, Weyhe, Germany; ²Institute of Organic Chemistry - Heidelberg University, Heidelberg, Germany
- MP 462 **Development of Vibrating Sharp-Edge Spray Ionization (VSSI) for Voltage-Free Mass Spectrometry Analysis**; [Peng Li](#)¹; Xiaojun Li²; Nandhini Ranganathan²; Chong Li²; Stephen Valentine²; ¹West Virginia University, Morgantown; ²West Virginia University.C. Eugene Bennett Department of Chemistry, Morgantown, WV



- MP 463 **Open Port Probe for Rapid Analysis of Biological Samples: Application to Drug Discovery;** Stefan Thibodeaux; *Novartis, Cambridge, MA*
- MP 464 **Next Generation Sample Introduction for High-Throughput Mass Spectrometry: Acoustic Droplet Ejection with an Open Port Probe;** Lucien Ghislain¹; Chang Liu²; Hui Zhang³; Jianjua Liu⁴; Wenyi Hua³; Timothy Foley³; Don W. Arnold⁵; Thomas R. Covey²; Sammy S. Datwani⁶; ¹*Labcyte Inc, San Jose, CA*; ²*SCIEX, Concord, ON*; ³*Pfizer, Groton, CT*; ⁴*Pfizer Inc., Groton, CT*; ⁵*SCIEX, Redwood Shores, CA*; ⁶*Labcyte Inc., San Jose, CA*
- MP 465 **All in One Paper-Based Sample Preparation Integrated with Instant Immunocapture for Targeted Protein Analysis;** Øystein Skjærve¹; Trine Grønhaug Halvorsen¹; Léon Reubsæet¹; ¹*University of Oslo, Oslo, Norway*
- MP 466 **Spray-Capillary: An Electrohydrodynamic Spray-Assisted Device for Quantitative Ultra-Low Volume Extraction;** Lushuang Huang¹; Zhe Wang¹; Si Wu¹; ¹*University of Oklahoma, Norman, OK*
- MP 467 **Regeneration of Dormant Soil Communities by Hydration: A New Platform for Assessing Soil Activity by Direct Real-Time Mass Spectrometry;** Karl Weitz¹; Montana L. Smith¹; Sheryl L. Bell¹; Ljiljana Paša-Tolić¹; Kirsten S Hofmockel¹; Nicole M. Lock²; Malak M. Tfaily^{1,3}; Rosalie K. Chu¹; Mary S. Lipton¹; ¹*Battelle Pacific Northwest National Laboratories, Richland*; ²*Shimadzu Scientific Instruments, Inc., Columbia, Maryland*; ³*University of Arizona, Tucson, AZ*
- MP 468 **A Microdroplet-Catalyzed Biginellireaction: Acceleration, Mechanisms and Separation of Isomers Using IMS-MS.;** Navneet sahota¹; Deyaa I. AbuSalim¹; Melinda L. Wang¹; Tarick J. El-Baba¹; Silas P. Cook¹; David E. Clemmer¹; ¹*Indiana University, Bloomington, IN*
- MP 469 **Development of a 70kV Water Cluster Source for High-Resolution 3D Bio-Imaging;** Allen Bellow¹; Sadia Sheraz née Rabbani²; Hua Tian³; Paul Blenkinsopp¹; Peter J Cumpson⁴; Nicholas Winograd⁵; ¹*Ionoptika Limited, Chandler's Ford, United Kingdom*; ²*Manchester Institute of Biotechnology, University of Manchester, United Kingdom*; ³*Department of Chemistry, Pennsylvania State University, PA*; ⁴*School of Mechanical and Systems Engineering, Newcastle University, United Kingdom*; ⁵*Department of Chemistry, Pennsylvania State University, University Park, PA*
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- MP 470 **Enrichment of Xenon Gas for Targeted Isotope Ratio Mass Spectrometry Utilizing a Digital Ion Trap;** Timothy Vazquez¹; Colette Taylor¹; Sean Williams¹; Emily Smith¹; Theresa Evans-Nguyen¹; ¹*University of South Florida, Tampa, FL*
- MP 471 **Back to Initial Ideas. Harmonized Kingdon Traps with Wire Internal Electrodes;** Eugene (evgeny) Nikolaev¹; Oleg Kharybin¹; Gleb Vladimirov¹; Petr Borisovets¹; Anton Lioznov¹; Anastasia Fursova¹; ¹*Skolkovo institute of science and technology, Moscow Region, Russian Federation*
- MP 472 **Analytical Solution for the Electric Field Inside Dynamically Harmonized FT-ICR Cell;** Anton Lioznov¹; Goekhan Baykut²; Eugene (evgeny) Nikolaev¹; ¹*Skolkovo institute of science and technology, Moscow Region, Russian Federation*; ²*Bruker Daltonik GmbH, Bremen, Germany*
- MP 473 **A Novel Ion Guide Achieving High Transmission Efficiency under a Strong Gas Flow;** Masuyuki Sugiyama¹; Hideki Hasegawa¹; Yuichiro Hashimoto²; ¹*Hitachi, Ltd., Tokyo, Japan*; ²*Hitachi high-technologies corporation, Hitachinaka, Japan*
- MP 474 **Charge Detection Mass Spectrometry of Microparticles Using Printed Circuit Board Electrode Arrays;** Elaura Gustafson¹; Halle V. Murray¹; Yixin Song¹; Jace Rozsa¹; Shih-hua Chiang¹; Aaron R. Hawkins¹; Daniel E. Austin¹; ¹*Brigham Young University, Provo, UT*
- MP 475 **Optimization of the Ions Trajectories in a Dynamically Harmonized Fourier-Transform Ion Cyclotron Resonance Cell Using a Design of Experiments Strategy;** Julien Maillard^{1,2}; Justine Ferey¹; Isabelle Schmitz-Afonso¹; Soumeia Bekri³; Thomas Gautier²; Nathalie Carrasco²; Carlos Afonso¹; Abdellah Tebani³; ¹*Université de Rouen, Laboratoire COBRA UMR 6014 & FR 3038, IRCOF, Mont St Aignan Cedex, France*; ²*LATMOS/IPSL, Université Versailles St Quentin, UPMC Université Paris 06, CNRS, Guyancourt, France*; ³*Department of Metabolic Biochemistry, Rouen University Hospital, Rouen, France*
- MP 476 **Simulation of a Quadrupole Mass Filter Employing a Digital Waveform and Discontinuous Ion Introduction to Obtain High Resolution and Transmission;** David Langridge¹; Martin Green¹; Benjamin Jeffrey²; Robert Appleby²; ¹*Waters Corporation, Wilmslow, United Kingdom*; ²*University of Manchester, Manchester, United Kingdom*
- MP 477 **Evaluation of Two-Dimensional Mass Spectrometry Scans Using a Linear Ion Trap;** Lucas Szalwinski¹; Dalton Snyder²; Zachary St. John³; Graham R. Cooks¹; ¹*Purdue University, West Lafayette, IN*; ²*Resource for Native Mass Spectrometry Guided Structural Biology, Columbus, OH*; ³*The College of New Jersey Department of Chemistry, Ewing Township, New Jersey*
- MP 478 **Application of CAN bus in Mass Spectrometer Design;** Ming Li¹; Kai Li¹; Xingbin Tang¹; ¹*NCS Testing Technology Co., Ltd, Beijing, China*
- MP 479 **Improvement of Electron Capture Efficiency in an RF Ion Trap by optimized Design of Magnetic Field;** Keqin Chen¹; Goran Ristic¹; Pavel Ryumin¹; Bill Loyd¹; Takashi Baba¹; ¹*SCIEX, Concord, ON*
- MP 480 **Advancement and Applications of Harmonic FTICR-MS Signals for Proteome Research;** Sung-Gun Park¹; Jared P. Mohr¹; Gordon Anderson²; James E. Bruce¹; ¹*University of Washington, Seattle, WA*; ²*GAA Custom Engineering, LLC, Benton, WA*
- MP 481 **Detection of Bacteria Growth by ESI Ion Trap Mass Spectrometer;** Chun-Jen Hsiao¹; Jung-Lee Lin¹; Abdil Özdemir²; Chung-Hsuan Chen¹; ¹*Genomics Research Center Academia Sinica, Taipei, Taiwan*; ²*Department of Chemistry, Faculty of Arts and Sciences, Sakarya University, Esentepe, Turkey*
- MP 482 **Characterization of Digital Mass Analysis in a Linear Trap without Resonant Ejection;** Margaret E. Reece¹; Adam P. Huntley¹; Peter T. A. Reilly¹; ¹*Washington State University, Pullman, WA*
- MP 483 **Methods to improve the Extraction Efficiency and Resolution of the Mass Selective Axial Ejection from a Linear Quadrupole Ion Trap;** Mircea Guna; *SCIEX, Concord, ON*
- MP 484 **Design and Performance Improvement of an Ion Cooling Cell for a Quadrupole Mass Spectrometer;** Tsung-Chi Chen¹; Eric C. Hemenway¹; Paul H. Gregory¹; Raman Mathur¹; Hans Schweingruber¹; Oleg Silivra¹; Viatcheslav V. Kovtoun¹; Michael Ugarov¹; Jae C. Schwartz¹; Alan E. Schoen¹; ¹*ThermoFisher, San Jose, CA*
- MP 485 **Improving the Coded Aperture Imaging in a Coded-Aperture Cycloidal Mass Spectrometer;** Raul Vyas¹; Philip J. Herr¹; Kathleen L Horvath¹; Tanouir Aloui¹; Matthew P. Kirley¹; Charles B. Parker¹; Adam D. Keil²; James B. Carlson³; Roger P. Sperline⁴; M Bonner Denton⁴; Brian R. Stoner¹; Michael E. Gehm¹; Jeffrey T Glass¹; Jason J Amsden¹; ¹*Duke University, Durham, NC*; ²*Broadway*



- MP 486 **Analytical, LLC, Monmouth, IL; ³RTI International, Research Triangle Park, NC; ⁴University of Arizona, Tucson, AZ**
A Method to Determine the Mathematical Form of a Toroidal Trap Potential Starting with a Trap Geometry in SIMION® 8.1.; Robert H. Jackson¹; Stephen A. Lammer²; Atanu K. Mohanty³; Xiao Wang⁴; ¹Instrumental Design Physics, Littleton, MA; ²PerkinElmer Inc., American Fork, UT; ³Indian Institute of Science, Bangalore, India; ⁴PerkinElmer, American Fork, UT
- MP 487 **Increasing the Mass Range of Ion-Ion Reactions in a Quadrupole Ion Trap with Waveform Switching;** Kenneth W Lee¹; Gregory S. Eakins¹; Mark S. Carlsen¹; Scott A. Mcluckey¹; ¹Purdue University, West Lafayette, IN
- MP 488 **Portable Ion Trap Mass Spectrometer with Paper Spray Ionization and Comprehensive Scan Modes for V-series Chemical Warfare Agent Identification;** Paul S.Demond¹; Dalton Snyder²; Ethan M McBride³; Carmany Daniel¹; Elizabeth S Dhummakupt³; Phillip M Mach³; R. Graham Cooks²; Trevor Glaros³; ¹Excet, Inc., Springfield, VA; ²Purdue University, West Lafayette, IN; ³ECBC, Aberdeen Proving Ground, Maryland
- MP 489 **Design and Performance of a Rotating Wall Analyzer for High-Throughput Ion Soft Landing;** Pei Su¹; Hang Hu¹; Don Gunaratne²; Julia Laskin¹; ¹Purdue University, West Lafayette, IN; ²Pacific Northwest National Laboratory, Richland, WA
- MP 490 **Theoretical and Experimental Validation of High-Resolution Linear Time-of-Flight Mass Spectrometry;** Sheng-Wei Wu^{1,2}; Yu-Meng Ou^{1,2}; Yi-Hong Cai¹; Chih-Hao Hsiao¹; Cheng-Kai Jan¹; Yi-Sheng Wang¹; ¹Academia Sinica, Taipei City, Taiwan; ²National Taiwan University, Taipei, Taiwan
- MP 491 **Recent Development in Improving the Precision of Quantitative Analysis for Linear Ion Trap(LIT) and LIT-Orbitrap Tandem Mass Spectrometry;** Linfan Li¹; Taoqing Wang²; Anyin Li²; Jae C Schwartz¹; ¹Thermo Fisher Scientific, San Jose, CA; ²University of New Hampshire, Durham, NH
- MP 492 **Application of a Triple Quadrupole MS with Acquisition Speed Improvements for Pesticide Analysis;** Harald Oser¹; Michael Ugarov²; Qingyu Song³; Michael Konicek¹; Claudia P.B. Martins⁴; Neloni Wijeratne⁴; ¹Thermo Fisher Scientific, San Jose, CA; ²Thermo Fisher Scientific, San Jose, California; ³ThermoFisher Scientific, San Jose, CA; ⁴ThermoFisher, San Jose, CA
- MP 493 **Negative Ions Detection with a Spaceflight-Designed Orbitrap-Based Mass Analyzer;** Barnabé Cherville¹; Christelle Briois¹; Laurent Thirkell¹; Bertrand Gaubicher¹; Fabrice Colin¹; ¹Laboratoire de Physique et de Chimie de l'Environnement et de l'Espace, Orléans, France
- MP 494 **High Throughput Charge Detection Mass Spectrometry;** Daniel Botamanenko¹; Aaron R. Todd¹; Martin F Jarrold¹; ¹Indiana University, Bloomington, IN
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- MP 495 **Quantitative Macrolipidomics of Human Whole Blood for the Discovery of Novel Biomarkers of omega-3 Polyunsaturate;** Juan Aristizabal-Henao¹; Ningombam Sanjib Meitei²; Anja Pia Bilttoft-Jensen³; Ken D. Stark¹; ¹University of Waterloo, Waterloo, ON; ²PREMIER Biosoft, Palo Alto, CA; ³Denmark Technical University, Lyngby, Denmark
- MP 496 **Untargeted Lipidomics Reveals Glycerolipid Compositional Changes in Fasted, Cold-Exposed MCAD KO Mice;** wenxuan zhang; University Medical center Groningen, Groningen, Netherlands
- MP 497 **A Rapid Ion Mobility Enabled LC-MS Plasma Lipid Profiling Assay for Breast Cancer Biomarker Discovery;** Adam M King¹; Jimmy Yuk²; Robert D Trengove³; Lauren G Mullin²; Paul D Rainville²; Giorgis Isaac²; Robert S Plumb²; Lee A Gethings⁴; Ian D Wilson⁵; ¹Waters corporation, Wilmslow, United Kingdom; ²Waters Corporation, Milford, MA; ³Murdoch University, Perth, Australia; ⁴Waters Corporation, Wilmslow, United Kingdom; ⁵Imperial College, London, United Kingdom
- MP 498 **AcquireX Workflow Evaluation for Deciphering Lipidome Analysis of Lipids from Whole Insects Using Chromatography Based Methods with High-Resolution Orbitrap MSn;** Daniel Gachotte¹; Yelena A Adelfinskaya¹; Jeffrey Gilbert¹; Reiko Kiyonami²; David Peake²; Yoko Yasuto³; ¹Corteva Agriscience, Indianapolis, IN; ²Thermo Fisher Scientific, San Jose, CA; ³Mitsui Knowledge Industry, Tokyo, Japan
- MP 499 **Red Blood Cell Membrane Fatty Acids in U. S. Blood Donors;** Carissa D. Powers¹; David C. Scully²; Rosemary L. Schleicher¹; ¹Centers for Disease Control and Prevention, Atlanta, GA; ²CDC Foundation, Atlanta, GA
- MP 500 **Tracking the Incorporation of Host Serum Lipids into the Membrane Lipids of Staphylococcus aureus with HILIC-IM-MS;** Kelly M. Hines¹; Gloria Alvarado²; Craig Gatto²; Antje Pokorny³; Brian J. Wilkinson²; Libin Xu¹; ¹University of Washington, Seattle, WA; ²Illinois state university, Normal, IL; ³University of North Carolina Wilmington, Wilmington, NC
- MP 501 **Lipid Pool Coupling Analysis Based on Tandem Mass Spectrometric Data;** Jakob Koch¹; Gregor Oemer²; Katrin Watschinger³; Sabrina Sailer³; Herbert Lindner⁴; Johannes Zschocke²; Markus A. Keller²; ¹Division of Human Genetics, Medical University of Innsbruck, Innsbruck, Austria; ²Division of Human Genetics, Medical University of Innsbruck, Innsbruck, Austria; ³Division of Biological Chemistry, Biocenter, Medical University of Innsbruck, Innsbruck, Austria; ⁴Division of Clinical Biochemistry, Biocenter, Medical University of Innsbruck, Innsbruck, Austria
- MP 502 **The Age of Dermal Fibroblasts in the Tumor Microenvironment Mediate Melanoma Cell Lipid Remodeling;** Aaron R. Goldman¹; Gretchen M. Alicea^{1,2}; Delaine M. Zayas-Bazán^{1,3}; Hsin-Yao Tang¹; Ashani T. Weeraratna¹; David W. Speicher¹; ¹The Wistar Institute, Philadelphia, PA; ²University of the Sciences, Philadelphia, PA; ³University of Pennsylvania, Philadelphia, PA
- MP 503 **Unconventional Synthesis of F-Series Prostaglandins from Lysate of C. elegans and their Identification by LC-MS/MS;** Ekta Tiwary¹; Muhan Hu¹; Landon S. Wilson¹; Taylor F. Berryhill¹; Michael A Miller¹; Jeevan Prasain¹; ¹University of Alabama at Birmingham, Birmingham, AL
- MP 504 **Sphingolipid Phenotype of Adipocyte APP-Overexpressing Mice by LC/MS/MS and SCF/MS/MS;** Yu An¹; Sarah Olive²; Benjamin Figard²; Philipp E. Scherer¹; Ruth Gordillo¹; ¹UTSouthwestern Medical Center, Dallas, TX; ²Shimadzu Scientific Instruments, Inc., Columbia, MD
- MP 505 **A New Lipidomics Software Workflow Demonstrates Disrupted Lipogenesis Induced with Drug Treatment in Leukemia Cells;** Mark Sartain¹; Genevieve Van de Bittner¹; Xiangdong Li¹; Jeremy Koelme²; Adithya Murali¹; Sarah Stow¹; ¹Agilent Technologies, Santa Clara, CA; ²Department of Chemistry, University of Florida, Gainesville, FL
- MP 506 **Desorption Electrospray Ionization Coupled to High Field Asymmetric Ion Mobility Mass Spectrometry Imaging for Investigating Cardiolipin Aberrations in Brain Cancer;** Anna C Krieger¹; Clara Feider¹; J. Clay Goodman²; Livia S. Eberlin¹; ¹The University of Texas at Austin, Austin, TX; ²Departments of Pathology & Immunology and Neurology, Houston, TX
- MP 507 **Lipid Profiling of Malaria Samples Using Orbitrap Velos Pro Mass Spectrometer with SimLipid Software;** Ningombam Sanjib Meitei^{1,2}; Himani Gupta²; Fatima



- MP 508 **Lipidomics Reveals Site-Specific and Circulatory Lipid Profile Dysregulation in Low Carbohydrate/High Protein Diet when Compared to Western Diet; Shama Naz^{1,2}; Lise Cougnaud^{1,3}; Fabiana A. Marques^{1,4}; Heng Jiang⁵; Olivia H. Koury⁶; Mathilde Triquigneaux¹; Andreas Bergdahl⁶; Dajana Vuckovic^{1,2}; ¹Department of Chemistry and Biochemistry, Concordia University, Montréal, QC; ²The Centre for Biological Applications of Mass Spectrometry (CBAMS), Concordia University, Montréal, QC; ³Department of Pharmaceutical Science, University of Bordeaux, Bordeaux, France; ⁴Institute of Chemistry, University of Sao Paulo, São Carlos, Brazil; ⁵The Centre for Biological Applications of Mass Spectrometry (CBAMS), Concordia University, Montréal, QC; ⁶Department of Health, Kinesiology and Applied Physiology, Concordia University, Montréal, QC**
- MP 509 **A Comprehensive Profiling Method for Regulatory Lipid Mediators Using UPLC TimSOF; Jun Yang¹; Xuejun Peng²; Debin Wan¹; Bruce D Hammock¹; ¹Department of Entomology and Nematology, University of California, Davis, Davis, CA; ²Bruker Daltonics Inc., San Jose, CA**
- MP 510 **MRM-Profiling as an Analytical Strategy to Perform the Analysis of Lipids in Extracellular Vesicles; Madison E. Edwards¹; Thomas De Luca²; Christina R. Ferreira¹; Tiago J. P. Sobreira¹; Eric A. Benson²; R. Graham Cooks¹; ¹Purdue University, West Lafayette, IN; ²Indiana University School of Medicine, Indianapolis, Indiana**
- MP 511 **Untargeted Lipidomic Profiling of Bis(monoacylglycerol) phosphate Lipids in Cancer Cells and Tumor Tissues Point to Transformation Specific Regulation of Acyl Chains; Megan Showalter¹; Anastasia Berg²; Michael Sa¹; Hiroshi Tsugawa³; Tobias Kind¹; Kermit Carraway, III²; Oliver Fiehn¹; ¹UC Davis West Coast Metabolomics Center, Davis, CA; ²Department of Biochemistry and Molecular Medicine UC Davis, Sacramento, CA; ³RIKEN Center for Sustainable Resource Science, Wako, Japan**
- MP 512 **Lipids is the Promising Biomarker to Classify HCC Cell Lines' Subtype Using SALDI-MS; Tao Wang¹; Jianmin Wu¹; ¹Zhejiang University, Hangzhou, China**
- MP 513 **Comprehensive LC-MS Lipidomic Analysis of Viral and Plasma Lipid Alterations in SIV-Infected Rhesus Macaques Treated with and without Antiretroviral Agents; Yong Jiang¹; Sijia Tao¹; Christina Gavegnano¹; Ruby R Kleinbard¹; Raymond F Schinazi¹; ¹Center for AIDS Research, Department of Pediatrics, Emory University, Atlanta, GA**
- MP 514 **Lipidomic Analysis of IKE-Induced Ferroptosis in Lymphoma Mouse Model; Fereshteh Zandkarimi^{1,2}; Yan Zhang³; Hui Tan³; Jacob D. Daniels⁴; Hengrui Liu³; Lewis M. Brown^{1,2}; Brent R Stockwell^{1,3}; ¹Department of Biological Sciences, Columbia University, New York, NY; ²Quantitative Proteomics and Metabolomics Center, New York, NY; ³Department of Chemistry, Columbia University, New York, NY; ⁴Department of Pharmacology, Columbia University Medical Center, New York, NY**
- MP 515 **Stools Lipid Profiling by HILIC LC-MS/MS – A Step Forward to a Non-Invasive Diagnostic of Diseases; Justine Hustin¹; Raphaël La Rocca¹; Johann Far¹; Delphine Debois²; Edwin De Pauw¹; Gauthier Eppe¹; Loïc Quinton¹; ¹University of Liege, MS Lab - GIGA, MolSys Research Unit, Liege, Belgium; ²ZenTech S.A., Liege, Belgium**
- MP 516 **Untargeted Lipidomics Analysis Reveals Effect of Abomasal Omega-3 Fatty Acid Infusion on Bovine Lipidome; William Myers¹; Eduardo Rico¹; Joseph W McFadden¹; Maria Elena Diaz Rubio¹; Sheng Zhang¹; ¹Cornell University, Ithaca, NY**
- MP 517 **Quantitative Analysis of Phospholipids and Triacylglycerol Lipids by Multiple Reaction Monitoring Profiling (MRM-Profiling); Zhuoer Xie¹; Christina R. Ferreira¹; Alessandra A. Vireque²; Tiago J. P. Sobreira¹; R. Graham Cooks¹; ¹Purdue University, West Lafayette, IN; ²Invitro, Assisted Reproductive Technologies Ltd., Ribeirão Preto, Brazil**
- MP 518 **Separating and Profiling Phosphatidylcholines and Triglycerides from Single Lipid Droplet in HepG2 Cells by In-Tip Solvent Microextraction Mass Spectrometry; Yaoyao Zhao¹; Hitoshi Chiba²; Shu-Ping Hui³; ¹Hokkaido University, Sapporo, Japan; ²Sapporo University of Health Sciences, Sapporo, Japan; ³Hokkaido University, Sapporo, Japan**
- MP 519 **Lipidomic Profiling of Pancreatic Cancer Extracellular Vesicles Reveals Unique Signatures; Shivani Bansal¹; Charles P. Hinzman¹; Michael Girgis¹; Giorgis Isaac²; Nyasha Munjoma²; Amrita K. Cheema¹; ¹Georgetown University Medical Center, Washington, DC; ²Waters Corporation, Milford, MA**
- MP 520 **Novel Findings in HILIC Based LC-MS/MS Methods for Targeted Lipidomics Profiling; Goncalo Vale¹; Sarah Martin²; Mackenzie Pearson³; Jeffrey G. McDonald¹; ¹UT Southwestern, Dallas, TX; ²Agios Pharmaceuticals, Cambridge, MA; ³Sciex, Redwood City, CA**
- MP 521 **Development and Deployment of a Lipidomics Platform for the Characterization of Lipid Composition Differences in Strains of *Bacillus subtilis*; David Reeves^{1,2}; Suresh Poudel³; Robert L. Hettich^{1,3}; ¹University of Tennessee, Knoxville, TN; ²Oak Ridge National Laboratory, Oak Ridge, TN; ³Oak Ridge National Laboratory, Oak Ridge, Tennessee**
- MP 522 **Separation and Detection Method for the Profiling of Glycosphingolipids Using Liquid Chromatography Fluorescence Mass Spectrometry (LC-FLD-MS); Bela Reiz¹; Radhika Chakraborty^{1,2}; Randy M. Whittall¹; Christopher W. Cairo^{1,2}; ¹Department of Chemistry, University of Alberta, Edmonton, Alberta; ²Alberta Glycomics Centre, Edmonton, Alberta**
- MP 523 **Combination of Distinctive Features Allows Rapid and Reliable Brain Tumor Tissue Identification; Anatoly Sorokin^{1,2}; Stanislav Pekov^{1,3}; Vsevolod Shurkhai^{1,4}; Vasilii Eliferov¹; Konstantin Bocharov¹; Veronika Storozhilova¹; Igor Popov^{1,3}; Alexander Potapov⁴; Eugene (evgeny) Nikolaev⁵; ¹Moscow Institute of Physics and Technology (State University), Dolgoprudny, Russia; ²Institute of Cell Biophysics RAS, Pushchino, Russia; ³Institute for Energy Problems of Chemical Physics RAS, Moscow, Russia; ⁴N. N. Burdenko Scientific Research Neurosurgery Institute, Moscow, Russia; ⁵Skolkovo institute of science and technology, Moscow Region, Russian Federation**
- MP 524 **Mapping the Lipid Transducers of Exercise in Rats and Human Subjects; David Gaul¹; Sam Moore¹; Alexandra Coomes²; Collin Douglas²; Karyn Esser²; Neil Johannsen³; Kate Early⁴; ¹Georgia Institute of Technology, Atlanta, GA; ²University of Florida, Gainesville, FL; ³Louisiana State University, Baton Rouge, LA; ⁴Columbus State University, Columbus, GA**
- MP 525 **Development of Phospholipids Profiling of Mouse Tissues by PRM and Quantitative MS1 Multiplexing; Xiaorong Fu¹; Goncalo Vale²; Jeffrey G. M. McDonald¹; Matthew Mitsche¹; ¹UT Southwestern Medical Center, Dallas, Texas; ²University of Texas Southwestern Medical Center, Dallas, Texas**
- MP 526 **S6K2 Inhibition Causes Lipid Remodeling and Reduced Growth in NRAS Mutant Melanoma Cells; Delaine M. Zayas-Bazan^{1,2}; Aaron R. Goldman²; Yun Hao^{2,3}; Hsin-Yi Chen²; Jessie Villanueva²; David W. Speicher²; ¹University of Pennsylvania, PA, PA; ²The Wistar Institute, Philadelphia, PA; ³University of Pennsylvania, Philadelphia**



- MP 527 **Rapid and Sensitive Characterization of FAHFA Lipids Using an Untargeted Lipidomics Approach;** Tong Shen¹; Bryan Roberts¹; Oliver Fiehn¹; ¹UC Davis West Coast Metabolomics Center, Davis, CA
- MP 528 **Mapping the Algal Lipidome to Expand the Biofuel and Bioproduct Portfolio;** Peter V. Shanta¹; Steven M. Rowland¹; Stefanie Van Wychen¹; Tao Dong¹; Lieve M. Laurens¹; ¹National Renewable Energy Laboratory, Golden, CO
- MP 529 **Effects of Various Temperature Related Storage Conditions on Human Plasma and Serum Lipid Profile;** Greg B. Reis¹; Jon Rees¹; Zsuzsanna Kuklenyik¹; ¹Centers for Disease Control and Prevention, Atlanta, Georgia
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- MP 530 **MSI and LC-MS Reveals Alterations of Phosphoinositides in Niemann-Pick Disease, Type C1;** Koralege Praneeth Chandimal Pathmasiri¹; Melissa R Pergande¹; Fernando Tobias¹; Stephanie M Cologna¹; ¹University of Illinois at Chicago, Chicago, IL
- MP 531 **Mass Spectrometric Assessment on the Biological Fate of Gemini Surfactants Used as Gene Delivery Agents;** Wei Jin¹; Mays Al-Dulaymi¹; Randy Purves²; Ildiko Badea¹; Anas El-Aneed¹; ¹University of Saskatchewan, Saskatoon, SK; ²Centre for Veterinary Drug Residues, Canadian Food Inspection Agency, Saskatoon, SK
- MP 532 **Ion Suppressing Contaminants Generated by Multiple Injections from the Same Sample Vial Negatively Impact Reverse Phase Based-Lipidomics Experiments;** Peter Benke¹; Bo Burla¹; Kim Ekroos²; Markus R Wenk¹; Federico Torta¹; ¹National University of Singapore, Singapore, Singapore; ²Lipidomics Consulting Ltd, Esbo, Finland
- MP 533 **High-Throughput, Comprehensive Lipid/Protein Composition and Particle Number Analysis of Lipoproteins in Normal and Dyslipidemic Patients;** John R. Barr¹; Michael Stephen Gardner¹; Zsuzsanna Kuklenyik¹; David Schieltz¹; Antony Lehtikoski²; Jennifer Kusovschi¹; Jon Rees¹; Christopher Toth¹; Michael S. Andrews¹; Bryan M. Parks¹; James L Pirkle¹; ¹CDC, Atlanta, GA; ²Battelle Memorial Institute at the Centers for Disease Control and Prevention, Atlanta, GA
- MP 534 **High-Throughput Targeted Lipidomics Analysis of Dihydroceramide Desaturase-1 (DES1) Knockout Mice;** Mackenzie Pearson¹; Santosh Kapil¹; Trevor S Tippets²; Scott A Summers²; ¹Sciex, Redwood City, CA; ²University of Utah, Salt Lake City, UT
- MP 535 **An Inhibitor of iPLA2 γ , R-BEL, Prevents Lipid Mediator Generation in the Ileum and Leads to Radiomitigation after Total Body Irradiation.;** Vladimir Tyurin¹; Yulia Tyurina¹; Andrew Amoscato¹; Louis J. Sparovero¹; Michael Epperly¹; Claudette St. Croix¹; Alan Watson¹; Simon Watkins¹; Joel Greenberger¹; Hulya Bayir¹; Valerian Kagan¹; ¹University of Pittsburgh, Pittsburgh, PA
- MP 536 ***P. aeruginosa* Lipoxigenase (pLoxA) Generates Ferroptotic Cell Death Signals in Host Human Bronchial Epithelial Cells: LC/MS Study.;** Yulia Tyurina¹; Dar Haider¹; Vladimir Tyurin¹; Andrew Amoscato¹; Joseph Joseph¹; Rama Mallampalli²; Hulya Bayir¹; Valerian Kagan¹; ¹University of Pittsburgh, Pittsburgh, PA; ²The Ohio State University, Columbus, OH
- MP 537 **A Rapid Quantitative Method for Analysis of Oxidation Products of Cholesteryl Linoleate, Total Cholesteryl Esters, and Free Cholesterol by LC-APCI-MS/MS;** Michael Gardner¹; Jon Rees²; Gregory Reis²; Lisa G. McWilliams²; Zsuzsanna Kuklenyik²; John R. Barr²; ¹Centers for Disease Control and Prevention, Atlanta, GA; ²Centers for Disease Control and Prevention, Atlanta, GA
- MP 538 **Improved High-Throughput Targeted Lipidomics Analysis with sMRM Pro Builder;** Santosh Kapil Kumar Gorti¹; Mackenzie Pearson²; Sean seymour³; Christie Hunter⁴; Paul Baker⁴; ¹SCIEX, Framingham, MA; ²Sciex, Framingham, MA; ³Seymour Data Science, San Francisco, California; ⁴Sciex, Redwood City, CA
- MP 539 **Enhanced Quantification of LPA 18:1 in Plasma with Differential Mobility Separation Technology;** Cyrus Papan¹; Joerg Dojahn¹; Sean Wu²; ¹SCIEX, Darmstadt, Germany; ²Sciex, Framingham, MA
- MP 540 **Quantifying the Lipidome for Respiratory Disease: A Rapid and Comprehensive HILIC-Based Targeted Approach;** Giorgis Isaac¹; Nyasha Munjoma²; Lee A Gethings²; Robert S Plumb¹; ¹Waters Corporation, Milford, MA; ²Waters Corporation, Wilmslow, United Kingdom
- MP 541 **Identification and quantitation of Lysophosphatidic Acid Regioisomeric Species in Mouse Plasma;** Juan Aristizabal-Henao¹; Maria Fernanda Fernandes¹; Robin E Duncan¹; Ken D. Stark¹; ¹University of Waterloo, Waterloo, ON
- MP 542 **Combinatorial Chemistry to Synthesize Glycerolipidomic Mixtures with an Arbitrary Number of Components of Known Concentration;** Tom Brenna¹; Dong Hao Park¹; ¹University of Texas at Austin, Austin, TX
- MP 543 **Semi-targeted Profiling of Fatty Acids Using Polycylamide Derivatization and C30 Reverse Phase Chromatography Coupled with High Resolution Tandem Mass Spectrometry;** Lucas Veillon¹; Marc O. Warmoes¹; Philip L Lorenzi¹; John N Weinstein¹; ¹MD Anderson Cancer Center, Houston, TX
- MP 544 **Ganglioside Lipidomics in Human Dried Blood Spots Utilizing micro-LC/MS and MS/MS;** Asoka Ranasinghe¹; Celia D'Arienzo²; Timothy Olah²; ¹Bristol-Myers Squibb Company, Princeton, NJ; ²Bristol-Myers Squibb Co., Princeton, NJ
- MP 545 **Dual Mass Spectrometry as a Tool to Improve Annotation and Quantification in Targeted Plasma Lipidomics;** Liang Gao¹; Amaury Cazenave-Gassiot²; Bo Burla¹; Markus R Wenk³; Federico Torta³; ¹Singapore Lipidomics Incubator (SLING), Life Sciences Institute, National University of Singapore, Singapore, Singapore; ²Department of Biochemistry, Yong Loo Lin School of Medicine, National University of Singapore, Singapore, Singapore; ³Department of Biochemistry, Yong Loo Lin School of Medicine, National University of Singapore, Singapore, Singapore
- MP 546 **Comprehensive Metabolic Profiling of Eicosanoids and Related Fatty Acids of Serum or Plasma by a Widely Targeted LC-MS/MS;** Masaki Yamada¹; Huan Lin¹; Takanari Hattori¹; ¹Shimadzu corp., Kyoto, Japan
- MP 547 **FIA-HRMS-Based Lipidomics Method: Comparing Measured Lipid Concentration Calculated Using Parent Molecular Ion Abundance Versus Sum of Product Ions Abundances;** Alexander Triebel¹; Federico Torta¹; Himani Gupta²; Ningombam Sanjib Meitei^{2,3}; Rupanjana Goswami²; ¹Singapore Lipidomics Incubator (SLING), Department of Biochemistry, YLL School of Medicine, National University of Singapore, Singapore, Singapore; ²PREMIER Biosoft, Indore, India; ³PREMIER Biosoft, Palo Alto, CA
- MP 548 **Alteration of Lipidome Due to Vitamin B12 Deficiency;** Akash Kumar Bhaskar^{1,2}; Khusbhoo Adlakha¹; Salwa Naushin^{1,2}; Arjun Ray¹; Praveen Singh^{1,2}; Monu Kumar¹; Akanksha Singh³; Dipankar Malakar³; Christie Hunter⁴; Shantanu Sengupta^{1,2}; ¹CSIR-Institute of Genomics and Integrative Biology, New Delhi, India; ²Academy of Scientific & Innovative Research, New Delhi, India; ³SCIEX, Gurgaon, India; ⁴Sciex, Redwood City, CA
- MP 549 **Analysis of Fatty Acids in GEMM Lymphatic Tumors with Mass Spectrometry: GC-MS Versus LC-MS;** Min Liu¹; Jayden Cline¹; Kristen E.N. Scott¹; David C. Koomen¹; John M. Koomen¹; John L. Cleveland¹; ¹Moffitt Cancer Center, Tampa, FL



- MP 550 **Steroid Analysis in Human Plasma: Comparative Evaluation of Sorbent-Based Platforms for Phospholipid Removal;** Karolina M. Krasinska¹; Allis S. Chien¹; ¹SUMS, Stanford University, Stanford, CA
- MP 551 **Fast Supercritical Fluid Chromatography Separation and Shotgun Lipidomics with High Resolution Mass Spectrometry for the Study of Breast Cancer Metastasis;** Sheher Mohsin¹; Ningombam Sanjib Meitei²; Peter Siegel³; Daina Avizonis⁴; Gaelle Bridon⁵; ¹Agilent Technologies, Schaumburg, IL; ²PREMIER Biosoft, Indore, India; ³Goodman Cancer Research Centre, Montreal, QC; ⁴Goodman Cancer Research Centre, Quebec, Montreal, Canada; ⁵Agilent Technologies, Inc., Wilmington, DE
- MP 552 **Analysis, Re-Analysis, and Quantitative Comparison of Lipidomics Using 13C-Labeled Cultures for Internal Standardization.;** Peining Xu¹; Joyce Liu²; Sophie Trefely^{1,2}; Clementina Mesaros³; Kathryn E. Wellen²; Nathaniel W Snyder¹; ¹Drexel University, Philadelphia, PA; ²University of Pennsylvania, Philadelphia, PA; ³University of Pennsylvania, Philadelphia, PA
- MP 553 **Stable Isotope Labeling to Study Synaptamide Biosynthesis in Neuronal Cell Culture;** Karl R Kevala¹; Michel Lagarde²; Arthur Spector¹; Hee-Yong Kim¹; ¹NIAAA/NIH, Rockville, MD; ²Universite de Lyon, INSA, Lyon, France
- MP 554 **in vivo Measurement of Oxylipins in Rat Brain Using Solid-Phase Microextraction and LC-MS;** Alexander Napylvov¹; Nathaly Reyes Garces²; Mariola Olkowicz²; Sofia Lendor²; Ezel Boyaci²; German Gomez-Rios²; Cian Monnin¹; Mustansir Diwan³; Barbara Bojko²; Clement Hamani³; Janusz Pawliszyn²; Dajana Vuckovic⁴; ¹Concordia University, Montreal, Qc; ²University of Waterloo, Waterloo; ³Sunnybrook Health Sciences Centre, Toronto, ON; ⁴Concordia University, Montreal, QC
- MP 555 **A Comparative Lipidomic Analysis between 2D and 3D Cell Culture of Adipocytes Derived from Mouse Primary Cell;** Jonghyun Kim¹; Kyoung-Jin Choi²; Sung Bum Park²; Yoon-Ju Na³; Ki Young Kim²; Tae-Young Kim¹; ¹Gwangju Institute of Science & Technology, Gwangju, South Korea; ²Therapeutics & Biotechnology Division, Korea Research Institute of Chemical Technology, Daejeon, South Korea; ³Department of New Drug Discovery and Development, Chungnam National University, Daejeon, South Korea
- MP 556 **Comparison of Various Orthogonal Instrumental Approaches to Lipidomics Analysis of Human Blood;** Ken Riedl¹; Ella Lin¹; Kiran Boyinepally¹; Ewy Mathe¹; ¹The Ohio State University, Columbus, OH
- MP 557 **Machine Learning Perspectives on Region of Interest Identification and Analysis in DESI Spectrometry;** Austin Ahlstrom¹; John C Price²; ¹Brigham Young University, Provo, UT; ²Brigham Young University, Provo, Utah
- MP 558 **Stable Isotope Labeling by Permethylation and Reversed-Phase LC/MS for Relative Quantification of Intact Neutral Glycolipids in Mammalian Cells;** Rodell Barrientos^{1,2}; Qibin Zhang^{1,2}; ¹Department of Chemistry and Biochemistry, University of North Carolina at Greensboro, Greensboro, NC; ²UNCG Center for Translational Biomedical Research, Kannapolis, NC
- METABOLOMICS: IDENTIFICATION OF UNKNOWN METABOLITES**
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- MP 559 **THE SPECTRUM FACTORY: A New Workflow for the Creation of Libraries of Unknown Mass Spectra from Known Precursor Compounds;** John M. Halket¹; Anna M. Caldwell²; W. Gary Mallard³; Stephen E. Stein³; ¹King's College London, London, United Kingdom; ²King's College London, London, United Kingdom; ³NIST, Gaithersburg, MD
- MP 560 **Using Stable Isotope Labeling to Facilitate Unknown Metabolite Identification: A Case Study of Yeast Gene YNL010W;** Wenyun Lu¹; Yifan Xu²; Joshua D. Rabinowitz¹; ¹Princeton University, Princeton, NJ; ²DuPont Industrial Biosciences, Wilmington, DE
- MP 561 **Novel Deep Annotation Strategies for Non-Targeted Plant Metabolomics Based on High Resolution Mass Spectrometry;** Zaifang Li¹; chunxia Zhao¹; Xiuqiong Zhang¹; Yueyi Xia¹; Hua Zhang¹; Xin Lu¹; Guowang Xu¹; ¹CAS Key Laboratory of Separation Science for Analytical Chemistry, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China
- MP 562 **Identification of Metabolites from *Avicennia camambola* L. Bark by Combination of Paper Spray & Electrospray Ionization Mass Spectrometry;** Syful Islam¹; Md Badrul Alam²; Arif Ahmed²; Sunghwan Kim²; ¹Department of Chemistry, Kyungpook National University, Daegu, South Korea; ²Kyungpook National University, Daegu, South Korea
- MP 563 **Discovery of Unknown Metabolic Interactions of Microbiota & Human Host – Combining Novel Metabolomics and Chemical Biology Methodologies;** Daniel Globisch^{1,2}; Louis P. Conway¹; Mario S. P. Correia¹; Caroline Ballet¹; Neeraj Garg¹; ¹Uppsala University, Uppsala, Sweden; ²SciLifeLab, Uppsala, Sweden
- MP 564 **Detecting Low Abundant Endogenous Cardiac Steroids from Biological Fluids Using Structure-Based MSn Approach On an OrbitrapTM TribridTM MS;** Reiko Kiyonami¹; Michael Harrington²; Alfred Fonteh²; Roger Biringer³; Andreas Huhmer¹; ¹Thermo Fisher Scientific, San Jose, CA; ²Huntington Medical Research Institutes, Pasadena, CA; ³LECOM Bradenton, Bradenton, FL
- MP 565 **Magnetic Resonance Mass Spectrometry Profiling of Myxobacterial Extracts – Higher Resolution, Deeper Insights?;** Chantal Bader¹; Patrick Haack¹; Fabian Panter¹; Matthias Witt²; Daniel Krug¹; Rolf Müller¹; ¹Helmholtz-Institute for pharmaceutical research Saarland (HIPS), Saarbrücken, Germany; ²Brüker Daltonik GmbH, Bremen, Germany
- MP 566 **Development of a *Caenorhabditis elegans* Reference Material for Long-Term LCMS Metabolomics Quality Control and Unknown Compound Identification;** Goncalo J. Gouveia¹; Brianna M Garcia²; Emerson Ferreira Queiroz³; Franklin E. Leach III⁴; David L. Blum¹; Jean-Luc Wolfender³; Lauren M. McIntyre⁵; I. Jonathan Amster²; Arthur S. Edison¹; ¹Department of Biochemistry and Molecular Biology, University of Georgia, Athens, GA; ²Department of Chemistry, University of Georgia, Athens, GA; ³School of Pharmaceutical Sciences, University of Geneva, Geneva, Switzerland; ⁴Department of Environmental Health Science, University of Georgia, Athens, GA; ⁵Department of Molecular Genetics and Microbiology, University of Florida, Gainesville, FL
- MP 567 **Novel Psychoactive Substances Detection Using a Novel Multi-Aspect Workflow Solutions;** Melissa Montoya¹; Tim Stratton¹; ¹Thermo Fisher Scientific, Austin, Texas
- MP 568 **Electrochemical Simulation of Phase I Metabolism of Three Novel Cardiovascular Drugs Using UHPLC-MS/MS;** Martin Eysberg¹; Małgorzata Szultka-Młyńska²; Jean-Pierre Chervet³; ¹Antec Scientific, Boston, MA 02108; ²Department of Environmental Chemistry and Bioanalytics, Nicolaus Copernicus University, Torun, Poland; ³Antec Scientific, Zoeterwoude, Netherlands
- MP 569 **Enabling Rapid and High-Confidence Metabolite Identification Using HILIC-QTOF Based MS/MS-RT library;** Shuang Zhao¹; Wan Chan¹; Ulrike Schweiger-Hufnagel²; Aiko Barsch²; Liang Li¹; ¹University of Alberta, Edmonton, AB; ²Brüker Daltonik GmbH, Bremen, Germany



- MP 570 **A Complete Workflow for Improved Untargeted Metabolome Annotation and Identification Using Ultra High-Resolution Accurate Mass and LC-MSn Orbitrap-Based Mass Spectrometry;** [David A. Peake](#)¹; Reiko Kiyonami¹; Ioanna Ntai¹; Amanda Souza¹; Ralf Tautenhahn¹; ¹Thermo Fisher Scientific, San Jose, CA
- MP 571 **Mass Spectrometry for Identification of Metabolites Secreted by Methamphetamine Treated Human Primary Macrophages;** [Katarzyna Lech](#)^{1,2}; Katarzyna Pawlak^{1,2}; Akou Vei¹; Emma Harwood¹; Spencer Marshall Jaquet¹; Brenda Morsey¹; Howard S. Fox¹; Pawel Ciborowski¹; ¹University of Nebraska Medical Center, Omaha, NE; ²Faculty of Chemistry, Warsaw University of Technology, Warsaw, Poland
- MP 572 **A Method of Calculating Retention Index of the Second Dimension Separation in Comprehensive Two-Dimensional Gas Chromatography Mass Spectrometry;** [Md Aminul Islam Proadhan](#)¹; Ahmed A Sleman¹; Xinmin Yin¹; Pawel Lorkiewicz¹; Seongho Kim²; Craig McClain¹; Xiang Zhang¹; ¹University of Louisville, Louisville, KY; ²Wayne State University, Detroit, MI
- MP 573 **Off-line fractionation of Complex Samples to Improve Depth-of-Coverage and Aid Compound Identification in Metabolomics;** [Charles R Evans](#)¹; Brady G Anderson¹; Maureen T Kachman¹; ¹University of Michigan, Ann Arbor, MI
- MP 574 **Comparison of Different Compound Spectral Libraries with DDA and DIA Analyzed Extracted Plasma for Metabolite Identification;** Robert Proos¹; Khatereh Motamedchaboki²; [Anthony Romanelli](#)¹; ¹Sciex, Framingham, MA; ²Sciex, Redwood City, CA
- MP 575 **IROA Approach Enabling Detection of Metabolites Whose Production is Initiated or Ceased in Response to Treatment;** Amy L. Lane¹; [Felice de Jong](#)²; Chris Beecher²; ¹University of North Florida, Jacksonville, FL; ²IROA Technologies LLC, Bolton, MA
- MP 576 **CHO Cell Culture Media Profiling and Unknown Identification by Liquid Chromatography and Accurate Mass High Resolution Mass Spectrometry;** [Richard Rogers](#)¹; Xuejun Peng²; Guillaume Tremintin²; ¹Just Biotherapeutics, Seattle, WA; ²Bruker Daltonics, San Jose, CA
- PEPTIDES: SEQUENCE ANALYSIS**
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- MP 577 **Applications of a Novel Hydrolysis System for Deconvolution of Cyclotides on a Bead and Super Rapid Amino Acid Analyses;** [Kiyoshi Nokihara](#)¹; Yuki Tominaga¹; Takeshi Kasama¹; Haruyuki Fujino¹; Atsushi Kitagawa¹; ¹HiPep Laboratories, Kyoto, Japan
- MP 578 **Electron Transfer Dissociation of Highly Acidic peptides Following Enhanced Protonation Using Chromium(III) with Electrospray Ionization;** [Surakshya Thapa](#)¹; Carolyn J. Cassidy¹; ¹University of Alabama, Tuscaloosa, AL
- MP 579 **Proteogenomics-Assisted Identification of Novel Variants Peptides after p53 Loss in Wild-Type p53 Harboring Human Melanoma Cell Lines;** [Satya Saxena](#)^{1,2}; Mohd M Khan³; Jakub Faktor⁴; Nathan P Manes⁵; Sachin Kote²; Georges Bedran²; Javier Alfaro²; Aleksandra Nita-lazar⁶; Borek Vojtesek⁴; Theodore Hupp^{2,6}; David R. Goodlett^{2,3}; ¹Deurion LLC, Seattle, WA; ²International Centre for Cancer Vaccine Science, University of Gdansk, Gdansk, Poland; ³University of Maryland, Baltimore, MD; ⁴RECAMO, Brno, Czech Republic; ⁵NIH/NIAID, Bethesda, MD; ⁶University of Edinburgh, Edinburgh, United Kingdom
- MP 580 **Analysis Platform for accurate amino acid sequencing combining with a benchtop MALDI-TOF MS and N/C-terminal sequencing;** [Nanami Sakashita](#)¹; Tomoko Kuriki¹; Brian J. Field²; Yuzo Yamazaki¹; ¹Shimadzu Corporation, Kyoto, Japan; ²Shimadzu Scientific Instruments, Inc., Columbia, MD
- MP 581 **Advances in Structural Elucidation Techniques for the Characterization of Cystine-Knot Peptides;** [Sarah J. Robinson](#)^{1,2}; Christopher M Crittenden¹; ¹Small Molecule Pharmaceutical Sciences, Genentech Inc., South San Francisco, CA; ²Discovery Chemistry, Genentech Inc., South San Francisco, CA
- MP 582 **Characterization of Five Commonly Used Chymotrypsins;** [Yunyun Zhu](#)¹; Alexander S. Herbert^{2,3,4}; Joshua J Coon^{2,3,4,5}; ¹University of Wisconsin-Madison, Madison, WI; ²Genome Center of Wisconsin, Madison, WI; ³Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI; ⁴Department of Biochemistry, University of Wisconsin, Madison, WI; ⁵Department of Chemistry, University of Wisconsin, Madison, WI
- MP 583 **Structural Characterization of Cyclic Peptides Using a Quadrupole Time-of-Flight Mass Spectrometer;** [Toshiya Matsubara](#)¹; Yusuke Inohana¹; Ichiro Hirano¹; ¹Shimadzu Corporation, Kyoto, Japan
- MP 584 **Investigating the Cleavage Capability of the Proteases LysN, LysArginase and Chymotrypsin in Complex, Biotinylated Samples;** [Peter Schein](#)¹; Volkmar Gieselmann¹; Marc Sylvester¹; ¹Institute of Biochemistry and Molecular Biology, Rheinische Friedrich-Wilhelms University of Bonn, Bonn, Germany
- PEPTIDOMICS**
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- MP 585 **Multiplex Dimethylated Leucine (DiLeu) Isobaric Tags to Probe Neuropeptidomic Response to Copper Toxicity in the Blue Crab, *Callinectes sapidus*;** [Chris Sauer](#)¹; Lingjun Li¹; ¹University of Wisconsin-Madison, Madison, WI
- MP 586 **Single Amino Acid Variant Discovery in 9 Panc-1 Cells;** [Zhijing Tan](#)¹; Xinpei Yi²; Nicholas J. Carruthers³; Paul M. Stemmer³; David M. Lubman⁴; ¹University of Michigan, Ann Arbor, MI; ²University of Chinese Academy of Sciences, Beijing, China; ³Wayne State University, Detroit, Michigan; ⁴University of Michigan, Ann Arbor, MI
- MP 587 **Capillary Zone Electrophoresis-Tandem Mass Spectrometry for Large-Scale Phosphoproteomics with over 11,000 Phosphopeptides IDs from the Colon Carcinoma HCT116 Cell Line;** [Daoyang Chen](#)¹; Katelyn R. Ludwig²; Oleg V. Krokhin³; Vic Spicer³; Zhichang Yang¹; Xiaojing Shen¹; Amanda B. Hummon⁴; Liangliang Sun¹; ¹Department of Chemistry, Michigan State University, East Lansing, MI; ²Department of Chemistry and Biochemistry, University of Notre Dame, Notre Dame, IN; ³Manitoba Centre for Proteomics and Systems Biology, University of Manitoba, Winnipeg, Manitoba; ⁴Department of Chemistry and Biochemistry, Comprehensive Cancer Center, The Ohio State University, Columbus, OH
- MP 588 **Single Cell MALDI MS Neuropeptidomics of the Aplysia Californica;** [Peter Andersen](#)¹; Thanh Do²; Stanislav S Rubakhin¹; Jonathan V. Sweedler¹; ¹University of Illinois at Urbana Champaign, Urbana, IL; ²University of Tennessee, Knoxville, TN
- MP 589 **Increasing the Analysis Depth of the HLA-Associated Peptide Repertoire by LC-MS/MS;** [Chris D McGann](#)¹; Scott P Goulding¹; Lia R Serrano¹; Michael R Nelson¹; Aman Makaju²; Jennifer G Abelin¹; Terri A Addona¹; ¹Neon Therapeutics, Cambridge, MA; ²Thermo Fisher Scientific, San Jose, CA
- MP 590 **Detection of Ultra-Low Abundance Epitopes by Parallel Reaction Monitoring (PRM);** [Jonas Förster](#)^{1,2}; Nitya Mohan^{1,2}; Rebecca Köhler^{1,3}; Mogjib Salek^{1,3}; Angelika B. Riemer^{1,3}; ¹German Cancer Research Center (DKFZ), Heidelberg, Germany; ²Faculty of Biosciences, Heidelberg University, Heidelberg, Germany, Heidelberg, Germany; ³Molecular Vaccine Design, German Center for Infection



- Research (DZIF), partner site Heidelberg, Heidelberg, Germany, Heidelberg, Germany
- MP 591 **A Mass Spectrometry Based Platform for Differential Diagnostics of Hypertensive Pregnancy Complications via Urine Peptidome Profiling;** Alexey Kononikhin^{1,2,3}; Victoria Sergeeva^{3,4}; Natalia Starodubtseva^{1,2}; Maria Indeykina^{2,4}; Anna Bugrova^{1,4}; Natalia V. Zakharova⁴; Vitaly Chagovets¹; Igor Popov^{1,2}; Vladimir Frankevich¹; Eugene (evgeny) Nikolaev⁵; ¹V. I. Kulakov National Medical Research Center for Obstetrics, Gynecology and Perinatology, Ministry of Healthcare of the Russian Federation, Moscow, Russia; ²Moscow Institute of Physics and Technology (State University), Dolgoprudny, Russia; ³V.L. Talrose Institute for Energy Problems of Chemical Physics, Russian Academy of Sciences, Moscow, Russia; ⁴Emanuel Institute for Biochemical Physics, Russian Academy of Sciences, Moscow, Russia; ⁵Skolkovo institute of science and technology, Moscow Region, Russian Federation
- MP 592 **Enhanced Detection of Short and Hydrophilic Peptides Fraction Using Porous Graphitic Carbon;** Susy Piovesana¹; Carmela Maria Carmela Maria Montone²; Chiara Cavaliere²; Giorgia La Barbera²; Aldo Laganà²; Anna Laura Capriotti²; Carlo Crescenzi³; ¹Department of Chemistry, Università di Roma "La Sapienza", Rome, Italy; ²Department of Chemistry, Università di Roma "La Sapienza", Rome, Italy; ³Salerno University, Fisciano (SA), Italy
- MP 593 **Intraspecific Comparison of the Venom Peptidome of *Conus purpurascens*;** Meghan K. Grandal^{1,2}; Mickelene F. Hoggard¹; Frank Marii¹; ¹National Institute of Standards and Technology, Charleston, SC; ²Medical University of South Carolina, Charleston, SC
- MP 594 **Optimized Mild Acid Elution and Sample Clean-Up of MHC Immunopeptides with Trapped Ion Mobility Spectrometry(tims)-TOF;** Teesha C Luehr¹; Queenie Chan¹; Leonard J Foster¹; ¹University of British Columbia, Vancouver, BC
- MP 595 **Quantitative Analysis of the Isoforms of the Master Iron Regulator Hcpidin in a Clinically Actionable Time Frame;** Robert Trengove^{1,2}; Garth Maker^{3,4}; ¹Murdoch University, Murdoch, Australia; ²Australian National Phenome Centre, Murdoch University, Perth, Australia; ³Murdoch University, Perth, Australia; ⁴Medical, Molecular and Forensic Sciences, Murdoch University, Murdoch, Australia
- MP 596 **Mass Spectrometry Based Immunopectidomics - Accelerating the Development of Personalized Cancer Immunotherapy;** Michal Bassani-sternberg^{1,2}; Markus Müller³; Florian Huber^{1,2}; Brian Stevenson³; Julien Racle⁴; Justine Michaux^{1,2}; Chloe Chong^{1,2}; David Gfeller^{4,5}; George Coukos^{1,2}; ¹Department of Oncology, University Hospital of Lausanne, Lausanne, Switzerland; ²Ludwig Institute for Cancer Research, Lausanne, Switzerland; ³Vital IT, Swiss Institute of Bioinformatics, Lausanne, Switzerland; ⁴Department of Oncology, University of Lausanne, Lausanne, Switzerland; ⁵Swiss Institute of Bioinformatics, Lausanne, Switzerland
- MP 597 **Characterization of Human Pancreatic Islet Peptidome Using Parallel Accumulation-Serial Fragmentation (PASEF) and Trapped Ion Mobility Spectrometry;** Elena V. Romanova¹; Stanislav S Rubakhin¹; David H. Mast¹; Jonathan V. Sweedler¹; ¹University of Illinois at Urbana-Champaign, Urbana, IL
- MP 598 **Enrichment of Zinc Finger Proteins by IMAC;** Stephanie Miller Lehman¹; Josue Baeza¹; Geoffrey P. Dann¹; Benjamin A Garcia¹; ¹University of Pennsylvania, Philadelphia, PA
- PHOSHOPEPTIDES: ENRICHMENT METHODS**
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- MP 599 **A Novel Automated and Highly Selective Phosphopeptide Enrichment Strategy for Successful Phosphopeptide Identification and Phosphosite Localization;** Shuai Wu¹; Kenneth Newton¹; Linfeng Wu¹; Jordy J. Hsiao¹; Valery G. Voinov^{2,3}; Joseph S. Beckman^{2,3}; ¹Agilent Technologies, Santa Clara, CA; ²e-Msion Inc., Corvallis, OR; ³Oregon State University, Corvallis, OR
- MP 600 **A Scalable Phosphopeptide Enrichment Strategy for Multiplexed Quantitative Phosphoproteomics;** Alison Erickson¹; Brian Erickson¹; Craig Braun¹; Ryan Kunz¹; ¹IQ Proteomics LLC, Cambridge, MA
- MP 601 **Large Scale EasyPepTM MS Sample Preparation for Phosphopeptide Enrichment Workflows;** Amarjeet Flora¹; Ryan D. Bomgarden¹; Sergei Snovida¹; Ashok Salunkhe¹; John C. Rogers¹; ¹Thermo Fisher Scientific, Rockford, IL
- MP 602 **Development of Fully Automated and High-Throughput Workflow for Phosphoproteomics;** Stoyan Stoychev^{1,2}; Ireshyn Govender¹; Previn Naciker¹; Sindisiwe Buthelezi¹; Siphso Mamputha¹; Isak Gerber^{1,2}; Justin Jordaan²; ¹CSIR, Pretoria, South Africa; ²ReSyn BioSciences, Pretoria, South Africa
- MP 603 **Using Quantitative Phosphoproteomics to Understand Key Phosphorylation Signaling Pathways in HCT116 Cells after Chemotherapy Drug Treatment;** Brian T Mullis¹; Lim Andrew Lee²; Rebekah J Woolsey³; David R Quilici³; Qian Wang¹; ¹University of South Carolina, Columbia, SC; ²Integrated Micro-Chromatography Systems, Irmo, SC; ³Mitch Hitchcock, Ph.D. Nevada Proteomics Center, Reno, NV
- PLANT "OMICS"**
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- MP 604 **Discovering Putative Mode of Action of Plant Protection Genes Using Metabolomics;** Jan Hazebroek¹; Teresa Harp¹; Chris Vlahakis¹; Leandro Perugini¹; Girma Tabor¹; ¹Corteva Agriscience, Johnston, IA
- MP 605 **Drought Metabolomics of Susceptible and Tolerant Soybean Cultivars;** Kevin J. Zemaitis¹; Philip Lindhorst¹; Troy D. Wood¹; ¹University at Buffalo, Buffalo, NY
- MP 606 **Application of Data-Independent Acquisition Approach to Study the Proteome Dynamics of Plant Pathogenesis Responses;** Kai-ting Fan¹; Kuo-Hsin Wang¹; Wei-Hung Chang¹; Jhih-Ci Yang Yang^{1,2}; Ching-Fang Yeh¹; Kai-Tan Cheng¹; Sheng-Chi Hung^{1,3}; Yet-Ran Chen¹; ¹Agricultural Biotechnology Research Center, Academia Sinica, Taipei, Taiwan; ²National Chiao Tung University, Hsinchu, Taiwan; ³Institute of Biotechnology, National Taiwan University, Taipei, Taiwan
- MP 607 **Using SWATH-MS to Understand Global Proteome Changes in Barley Lines with Reduced Storage Protein Synthesis;** Utpal Bose¹; Keren Byrne¹; Malcolm J. Blundell²; Crispin A. Howitt²; Michelle L. Colgrave¹; ¹Agriculture and Food, CSIRO, St Lucia, Australia; ²Agriculture and Food, CSIRO, Canberra, Australia
- MP 608 **Dynamic Proteome Response of Different Rice Varieties to Drought Stress;** Sara Hamzelou¹; Dana Pascovici¹; Mehdi Mirzaei¹; Ardeshir Amirkhani¹; Matthew J. McKay¹; Brian J. Atwell¹; Paul A. Haynes¹; ¹Macquarie University, North Ryde, Australia
- MP 609 **Simple and High-Throughput Method for Plant Metabolites by PESI/MS/MS: First Application to Plant Metabolite Analysis and Agricultural Industry;** Ryota Harada¹; Moeko Taki¹; Yumi Hayashi^{2,3}; Kei Zaitsumi²; Katsuhiko Shiratake¹; ¹Laboratory of Horticultural Science, Graduate School of Bioagricultural Sciences, Nagoya University, Nagoya, Japan; ²In Vivo Real-Time Omics Laboratory, Institute for Advanced Research, Nagoya



- University, Nagoya, Japan; ³Pathophysiological Laboratory Sciences, Department of Radiological and Medical Laboratory Sciences, Nagoya University Graduate School of Medicine, Nagoya, Japan
- MP 610 **Dissection of Flag Leaf Metabolic Shifts and Relationship with Those Occurring Simultaneously in Developing Seed by Application of Non-Targeted Metabolomics**; Chaoyang Hu¹; Jianxin Shi²; Yue Song³; Shan-an Chan⁴; ¹Ningbo University, Ningbo, China; ²Shanghai Jiao Tong University, Shanghai, China; ³Agilent Technologies, Shanghai, China; ⁴Agilent Technologies, Taipei, Taiwan
- MP 611 **Metabolic Disturbance in the Beet Necrotic Yellow Vein Virus/Sugar Beet Pathosystem**; Fabio C. Chaves¹; Kimberly M. Webb²; William M. Wintermantel³; Lisa M Wolfe¹; Linxing Yao¹; Corey D. Broeckling¹; ¹Proteomics and Metabolomics Facility of Colorado State University, Fort Collins, CO; ²USDA-ARS, Soil Management and Sugar Beet Research Unit, Fort Collins, CO; ³USDA-ARS, Crop Improvement and Protection Research Unit, Salinas, CA
- MP 612 **Phosphoproteomics Reveals the Downstream Phosphorylation Signaling Targets of the Lectin Receptor-Like Kinase PtLecRLK1 Involved in Plant / Mycorrhizal symbiosis**; Him K Shrestha¹; Paul Abraham²; Jin-Gui Chen²; Robert L. Hettich²; ¹University of Tennessee, Knoxville, TN; ²Oak Ridge National Laboratory, Oak Ridge, TN
- MP 613 **A Quantitative Strategy for Deep Coverage of the Algal Phosphoproteome**; Megan M. Ford¹; Emily G. Werth¹; Leslie M. Hicks¹; ¹University of North Carolina, Chapel Hill, NC
- MP 614 **Characterization and Identification of Di-Isodityrosine and Pulcherosine Cross-linkages Occurring in the Plant Cell Wall Extensin Scaffold**; Lawrie Gainey¹; Steven D. Hartson¹; Michelle English²; Marshall Bern²; Andrew J. Mort¹; ¹Oklahoma State University, Stillwater, OK; ²Protein Metrics Inc., San Carlos, CA
- MP 615 **Enhancement of Nodule-Specific Cysteine-Rich Peptide Detection in Medicago truncatula by MALDI-MSI through Inclusion of a Simple Wash**; Caitlin Keller¹; Nhu Q. Vu¹; Bailey Kleven¹; Sanhita Chakraborty¹; Junko Maeda¹; Dhileepkumar Jayaraman¹; Michael R. Sussman¹; Jean-Michel Ané¹; Lingjun Li¹; ¹University of Wisconsin-Madison, Madison, WI
- MP 616 **Elucidating Protein-Protein Interactions in Chlamydomonas reinhardtii Using Immunoprecipitation and Liquid Chromatography-Mass Spectrometry**; Anthony A Iannetta¹; Leslie M Hicks¹; ¹University of North Carolina, Chapel Hill, NC
- MP 617 **Development and Characterization of IR-MALDESI Specifically for Mass Spectrometry Imaging of Plants**; Michael C Bagley¹; Rika S Judd¹; Anna N Stepanova¹; Yogini S Jaiswal²; Måns Ekelöf¹; Kenneth P Garrard¹; Leonard L Williams²; Jose M Alonso¹; De-Yu Xie¹; David C Muddiman^{1,3}; ¹North Carolina State University, Raleigh, NC; ²Center for Excellence in Post Harvest Technologies, North Carolina Agricultural and Technical State University, The North Carolina Research Campus, Kannapolis, North Carolina; ³Molecular Education, Technology, and Research Innovation Center (METRIC), North Carolina State University, Raleigh, NC
- MP 618 **Proteoform Profiling of Canadian Breadwheat Glutenins Reveals Unexpected C-Terminal Tyrosine Truncation in Low Molecular Weight Glutenins**; Ray Bacala^{1,2}; Katherine Cordova¹; Helene Perreault²; Dave Hatcher¹; ¹Canadian Grain Commission, Winnipeg, MB; ²Department of Chemistry, University of Manitoba, Winnipeg, MB
- MP 619 **The Metabolome of Early Season Sorghum Plant Tissue is Predictive of End of Season Biomass**; Amy M Sheflin¹; Stephen Kresovich²; Ismail Dweikat³; Ellen Marsh³; Daniel Schachtman³; Jessica Prenni¹; ¹Colorado State University, Fort Collins, CO; ²Clemson University, Clemson, SC; ³University of Nebraska Lincoln, Lincoln, NE
- MP 620 **Proteomic Analysis of Translational Control of Gene Expression under Light Treatment in Arabidopsis thaliana**; Yixiang Zhang^{1,2}; Xuhong Yu³; Scott D. Michaels³; Jonathan C. Trinidad^{1,2}; ¹Department of Chemistry, Indiana University, Bloomington, IN; ²Laboratory for Biological Mass Spectrometry, Indiana University, Bloomington, IN; ³Department of Biology, Indiana University, Bloomington, IN
- MP 621 **Regulation at the Plant-Microbe Interface: Discovery and Characterization of Signaling Polypeptides Using High-Performance Tandem Mass Spectrometry**; Paul E. Abraham¹; Suresh Poudel¹; Anna Matthiadis¹; Udaya Kalluri¹; Robert L. Hettich¹; ¹Oak Ridge National Laboratory, Oak Ridge, TN
- MP 622 **Profiling of Histone Acetylation and Methylation Marks Associated with Embryo and Aleurone Tissue-Specific Epigenetic Regulation of Seed Dormancy in Wheat**; Michelle Rampitsch¹; Mei Huang¹; Yao Zhen¹; Nataša Radovanovic¹; Wayne Xu¹; Christof Rampitsch¹; Natalia V. Bykova¹; ¹Agriculture and Agri-Food Canada, Morden, Manitoba
- MP 623 **Metabolome-Based Genome Wide Association Profiling of Innate Immunity in Rice**; Joshua Blakeslee¹; Pengfei Bai²; Yun Li¹; Matthew Bernier²; Guo-Liang Wang²; ¹The Ohio State University, Wooster, OH; ²The Ohio State University, Columbus, OH
- MP 624 **Molecular and Microbial Responses to Drought in Field-Grown Sorghum**; Kim K. Hixson¹; Kristin M. Engbrecht¹; Daniel J. Orton¹; Kent J. Bloodsworth¹; Aivett Bilbao¹; Joon-Yong Lee¹; Young-Mo Kim¹; Jamie R. Nunez¹; Bryan A. Stanfill¹; Erika M. Zink¹; Karl K. Weitz¹; Ling Xu^{2,3}; Pubudu P. Handakumbura¹; Mary A. Madera²; Julie A. Sievert⁴; Joy Hollingsworth⁴; Ronald J. Moore¹; Ryan S. Renslow¹; Thomas O. Metz¹; Ljiljana Pasa-Tolic¹; Robert Hutmacher⁵; Jeffery A. Dahlberg⁴; Devin Coleman-Derr^{2,3}; Peggy G. Lemaux²; Christer Jansson¹; ¹Pacific Northwest National Laboratory, Richland, WA; ²University of California, Berkeley, Berkeley, CA; ³US Department of Agriculture-Agricultural Research Service, Albany, CA; ⁴Kearney Agricultural Research & Extension Center, Parlier, CA; ⁵Westside Research & Extension Center, University of California, Davis, Five Points, CA
- MP 625 **Utilization of Substructure Identification through MSn Analysis for Unknown Structure Determination Assisted with in silico Fragmentation Prediction**; Tim Stratton; Thermo Fisher Scientific, San Jose, CA
- MP 626 **Spatial Distribution Mapping of Molecules in the Grains of Different Rice Landraces, Using Desorption Electrospray Ionization Mass Spectrometry**; Arunan Suganya¹; Debal Deb²; Thalappil Pradeep¹; ¹Indian Institute of Technology - Madras, Chennai, India; ²Centre for Interdisciplinary Studies, Barrackpore, Kolkata 700 123, India

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- MP 627 **Gaseous Polylactide Ions Retain Structural Memory of How They Were Produced by ESI: An Ion Mobility Spectrometry/Molecular Dynamics Simulation Study**; Quentin Duez^{1,2}; Haidy Metwally²; Sébastien Hoyas¹; Vincent Lemaury¹; Jérôme Cornil¹; Pascal Gerbaux¹; Lars Koneremann²; Julien De Winter¹; ¹University of Mons, Mons, Belgium; ²University of Western Ontario, London, ON
- MP 628 **Analysis of an Ethoxylated Caprylic/Capric Polyglyceride Surfactant Mixture via Liquid Chromatography Coupled to Ion Mobility Mass Spectrometry**; Jason Michael O'Neill¹; Chrys Wesdemiotis¹; ¹The University of Akron Chemistry Department, Akron, OH



- MP 629 **A Mass Spectrometry Imaging Method for Visualizing Synthetic Polymers Combining with Kendrick Mass Defect Analysis;** Takaya Satoh¹; Sayaka Nakamura²; Thierry Fouquet²; Hiroaki Sato²; Yoshihisa Ueda³; Mike H. Frey⁴; ¹JEOL Ltd. MSBU Application division Group1, Akishima, Tokyo, Japan; ²Research Institute for Sustainable Chemistry, National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan; ³JEOL Ltd. MSBU, Akishima, Japan; ⁴JEOL USA, Inc., Peabody, MA
- MP 630 **Molecular Coding/Decoding of Oligomer Sequences via Advanced Polymer Chromatography – Ion Mobility Separation - Mass Spectrometry Hyphenation;** Marie-Theres Picker¹; Chiel Mertens²; Filip Du Prez²; Dirk Kuckling¹; ¹Paderborn University, Paderborn, Germany; ²Ghent University, Ghent, Belgium
- MP 631 **Characterization of MQ Silicone Resins by GPC-MALDI-MS;** Tianlan Zhang¹; Wei Gao¹; Donald Eldred²; Tom Bekemeier²; ¹The Dow Chemical Co, Collegeville, PA; ²Dow Chemical Company, Auburn, MI
- MP 632 **Molecular Characterization of Oligomeric Pyrolysis Compounds of Ethyl Acrylate-Butyl Acrylate Copolymer Using Thermal Desorption/Pyrolysis DART-MS;** Chikako Takei¹; Kenichi Yoshizawa¹; Sayaka Nakamura²; Hiroaki Sato²; Hajime Ohtani³; ¹BioChromato, Inc., Fujisawa, Japan; ²National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan; ³Nagoya Institute of Technology, Nagoya, Japan
- MP 633 **Structural Elucidation of Multiply Charged Gaseous Organosilicon Cations via Solution Phase Additives;** Tanya Habitz¹; Ron Tecklenburg¹; John Stutzman¹; ¹The Dow Chemical Company, Midland, MI
- MP 634 **Optimizing the Performance of Organic Memory Devices – A Complementary Multi-Technique Analytical Approach;** Lothar Veith¹; Minye Jin¹; Hans Joachim Räder¹; Jasper Michels¹; Rüdiger Berger¹; Paul Blom¹; Tanja Weil¹; ¹Max Planck Institute for Polymer Research, Mainz, Germany
- MP 635 **A Study on Matrix Preparation towards MALDI-Imaging of Synthetic Polymer Samples;** Toshiji Kudo¹; Takashi Nirasawa²; Shigeru Sakamoto¹; ¹Bruker Japan K.K., Yokohama, Japan; ²Bruker Japan K.K., Yokohama, Japan
- MP 636 **A High Performance Liquid Chromatography/Mass Spectrometry (LC/MS) Method for the Characterization of Stressed Polysorbate 20 and 80;** Paul W. Brown¹; Yan He¹; Olga Friese²; Jason Rouse³; ¹Pfizer, Wildwood, MO; ²Pfizer, Wildwood, MO; ³Pfizer, Andover, MA
- MP 637 **Chemical Depolymerization and Analysis of Synthetic and Natural Insoluble Polymers by 1D and 2D High Resolution FT-ICR Mass Spectrometry;** Ziad Mahmoud¹; Sergui Mansour¹; Fabrice Bray¹; Laëtitia Chausset-Boissarie¹; Christian Rolando²; ¹Université de Lille, Villeneuve d'Ascq, France; ²Univ. de Lille, Sciences et Technologies, Villeneuve D'ascq, France
- MP 638 **Determination of the Detailed Electron Impact Fragmentation Pathways for Mercaptopropyl and Chloropropyl Containing Silane Coupling Agents and Siloxane Polymers;** Ron Tecklenburg¹; Tanya Habitz¹; ¹The Dow Chemical Company, Midland, MI
- MP 639 **ケンド(リック): “Kendo” Open File for the Advanced Kendrick Mass Defect Analysis of Mass Spectra From Polymeric Materials;** Thierry Nicolas Jean Fouquet¹; Sayaka Nakamura¹; Robert Cody²; Hiroaki Sato³; ¹National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan; ²JEOL USA, Inc., Peabody, MA
- PROTEIN THERAPEUTICS: QUANTITATIVE ANALYSIS I**
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- MP 640 **Effect of Amino Acid Supplementation on Host Cell Protein Profile for Recombinant *Pramlintide concatemer* Production in *E. coli*;** Rohan Shah¹; Saurabh Nagpal²; Anurag Rathore¹; Jashwant Kumar¹; ¹Indian Institute of Technology, delhi, India; ²Agilent Technologies, Gurgaon, India
- MP 641 **Compiling a Method Toolbox to Improve Detection of Host Cell Proteins;** Martha Stapels¹; Helena Awad¹; Michelle Busch¹; Joanne Cotton¹; Fateme Tousi¹; ¹Sanofi, Framingham, MA
- MP 642 **Monitoring of Non-Human Glycan Motif in Biotherapeutics for Immunogenicity Prediction;** Unyong Kim¹; Myung Jin Oh^{2,3}; Nari Seo^{2,3}; Hyun Joo An^{2,3}; ¹GLYCAN Co., Ltd., Seongnam, South Korea; ²Asia-Pacific Glycomics Reference Site, Daejeon, South Korea; ³Chungnam National University, Daejeon, South Korea
- MP 643 **Quantitative Analysis of Intact Monoclonal Antibodies from Mouse Serum Using LC/MS and CE/MS Techniques;** David Wong¹; Omar S. Barnaby²; Mei Han³; Yanan Yang¹; Christopher A. James⁴; ¹Agilent Technologies, Inc., Santa Clara, CA; ²Amgen, Inc., Thousand Oaks, CA; ³Amgen Inc., South San Francisco, CA; ⁴Amgen, Inc., Thousand Oaks, CA
- MP 644 **Spatially-Resolved, 3D-Printed Micro-Sampling Coupled to Sensitive Nano-LC-MS to Quantify the Absolute Levels of Heterogeneous Distribution of mAb/Targets in Tissues;** Ming Zhang¹; Bo An¹; Jun Qu¹; ¹SUNY at Buffalo, Buffalo, NY
- MP 645 **Characterization of Commercial Vaccines by Charge Detection Mass Spectrometry;** Kevin Bond¹; Che-Yen (Joe) Wang²; Martin F Jarrold¹; ¹Indiana University Bloomington, Bloomington, IN; ²Indiana University, Bloomington, IN
- MP 646 **High-Resolution Isolation LC/SRM-MS Enabled Improved Selectivity via the Isolated Isotopic Precursor/Product Transitions;** Shihan Huo¹; Jie Pu¹; Ming Zhang^{1,2}; Xiaoyu Zhu¹; Jun Qu^{1,2}; ¹University at Buffalo, Buffalo, NY; ²New York State Center of Excellence in Bioinformatics & Life Sciences, Buffalo, NY
- MP 647 **A Peptide Mapping Based Quality-by-Design Study of Biopharmaceuticals Oxidation during Formulation Development;** Bo Zhai¹; Danika Rodrigues²; Dwaine Banton³; Andrew D Mahan¹; Stuart Ember²; Jeffrey Brelsford¹; Santosh Thakkar²; Hirsh Nanda¹; ¹Janssen Research & Development, Cell & Developability Sciences, Spring House, PA; ²Janssen Research & Development, Large Molecule Drug Product Development, Malvern, PA; ³Janssen Research & Development, Manufacturing and Applied Statistics, Spring House, PA
- MP 648 **A Generic Anti-Peptide Capture Coupled to LC/MS MRM for Low Level Pharmacokinetic Measurements of Therapeutic Proteins;** Bao-Jen Shyong¹; Weixun Wang²; Huaibing He²; Bernard Choi²; Lucinda Hittle²; Kevin Bateman¹; Daniel Spellman¹; ¹Merck & Co., Inc., West Point, PA; ²Merck & Co., Inc., Rahway, NJ
- MP 649 **Comparison of Methods for Plate-Based Capture and Quantification of Monoclonal Antibodies by LC-MS;** Nicolas Caffarelli¹; Yue Lu¹; Pegah Jalili¹; Thomas Juehne¹; Jeffrey Turner¹; Kevin Ray¹; ¹MilliporeSigma, St. Louis, MO
- MP 650 **Engineering the XS® Pichia Expression System to Reduce Host Cell Protein Impurities in Biopharmaceuticals Production;** Sylwia Jozwiak¹; Katrien Claes²; Christoph Kiziak²; James Graham¹; ¹Research and Development, Pharma&Biotech, Lonza Biologics plc, Slough, United Kingdom; ²Research and Development Microbial, Pharma&Biotech, Lonza AG, Visp, Switzerland



- MP 651 **A High-Resolution Multi-Attribute Method for Product Characterization, Process Characterization, and Quality Control of Therapeutic Proteins;** Xiaoyan Guan¹; Le Zhang¹; Da Ren¹; Tamer Eris¹; ¹*Amgen, Thousand Oaks, CA*
- MP 652 **The Development of a Point-of-Need Miniaturized ESI-MS for Upstream Bioprocessing Applications;** Richard W Moseley¹; Alex I McIntosh¹; ¹*Microsaic Systems, Woking, United Kingdom*
- MP 653 **Evaluation of nSMOL Methodology for the Analysis of the mAb Bevacizumab in Human Plasma by LC-MS/MS;** Mike Buonarati¹; Stephen Kurzyniec²; Vikki Johnson²; Reed Lyon¹; Laurence M. Brill¹; Dale Schoener¹; ¹*Intertek Pharmaceutical Services, San Diego, CA*; ²*Shimadzu Scientific Instruments, Inc, Carlsbad, CA*
- MP 654 **Comprehensive and Streamlined Approach for Host Cell Protein Identification and Quantification;** Sean McCarthy¹; Zoe Zhang²; Lei Xiong²; Elliott Jones²; ¹*SCIEX, Framingham, MA*; ²*Sciex, Redwood City, CA*
- MP 655 **Tandem Quadrupole MS for the Quantification of Monoclonal Antibody Subunit Light Chains in Plasma;** Caitlin M Dunning¹; Mary E Lame¹; Yun W Alelyunas¹; Mark D Wrona¹; ¹*Waters Corporation, Milford, MA*
- MP 656 **Comparison of Sample Preparation Methods for Hybrid Ligand Binding Assay-Liquid Chromatography Tandem Mass Spectrometry;** Maria-Christina S Malinao¹; Chad Eichman¹; Brian Rivera¹; ¹*Phenomenex, Torrance, CA*
- MP 657 **An Improved Immunoaffinity LC-MS/MS Workflow for the Quantitation of IgG's during Preclinical PK Studies;** Michael M. Rosenblatt¹; Lyndsey Jager¹; Nidhi Nath¹; Marjeta Urh¹; ¹*Promega Corporation, Madison, WI*
- MP 658 **Ultra-sensitive Quantification of Monoclonal antibodies and ADCs in Mouse Plasma using Trap-Elute MicroLC-MS/MS method;** Lei Xiong¹; Ji Jiang¹; Remco van Soest¹; ¹*Sciex, Redwood City, CA*
- MP 659 **Efficient Data Processing Workflows for In-Depth, MS-Based Glycoanalysis of Biopharmaceuticals;** Aude Tartiere¹; Albert Van Wyk²; Joe Shambaugh³; John McCarter³; Cassandra Wigmore⁴; Peter Haber⁵; ¹*Genedata, Inc., San Francisco, CA*; ²*Genedata Ltd, Cambridge, United Kingdom*; ³*Genedata Inc, Lexington, MA, USA, Lexington, MA*; ⁴*Genedata AG, Basel, Switzerland, Basel, Switzerland*; ⁵*Genedata GmbH, Munich, Germany, Munich, Germany*
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- MP 660 **Isotopically Resolved Analysis of Protein Subunits Using High Resolution Accurate Mass;** Sean McCarthy¹; Melanie Juba²; Zoe Zhang³; ¹*SCIEX, Framingham, MA*; ²*Sciex, Framingham, MA*; ³*Sciex, Redwood City, CA*
- MP 661 **Laser-Free FPOP Hydroxyl Radical Protein Footprinting with In-Line Radical Dosimetry for Biopharmaceutical Higher Order Structural Analysis;** Scot R Weinberger¹; Ron C. Orlando^{1,2}; Joshua S Sharp^{1,3}; ¹*GenNext Technologies, Inc., Montara, CA*; ²*University of Georgia, Athens, GA*; ³*University of Mississippi, University, MS*
- MP 662 **Mass Spectrometric Characterization of Acidic Species Generated in Cell Culture and Stability Studies of Monoclonal Antibodies;** Ioannis A Papayannopoulos¹; Shannon Renn-Bingham¹; ¹*Celldex Therapeutics, Fall River, MA*
- MP 663 **Mapping Glycation Sites of an Antitumor Tn-BSA Neoglycoconjugate by Mass Spectrometry;** Simin Tavangari¹; Rene Roy¹; Alexandra M Furtos²; ¹*Universite du Quebec a Montreal, Montreal, Québec*; ²*University of Montreal, Montreal, QC*
- MP 664 **A Single Injection LC-MS Analysis Scheme for Simultaneous Analysis of Biotherapeutics and Host-Cell Impurities via Online Digestion LC-MS/MS;** Joshua Emory¹; Brian Feild¹; Harsha P. Gunawardena²; ¹*Shimadzu Scientific Instruments, Inc., Columbia, Maryland*; ²*Janssen Research and Development, Spring House, PA*
- MP 665 **On-Line Aggregate and Fragment Analysis of Therapeutic Monoclonal Antibodies Using Native Size Exclusion Chromatography Mass Spectrometry;** Chongfeng Xu¹; Zoran Susic¹; Sean McCarthy²; Esme Candish²; Fan Zhang³; Elliott Jones²; ¹*Biogen, Cambridge, MA*; ²*Sciex, Framingham, MA*; ³*Sciex, Redwood City, CA*
- MP 666 **Hydroxyl Radical Protein Footprinting Reveals Buffer Effects in Adalimumab Biosimilar Aggregation and Heat Shock Tolerance;** Joshua S. Sharp¹; Sandeep K. Misra¹; Scot R Weinberger²; Ron C. Orlando^{2,3}; ¹*University of Mississippi, University, MS*; ²*GenNext Technologies, Inc., Montara, CA*; ³*University of Georgia, Athens, GA*
- MP 667 **CESI-MS: A Useful Tool to Analyze the Charge Variants and Disulfide Structural Heterogeneity of IgG2;** Prashant Dour¹; Faraz Rashid¹; Dipankar Malakar¹; Manoj Pillai¹; ¹*SCIEX INDIA, Gurugram, India*
- MP 668 **Structural Study of a PEGylated Therapeutic Protein by MALDI-MS/MS and ESI-QTOF;** Sergei Dikler¹; Anjali Alving¹; ¹*Bruker Scientific, Billerica, MA*
- MP 669 **Automated Chemical Footprinting Enables Monitoring of Conformational Change of Protein Therapeutics;** Sonya Entova¹; Nina Chen¹; Mohammed Sahar¹; Alla Polozova¹; Hao Zhang¹; ¹*Amgen Inc., Cambridge, MA*
- MP 670 **Time-resolved Deconvolution for Automated, In-depth Characterization of an IgG-type Monoclonal Antibody by Intact Mass Analysis;** Peter Haber¹; John McCarter²; Aude Tartiere³; Albert Van Wyk⁴; Cassandra Wigmore⁵; Joe Shambaugh²; ¹*Genedata GmbH, Munich, Germany*; ²*Genedata, Inc., Lexington, MA*; ³*Genedata, Inc., San Francisco, CA*; ⁴*Genedata Ltd, Cambridge, United Kingdom*; ⁵*Genedata AG, Basel, Switzerland*
- MP 671 **Improving Sequence Coverage of Hydrophobic Regions of Bispecific Antibody Cancer Therapeutics with Top-Down Mass Spectrometry and Enzymatic Digestion;** Jennifer Lippens¹; Burton Lee¹; Andrew Dykstra¹; Tawnya Flick¹; ¹*Amgen, Inc., Thousand Oaks, CA*
- MP 672 **A Workflow-Driven Platform Solution for MAM-Based Critical Quality Attribute Monitoring of Biotherapeutics in Process Development and QC;** Nilini Ranbaduge¹; Henry Shion¹; Ying Qing Yu¹; Min Du¹; Weibin Chen¹; ¹*Waters Corporation, Milford, MA*
- MP 673 **Characterization and Relative Quantitation of Sequence Variants in Protein Therapeutics by Liquid Chromatography Tandem Mass Spectrometry;** Scott Ugrin¹; Colin G. Barry¹; Michelle English²; ¹*Alliance Pharma, Malvern, PA*; ²*Protein Metrics Inc., San Carlos, CA*
- MP 674 **High-Throughput Analysis of Antibody Charge Heterogeneity by Native Microfluidic Capillary Electrophoresis- Mass Spectrometry;** Hongxia (jessica) Wang¹; Haibo Qiu¹; Jikang Wu¹; Thomas Daly¹; Ning Li¹; ¹*Regeneron Pharmaceuticals Inc., Tarrytown, NY*
- MP 675 **Streamlining mAb Characterization with a PASEF Based Disulfide Analysis Workflow;** Stuart Pengelley¹; Waltraud Evers¹; K. Ilker Sen²; Guillaume Tremintin³; Eric Carlson²; Detlev Suckau¹; Anja Resemann¹; Marshall Bern²; ¹*Bruker Daltonik GmbH, Bremen, Germany*; ²*Protein Metrics Inc., Cupertino, CA*; ³*Bruker Daltonics Inc., Billerica, MA 01821*
- MP 676 **Improved Middle-Down Characterization of Antibodies Using Multiple Ion Activation Techniques and Proton Transfer Reaction on a Modified Orbitrap Mass Spectrometer;** Romain Huguet¹; Kristina Szrentic²; John E. P. Syka¹; Christopher Mullen¹; Joshua A Silveira¹; Jennifer Sutton¹; Luca Fornelli³; ¹*Thermo Fisher Scientific, San Jose*



MP 677 **Optimization of Capillary Nondenaturing Size Exclusion Chromatography of Proteins Coupled to a Multinozzle Electrospray Source;** Theresa McLaughlin¹; Yue Ju²; Pan Mao³; Guillaume Tremintin⁴; Allis S. Chien¹; Mel Park⁴; ¹Stanford University, Stanford, CA; ²Bruker Daltonics Inc., Billerica, MA 01821; ³Newomics Inc., Berkeley, CA; ⁴Bruker Daltonics Inc., Billerica, MA

MP 678 **Data Independent Top-down Mass Spectrometry Facilitated by a New MSE Processing Tool;** Lindsay J Morrison¹; Barbara J Sullivan¹; ¹Waters Corporation, Beverly, MA

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MP 679 **Composition and Particle Size Characterization of ApoL1 Containing Molecular Assemblies in Human Plasma in Relation to Kidney Filtration Rate;** Michael Andrews¹; Andrew N Hoofnagle²; Yulanda Williamson¹; David Schieltz¹; Zsuzsanna Kuklenyik¹; John R Barr¹; ¹Centers for Disease Control and Prevention, Chamblee, GA; ²University of Washington, Seattle, WA

MP 680 **The Investigation of High Intensity Interval Training on Left Ventricular Fibrosis in Cardiac Patients by Proteomics;** Meng-chu Liu¹; Pang-Hung Hsu¹; Chih-Chin Hsu²; ¹Department of Bioscience and Biotechnology, National Taiwan Ocean University, Keelung City, Taiwan; ²Department of Physical Medicine and Rehabilitation, Keelung Chang Gung Memorial Hospital, Keelung City, Taiwan

MP 681 **Total Solubilization of FFPE Samples for One Pot High Throughput, High Yield Clinical Proteomics;** John P. Wilson¹; Ilyana Ilieva²; Darryl J Pappin^{1,3}; John B. Wojcik²; ¹ProtiFi, LLC, Farmingdale, NY; ²University of Pennsylvania, Philadelphia, PA; ³Cold Spring Harbor laboratory, Cold Spring Harbor, NY

MP 682 **Identification of Aggressive Prostate Cancers: In-depth Proteomics of Tissues and Urines;** Andrew Maclin¹; Amanda Khoo²; Katharina Fritsch²; Ankit Sinha²; Vladimir Ignatchenko¹; Joseph J. Otto³; Lydia Y. Liu²; Vincent Huang⁴; Julie Livingstone⁴; Danny Vesprini⁵; Julius O. Nyalwidhe³; O. John Semmes³; Paul C. Boutros⁶; Stanley Liu⁵; Thomas Kislinger¹; ¹Princess Margaret Cancer Centre, Toronto, ON; ²University of Toronto, Toronto, ON; ³Eastern Virginia Medical School, Norfolk, VA; ⁴Ontario Institute for Cancer Research, Toronto, ON; ⁵Sunnybrook Health Sciences Centre, Toronto, ON; ⁶UCLA, Los Angeles, CA

MP 683 **Identifying Quantitative Protein Changes in the Iris of Glaucoma Patients Using Label Free Proteomics;** Craig P Dufresne¹; Richard D Semba²; Pingbo Zhang²; Min Zhu²; Jiang Qian³; Tianshun Gao²; Ibrahim AlJadaan⁴; Sami AlShahwan⁴; Ohood Owaidha⁴; Randy Craven²; Deepak Edward^{2,4}; Alka Mahale⁴; ¹Thermo Fisher Scientific, West Palm Beach, FL; ²Johns Hopkins University, Baltimore, MD; ³National Institute on Aging, National Institutes of Health, Baltimore, MD; ⁴King Khaled Eye Specialist Hospital, Riyadh, Saudi Arabia

MP 684 **Protein Signatures for Diagnosis of Ovarian Cancer in a Murine Model;** Melissa M Galey¹; Alexandria N Young¹; Valentina Petukhova¹; Jian Wang²; Mingxun Wang²; Joanna E Burdette¹; Laura M Sanchez¹; ¹University of Illinois at Chicago, Chicago, IL; ²Ometa Labs, San Diego, CA

MP 685 **Application of Plasma Proteomics in Alzheimer's Disease;** Mostafa J Khan¹; Renā A.S. Robinson¹; ¹Vanderbilt University, Nashville, TN

MP 686 **Using iTRAQ-labeling nanoLC-MS/MS Proteomic Approaches to Discovery Urinary Protein Biomarkers of Urothelial Carcinoma;** Chao-Jung Chen¹; Chieh Yang²;

Che-Yi Chou^{1,3}; Chiu-Ching Huang^{4,5}; ¹China Medical University, Taichung, Taiwan; ²China Medical University Hospital, Taichung, Taiwan; ³Asia University Hospital, Taichung, Taiwan; ⁴China Medical University Hospital, Taichung, Taiwan; ⁵China Medical University, Taichung City, Taiwan

MP 687 **Proteomics Analysis of Acid Bone Lysate Using Micro Pillar Arrayed Columns;** Goran Mitulovic¹; Franz Josef Strauss^{2,3}; Alexandra Stähli^{2,4}; Lucian Beer²; Valentina Gilmozzi²; Nina Haspel²; Gerhild Schwab²; Rainhard Gruber²; ¹Medical University of Vienna, KIMCL, Vienna, Austria; ²Medical University of Vienna, Vienna, Austria; ³University of Chile, Santiago, Chile; ⁴University of Bern, Bern, Switzerland

MP 688 **Optimized Sample Preparation for the Assessment of Formalin-Fixed and Paraffin Embedded (FFPE) Tissue Specimen for Mass-Spectrometry Based Proteogenomics;** Georgia Mitsa¹; Adriana Aguilar²; Mark Basik³; Sonia del Rincon¹; Rene Zahedi¹; Christoph H. Borchers^{1,3,4,5}; ¹Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; ²Segal Cancer Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; ³Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC; ⁴University of Victoria-Genome BC Proteomics Centre, Victoria, BC; ⁵Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC

MP 689 **Proteomic Analysis of Dpy1912-Deficient Human Globozoospermia Reveals Multiple Molecular Defects;** Xuejiang Guo¹; Yueshuai Guo¹; Daozhen Chen²; Xiaoyu Yang¹; ¹Nanjing Medical University, Nanjing, China; ²Wuxi Maternal and Child Health Care Hospital Affiliated to Nanjing Medical University, Wuxi, China

MP 690 **Mass Spectrometry-Based Proteomes of Paired Human Cerebrospinal Fluid and Plasma in Relation to the Blood-Brain Barrier;** Loïc Dayon¹; Ornella Cominetti¹; Jérôme Wojcik²; Antonio Núñez Galindo¹; Aikaterini Oikonomidi³; Hugues Henry⁴; Eugenia Migliavacca¹; Martin Kussmann^{1,5}; Gene L. Bowman^{1,6,7}; Julius Popp^{3,8}; ¹Nestlé Institute of Health Sciences, Nestlé Research, Lausanne, Switzerland; ²Precision for Medicine, Geneva, Switzerland; ³CHUV, Old Age Psychiatry, Department of Psychiatry, Lausanne, Switzerland; ⁴CHUV, Department of Laboratories, Lausanne, Switzerland; ⁵Frontiers Media S.A., Lausanne, Switzerland; ⁶Marcus Institute for Aging Research, Hebrew Senior Life, Boston, MA; ⁷Department of Medicine, Beth Israel Deaconess Medical Center and Harvard Medical School, Boston, MA; ⁸HUG, Geriatric Psychiatry, Department of Mental Health and Psychiatry, Geneva, Switzerland

MP 691 **Proteomic Characterisation of Chronic Lymphocytic Leukaemia Identifies Putative Subtype-Independent Clinical Targets and Dysregulation of the Spliceosome;** Harvey Johnston^{1,2}; Matthew J Carter²; Marta Larrayoz²; James Clarke²; Spiros D Garbis²; David Oscier²; Jonathan C Strefford²; Andrew J Steele²; Renata Walewska²; Mark S Cragg²; ¹UCL, London, United Kingdom; ²University of Southampton, Southampton, United Kingdom

MP 692 **Proteomic Characterization of Microneedle-Extracted Dermal Interstitial Fluid;** Gabrielle Rizzo¹; Bao Q. Tran²; Phillip Miller³; C Nicole Rosenzweig⁴; Ronen Polsky³; Trevor Glaros⁴; Phillip Mach⁵; ¹Excet, Inc., Springfield, VA; ²20th CBRNE Command, APG, MD; ³Sandia National Laboratory, Albuquerque, NM; ⁴ECBC, Aberdeen Proving Ground, MD; ⁵US Army ECBC, Aberdeen Proving Ground, MD



- MP 693 **MiCIdGUI: A User Friendly Graphical Interface for MiCId a Tool for Microorganism Classification and Identification**; Gelio Alves¹; Aleksey Ogurtsov¹; Oleg Obolensky¹; Yi-Kuo Yu¹; ¹National Center for Biotechnology Information, NLM, Bethesda, MD
- MP 694 **MHCquant: Automated and Reproducible Data Analysis for Immunopeptidomics**; Leon Bichmann¹; Annika Nelde^{2,3}; Michael Ghosh²; Timo Sachsenberg¹; Christopher Mohr⁴; Alexander Peltzer⁴; Leon Kuchenbecker¹; Juliane S. Walz³; Stefan Stevanović^{2,5}; Hans-Georg Rammensee^{2,5}; Oliver Kohlbacher^{1,4,6,7}; ¹Applied Bioinformatics, Department of Computer Science, University of Tübingen, Tübingen, Germany; ²Institute for Cell Biology, Department of Immunology, University of Tübingen, Tübingen, Germany; ³Department of Hematology and Oncology, University of Tübingen, Tübingen, Germany; ⁴Quantitative Biology Center, University of Tübingen, Tübingen, Germany; ⁵German Cancer Consortium (DKTK), DKFZ partner site, Tübingen, Germany; ⁶Biomolecular Interactions, Max Planck Institute for Developmental Biology, Tübingen, Germany; ⁷Institute for Translational Bioinformatics, University Hospital Tübingen, Tübingen, Germany
- MP 695 **Evaluation of Instrumental Variability Utilizing 2D LC-MS/MS Proteomic HeLa Standard Data to Enhance Quality Control Metrics in Clinical Proteomics**; Richard M. Searfoss¹; Punit Shah¹; Kennedy Ofori-Mensa¹; Kiki Panagopoulos¹; Rangaprasad Sarangarajan¹; Niven R. Narain¹; Michael A. Kiebish¹; ¹BERG, LLC, Framingham, MA
- MP 696 **Plasma-Based Protein Panel Can Predict Risk of Acute Graft-Versus-Host Disease and Non-Relapse Mortality in Patients Undergoing Allogeneic Hematopoietic Stemcell Transplantation**; Kisoon Dan¹; Junghoon Shin²; Dohyun Han¹; Ji-Won Kim³; Kyungkon Kim⁴; Sang Hoon Song²; Inho Kim²; ¹Proteomics Core Facility, Biomedical Research Institute, Seoul National University Hospital, Seoul, South Korea; ²Department of Internal Medicine, Seoul National University Hospital, Seoul, South Korea; ³Department of Internal Medicine, Seongnam Hospital, Seongnam, South Korea; ⁴Department of Convergence Medicine, Asan Institute for Life Sciences, Asan Medical Center, Seoul, South Korea
- MP 697 **Proteomic Analysis of Liver Tissue Reveals Chronic Low Level Oxidative Stress in a Mouse Model of Primary Hyperoxaluria Type 1**; Brianna E Buchalski¹; John Knight¹; Ross Holmes²; James A Mobley³; ¹University of Alabama at Birmingham, Birmingham, Alabama; ²University of Alabama at Birmingham, AL; ³University of Alabama at Birmingham, AL
- MP 698 **Profiling of Advanced Glycation End Products (AGE) PTM on Antigen Processing Machinery and MHC-II Molecules in Diabetes and T2DM Syndrome**; Cristina C Clement¹; Pia Negroni²; Kateryna Morozova¹; Lawrence Stern²; Laura Santambrogio¹; ¹Albert Einstein College of Medicine, Bronx, NY; ²University of Massachusetts Medical School, Worcester, MA
- MP 699 **Parallelizable Quantitative Characterization of Proteome and Targeted Metabolome from Laser Capture Microdissected Tissue Cells**; Shichen Shen¹; Jun Li¹; Min Ma²; Sailee Rasam¹; Xiaotao Duan³; Jun Qu¹; ¹University at Buffalo, Buffalo, NY; ²Roswell Park Comprehensive Cancer Center, Buffalo, NY; ³Beijing Institute of Pharmacology and Toxicology, Beijing, China
- MP 700 **Kinome Profiling Identifies Drug Resistance Pathways in Hepatocellular Carcinoma**; Martin Golkowski¹; Ho-Tak Lau¹; Marina Chan²; Heidi Kenerson³; Venkata Narayana Vidadala⁴; Anna Shoemaker¹; Dustin J Maly⁴; Raymond S Yeung³; Taranjit S Gujral²; Shao-En Ong¹; ¹Department of Pharmacology, University of Washington, Seattle, WA; ²Human Biology Division, Fred Hutchinson Cancer Research Center, Seattle, WA; ³Department of Surgery, University of Washington, Seattle, WA; ⁴Department of Chemistry, University of Washington, Seattle, WA
- MP 701 **Contraceptive Pills Alter Proteome of Erythrocytes and Induce Redox Damages**; Laurence Servais¹; Clovis Wouters¹; France Baumans¹; Dominique Baiwir²; Irina Lobysheva³; Flavia Dei Zotti³; Edwin De Pauw¹; Gauthier Eppe¹; Jean-Luc Balligand³; Gabriel Mazzucchelli^{1,2}; ¹University of Liege, Mass Spectrometry Laboratory, MolSys Research Unit, Liege, Belgium; ²University of Liège, GIGA Proteomics Facility, Liege, Belgium; ³Institute for Experimental and Clinical Research (IREC) and Pole of Pharmacology and Therapeutics (FATH)/UCL, Brussels, Belgium
- MP 702 **A Fast Sample Processing Strategy for Deep Urine Label-Free Quantification Proteomic Analysis**; Pamela S Cantrell¹; Xuemei Zeng¹; Nathan A Yates^{1,2}; ¹Biomedical Mass Spectrometry Center, University of Pittsburgh Schools of the Health Sciences, Pittsburgh, PA; ²Department of Cell Biology, University of Pittsburgh School of Medicine, Pittsburgh, PA
- MP 703 **Method Development for the Identification of Proteins in Fingertip Smears by Using MALDI-MS**; Cristina Russo¹; Laura Cole¹; Lynda Wylde²; Simona Francese¹; ¹Sheffield Hallam University, Sheffield, United Kingdom; ²The University of Sheffield, Sheffield, United Kingdom
- MP 704 **Carbonylated Proteome Signatures Caused by Stress during Development of Human Pregnancy in GARBH-Ini cohort**; Abhishek Kumar Singh¹; Amit Kumar Dey¹; Pallavi Kshetrapal Kshetrapal²; Nitya Wadhwa²; Shinjini Bhatnagar²; Arindam Maitra³; Dipankar Malakar⁴; Faraz Rashid⁴; Manoj Pillai⁴; Dinakar M Salunke⁵; Tushar Kanti Maiti¹; ¹Regional Centre for Biotechnology, Faridabad, India; ²Translational Health Science and Technology Institute, Faridabad, India; ³National Institute of Biomedical genomics, Kalyani, India; ⁴SCIEX INDIA, Gurugram, India; ⁵International Centre for Genetic Engineering and Biotechnology, Delhi, India
- MP 705 **Quantitative Mass Spectrometry-Based Global Proteome and Phosphoproteome Analyses of Thymic Epithelial Tumors (TET)**; Xu Zhang¹; Fatos Kirkali¹; Yue Qi¹; Ting Huang²; Tapan Maity¹; Khoa Dang Nguyen¹; David S. Schrupp³; Olga Vittek²; Arun Rajan¹; Udayan Guha¹; ¹Thoracic and GI Malignancies Branch, Center for Cancer Research, NCI, NIH, Bethesda, MD; ²Khoury College of Computer Sciences, Northeastern University, Boston, MA; ³Thoracic Surgery Branch, Center for Cancer Research, NCI, NIH, Bethesda, MD
- MP 706 **Serum Multi-omics Revealed the Effect of Sport Activity**; Marcello Manfredi¹; Elisa Robotti¹; Elettra Barberis¹; Maria Teresa Valenti²; Emilio Marengo¹; ¹University of Piemonte Orientale, Alessandria, Italy; ²University of Verona, Verona, Italy
- MP 707 **Proteogenomics Identifies Common Drugable Pathways in Undifferentiated Pleiomorphic Sarcoma**; Marcos Y Mayordomo^{1,2}; Javier A Alfaro²; Georges Bedran^{1,2}; Nathan a Grimes³; Larry Hayward¹; Jakub Factor¹; Rob O'Neill⁴; Borek Vojtesek⁵; Helen Creedon¹; Satya Saxena⁶; Katy Teo¹; Val Brunton¹; Donald Salter¹; Ted Hupp^{1,2}; Javier A Alfaro^{1,2}; ¹University of Edinburgh, Edinburgh, United Kingdom; ²University of Gdansk, Gdansk, Poland; ³University of Edinburgh, Edinburgh, United Kingdom; ⁴University of Cambridge, Cambridge, United Kingdom; ⁵Masaryk Memorial Cancer Institute, Oncology, Czech Republic; ⁶University of Baltimore, Baltimore, MD
- MP 708 **Identifying Breast Cancer Vulnerabilities by Mapping Interactome Dysregulations in Primary Tumor Samples**; Johannes Kreuzer¹; Robert Morris¹; Ridwan Ahmad¹; Cyril H. Benes¹; Dennis C. Sgroi¹; Wilhelm Haas¹; ¹Massachusetts General Hospital and Harvard Medical School, Charlestown, MA



- MP 709 **A Fully GLP Compliant Multiplexed Protein Quantification MRM Assay Panel**; Paul-Gerhard Lassahn¹; Claudia Escher²; Tobias Treiber²; Alexandre Kornfeld¹; Jakob Vowinkel²; Gregor Schütze¹; ¹SYNLAB Analytics & Services Switzerland AG, Birsfelden, Switzerland; ²Biognosys AG, Schlieren, Switzerland
- MP 710 **Evaluation of Different Sample Preparation Workflows for Reproducible, Quantitative, and In-Depth Analysis of Urine Proteomics**; Hua Ding¹; Hossein Fazelinia¹; Lynn A. Spruce¹; Dana A. Weiss¹; Stephen A. Zderic¹; Steven H. Seeholzer¹; ¹Children's Hospital of Philadelphia, Philadelphia, PA
- MP 711 **Biomarker Discovery in Serum and Plasma Using Protein Profiling by MALDI-TOF Mass Spectrometry**; Eric Weaver¹; Robert English²; Matthew Texter²; Ryan Walsh²; ¹University of Texas, Arlington, Arlington, TX; ²Shimadzu Scientific Instruments, Inc., Columbia, Maryland
- MP 712 **Providing Absolute Certainty without Absolute Quantity**; Meghan Bradley¹; Christopher M. Shuford¹; Patricia L. Holland¹; Michael Levandoski¹; Russell P. Grant¹; ¹LabCorp, Burlington, NC
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- MP 713 **MS-Based Deep Proteome Profiling of AD Related Mouse Model Defective in RNA Splicing**; Mingming Niu¹; Ping-Chung Chen²; Yun Jiao²; Hong Wang²; Junmin Peng²; ¹St Jude Children's Research Hospital, Memphis, TN; ²St Jude Children's Research Hospital, Memphis, TN
- MP 714 **Docosahexaenoic Acid Attenuates Metabolic Dysfunctions Induced by Lipopolysaccharide in BV-2 Microglial Cells**; Bo Yang^{1,2}; Runting Li¹; Brian P. Mooney^{1,2}; Kevin L. Fritsche¹; David Q. Beversdorf¹; Grace Y. Sun¹; C. Michael Greenleaf^{1,2}; ¹University of Missouri, Columbia, MO; ²Charles W. Gehrke Proteomics Center, Columbia, MO
- MP 715 **Comparison of Quantitative LC/MS/MS Plant Protein Assay Design and Impact on Precision of Results**; Kristi Harkins¹; Danielle Baker¹; Michaela Owens¹; ¹DowDuPont, Johnston, IA
- MP 716 **Increasing the Breadth and Depth of Multiplexed Quantitation Using Advanced Instrumentation and Methods**; Devin Schweppe¹; Qing Yu¹; Aaron Robitaille²; Graeme McAlister²; Derek J Bailey²; Jose Navarrete-Perea¹; Joao A. Paulo¹; Romain Huguet²; Steven Gygi¹; ¹Harvard Medical School, Boston, MA; ²ThermoFisher, San Jose, CA
- MP 717 **Quantitative Proteomic Analysis of Cell Cycle Regulation in Golgi-Matrix Assembly and Disassembly**; Hye Kyong Kweon¹; Shijiao Huang¹; Yanzhuang Wang¹; Philip C. Andrews¹; ¹University of Michigan, Ann Arbor, MI
- MP 718 **Systematic Investigation of Protein Dynamics to Unveil Their Degradation Pathways in Human Cells**; Ming Tong¹; Ronghu Wu¹; ¹Georgia Institute of Technology, Atlanta, GA
- MP 719 **Developing Mass Spectrometry Based Proteomic Methods to Identify and Quantify Protein Carbonylation in Plants**; Georgina H Charlton¹; Cleidiane G Zampronio¹; John Sinclair²; Peter Kilby²; Alex Jones¹; ¹University of Warwick, Coventry, United Kingdom; ²Syngenta Jealott's Hill International Research Centre, Bracknell, United Kingdom
- MP 720 **Surpassing 10,000 Proteins Quantified in Human Tissue by Augmenting Single Shot Data-Independent Acquisition (DIA) with Hybrid Libraries**; Jan Muntel¹; Tejas Gandhi¹; Lynn Verbeke¹; Oliver M. Bernhardt¹; Roland Bruderer¹; Lukas Reiter¹; ¹Biognosys AG, Schlieren, Switzerland
- MP 721 **Dynamic Proteome Changes during Macrophage Polarization Induced by Mouse Colon Cancer Cell-Derived Exosomes**; Yifan Tan¹; Lei Sun²; Meishuang Yan³; Yang Li³; Lin Wu²; Yan Ren¹; Xiaomin Lou²; Siqi Liu¹; ¹BGI
- Shenzhen, Shenzhen, China; ²Beijing Institute of Genomics, Beijing, China; ³Beijing Protein Innovation, Beijing, China
- MP 722 **Proteome-Wide Differences in Turnover Rates Among Rodents are Correlated to Their Lifespans and Energetic Demands**; Kyle Swovick¹; Kevin A Welle¹; Jennifer R Rhyhorenko¹; Andrei Seluanov¹; Vera Gorbunova¹; Sina Ghaemmaghami¹; ¹University of Rochester, Rochester, NY
- MP 723 **Absolute and Multiplex Protein Quantification Using Cell-Free Protein Synthesis and Mass Spectrometry**; Keiko Masuda¹; Keiko Kasahara²; Ryohei Narumi²; Yoshihiro Shimizu³; ¹RIKEN, Suita, Japan; ²National Institutes of Biomedical Innovation, Health and Nutrition, Ibaraki, Japan; ³RIKEN, Suita, Osaka, Japan
- MP 724 **A Novel Microduplication of ARID1B: Clinical, Genetic and Proteomic Findings**; Kathleen C Lundberg¹; Nicholas Szoko²; Daniela M. Schlatzer¹; Marvin Natowicz²; ¹Case Western Reserve University, Cleveland, OH; ²Cleveland Clinic, Cleveland, OH
- MP 725 **Global Proteomics Analysis to Decipher Common Proteostatic Stress Rescue Pathways of the Antioxidants Tempol and MitoTEMPO**; Silas D Wood¹; Maggie PY Lam¹; ¹Department of Medicine, Division of Cardiology, Consortium for Fibrosis Research and Translation, Anschutz Medical Campus, Aurora, CO
- MP 726 **Histone H3K56-acetylation is Epigenetic Barrier for Embryonic Stem Cell Differentiation into Trophoblasts**; Jennifer Nance¹; Feixia Chu¹; Thomas Fazzio²; Taylor Hickman¹; Amanda Chasse¹; ¹University of New Hampshire, Durham, NH; ²University of Massachusetts Medical School, Worcester, MA
- MP 727 **Increasing Protein Overlap between Multiple Isobaric Mass Tag Experiments with Comprehensive Precursor Ion Inclusion**; Simion Kreimer¹; Robert N. Cole¹; ¹Johns Hopkins, Baltimore, MD
- MP 728 **Protein Assisted Digestion Improves Sensitivity of Immunocapture-MRM Method to Quantify Stool Biomarker of Colorectal Cancer**; Rebecca Beard¹; Baochuan Guo¹; ¹Cleveland State University, Cleveland, OH
- MP 729 **In vivo Protein Turnover Rates in Mouse and Human Tissues**; Brian L. Frey¹; Zach Rolfs¹; Xudong Shi¹; Yoshitaka Kawai²; Bruce A. Buchholz²; Lloyd M. Smith¹; Nathan V. Welham¹; ¹University of Wisconsin - Madison, Madison, WI; ²Lawrence Livermore National Laboratory, Livermore, CA
- MP 730 **Characterization of the Ubiquitination Signaling on Hypoxia-Inducible Factor with Quantitative Chemical Proteomics Analysis**; Yunan Li¹; Ang Luo¹; Luke Erber¹; Yue Chen¹; ¹University of Minnesota at Twin Cities, Minneapolis, MN
- MP 731 **Identification and Characterizations of O2- and O4-Alkylthymidine DNA-Binding Proteins**; Xiaomei He¹; Pengcheng Wang¹; Hong Wang¹; ¹University of California, Riverside, Riverside, CA
- MP 732 **Evaluation of the Accuracy of Synchronous Precursor Selection (SPS) in Public Datasets**; Conor Jenkins^{1,2}; Aimee Rinas³; Benjamin Orsburn¹; ¹Think20 Labs, Columbia, MD; ²Hood College Bioinformatics Program, Frederick, MD; ³AIT BioSciences, Indianapolis, IN
- MP 733 **Applications of Mass Spectrometry Targeted Assays for Quantitative Analysis of Cancer Signaling Proteins**; Penny Jensen¹; Bhavin Patel¹; Leigh A Foster¹; Aaron S. Gajadhar²; Sebastien Gallien³; Jonathan R Krieger⁴; Jiefei Tong⁵; Michael F. Moran⁴; Rosa Viner²; Andreas Huhmer²; Kay Opperman¹; John C Rogers¹; ¹Thermo Fisher Scientific, Rockford, IL; ²Thermo Fisher Scientific, San Jose, CA; ³Thermo Fisher Scientific, Precision Medicine Science Center, Cambridge, MA; ⁴SPARC BioCentre, Hospital for Sick Children, Toronto, Ontario; ⁵Program in Cell Biology, The Hospital for Sick Children, Toronto, Ontario



- MP 734 **A Modified Orbitrap™ Tribrid Mass Spectrometer with Real-Time Search and Advanced Spectral Processing Enhances Multiplexed Proteome Coverage and Quantification Accuracy;** Aaron M Robitaille¹; Romain Huguet¹; Derek J Bailey¹; Graeme McAlister¹; Arne Kreutzmann²; Daniel Mourad²; Daniel Lopez-Ferrer¹; Andreas Huhmer¹; Vlad Zabrouskov¹; ¹Thermo Fisher Scientific, San Jose, CA; ²Thermo Fisher Scientific, Bremen, Germany
- MP 735 **Improved Identification, Quantification Accuracy, and Workflow Efficiency Using a Modified Quadrupole Orbitrap™ Mass Spectrometer and Tandem Mass Tags™ (TMT™) Approach;** Aaron Robitaille¹; Tabiwang N. Arrey²; Markus Kellmann²; Arne Kreutzmann²; Daniel Mourad²; Daniel Lopez-Ferrer¹; Andreas Huhmer¹; Alexander Harder²; ¹Thermo Fisher Scientific, San Jose, CA; ²Thermo Fisher Scientific, Bremen, Germany
- MP 736 **Strategies for Sample Normalization Post-Acquisition for Tandem Mass Tag (TMTM) Quantitative Workflow;** Pedro Navarro¹; Fernando J García Marqués²; Woong Kim³; Greg Foster³; Sharon J. Pitteri²; Daniel Lopez-Ferrer³; ¹Thermo Fisher Scientific, Bremen, Germany; ²Stanford University School of Medicine, Canary Center at Stanford for Cancer Early Detection, Palo Alto, CA; ³Thermo Fisher Scientific, San Jose, CA
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- MP 737 **Top-down Mass Spectrometry Characterization of Phospholamban Proteoforms in Cardiac Tissue Enabled by A Novel Photo-cleavable Surfactant;** Austin Carr¹; Kyle Brown¹; Song Jin¹; Ying Ge^{1,2,3,4}; ¹Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706; ²Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI; ³Molecular and Cellular Pharmacology Program, University of Wisconsin, Madison, WI; ⁴Human Proteomics Program, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI
- MP 738 **BirA* Mice Enable Cell Type Specific Proteomics in vivo;** Shiva Ahmadi^{1,2}; Elham Pourbarkhordariesfandabadi^{1,2}; Angela Egert²; Martin Breitbach²; Caroline Geissen²; Michael Hesse²; Kenichi Kimura²; Bernd K Fleischmann²; Hubert Schorle²; Volkmar Gieselmann^{1,2}; Dominic Winter^{1,2}; ¹IBMB Bonn, Bonn, Germany; ²University of Bonn, Bonn, Germany
- MP 739 **Identification Commutability in Proteomics and Metabolomics Utilizing Human Tissue Reference Materials;** Clay Davis¹; Benjamin Neely¹; Tracey Schock¹; Lisa Kilpatrick²; Debra Ellisor¹; Rebecca Pugh¹; ¹NIST, Charleston, SC; ²NIST, Gaithersburg, MD
- MP 740 **Alterations in Extracellular Matrix Composition during Aging and Photoaging of the Skin;** Maxwell McCabe¹; Kirk Hansen¹; Ryan Hill¹; Gary Fisher²; Taihao Quan²; ¹University of Colorado Anschutz Medical Campus, Aurora, CO; ²University of Michigan, Ann Arbor, MI
- MP 741 **Proteomic Profiling of Mitochondrial Complexomes; Naked Mole Rat Versus Mouse;** Satomi Miwa¹; Andrew J Porter¹; Graham Smith¹; Achim Treumann¹; Pawel Palmowski¹; Andrei Seluanov²; Vera Gorbunova²; Thomas Von Zgliniki¹; ¹Newcastle University, Newcastle Upon Tyne, United Kingdom; ²Rochester Institute of Technology, Rochester, NY
- MP 742 **Proteomics on Immune Competent Mouse Models Reveals Differences in Immunogenicity;** Fang Wang¹; Wenyan Zhong¹; Edward Rosfjord¹; Xiaoran S. Yang¹; Luanna Lemon¹; Jeremy S. Myers¹; ¹Pfizer WRD, Pearl River, NY
- MP 743 **A Proteomic Investigation of Changes in the Collagen Types Present in the Anterior Cruciate Ligament during Post-Natal Growth;** Jeffrey R. Enders^{1,2}; Stephanie G. Cone¹; Matthew B. Fisher¹; ¹North Carolina State University, Raleigh, NC; ²Molecular Education, Technology, and Research Innovation Center (METRIC), North Carolina State University, Raleigh, NC
- MP 744 **Body-Wide Proteome Dynamics in the Understanding and Assessment of Multiorgan Drug Response;** Bingyun Sun; Simon Fraser University, Burnaby, BC
- MP 745 **Bone Proteomics: Enhancing Homogenization of Bone Samples for Increased Proteomic Depth;** Rowan Matney¹; Kratika Singhal¹; Fang Liu¹; Ryan D. Leib¹; Allis S. Chien¹; ¹Stanford University Mass Spectrometry, Stanford, CA
- MP 746 **Elucidating Alternative Biological Pathways with Tailored Enrichment Strategies from Clinical Tissue Samples;** Kratika Singhal¹; Rowan Matney¹; Fang Liu¹; Ryan Leib¹; Allis Chien¹; ¹Stanford University Mass Spectrometry, Stanford, CA
- MP 747 **Distinct Blubber Proteome Responses to Single and Repeated ACTH Challenges in a Marine Mammal;** Jared Deyarmin¹; Molly McCormley¹; Cory Champagne²; Alicia Stephan¹; Laura Pujade Busqueta¹; Dorian Houser²; Daniel Crocker³; Jane Khudyakov^{1,2}; ¹University of the Pacific, Stockton, CA; ²National Marine Mammal Foundation, San Diego, CA; ³Sonoma State University, Rohnert Park, CA
- MP 748 **Identification of Estradiol-Regulated Protein Networks and Associated Biological Processes in the Rat Retina by Label-Free Quantitative Proteomics;** Laszlo Prokai¹; Khadiza Zaman¹; Fatima Rahlouni¹; Vien Nguyen¹; Vladimir Shulaev²; Katalin Prokai-Tatrai¹; ¹University of North Texas Health Science Center, Fort Worth, TX; ²University of North Texas, Denton, TX
- MP 749 **A Novel Proteomic Method Defines Extracellular Matrix Proteins and Their Post-Translational Modifications from Formalin-Fixed, Paraffin-Embedded Specimens of Heart Valve Disease;** Cassandra L. Clift¹; Susana Comte-Walters¹; Lauren E Ball¹; David Bichell²; Yan Ru Su³; Anand Mehta¹; Richard R Drake¹; Pegg M. Angel¹; ¹Department of Cell and Molecular Pharmacology and Experimental Therapeutics, Medical University of South Carolina, Charleston, SC; ²Division of Pediatric Cardiac Surgery, Vanderbilt University Medical Center, Nashville, TN; ³Department of Cardiovascular Medicine, Vanderbilt University Medical Center, Nashville, TN
- MP 750 **Comprehensive Proteomic Analysis of Gray and White Matter from Human Post-Mortem Brain Tissue;** Duc M Duong^{1,2}; Luming Yin^{1,2}; James J. Lah^{2,3}; Allan I. Levey^{2,3}; Nicholas T. Seyfried^{1,2,3}; ¹Department of Biochemistry, Emory University, Atlanta, GA; ²Center for Neurodegenerative Diseases, Emory School of Medicine, Atlanta, GA; ³Department of Neurology, Emory University, Atlanta, GA
- MP 751 **Proteomic Analysis of Extracellular Matrix Dynamics during Mouse Forelimb Development;** Kathryn R. Jacobson¹; Sarah L Lipp¹; Alex R. Ocken¹; Tamara L. Kinzer-Ursem¹; Sarah Calve¹; ¹Purdue University, West Lafayette, IN
- MP 752 **Extensive Intratumor Proteogenomic Heterogeneity Revealed by Multiregion Sampling in a High-Grade Serous Ovarian Tumor Specimen;** Thomas P. Conrads^{1,2}; Allison L. Hunt¹; Guisong Wang²; Julie Oliver²; Dave Mitchell²; Glenn Gist²; Brian Hood²; Ming Zhou¹; Brian Blanton²; Kelly Conrads²; Chad Hamilton²; Kathleen Darcy²; Craig Shriver³; Yovanni Casablanca²; George Larry Maxwell²; Nicholas W. Bateman²; ¹Inova Schar Cancer Institute, Annandale, VA; ²Gynecologic Cancer Center of Excellence, Annandale, VA; ³John P. Murtha Cancer Center, Bethesda, MD



- MP 753 **MMP-28 Alters Immunometabolic and Bioenergetic Profile of Activated Macrophages;** Dorota Tokmina-Roszyk^{1,2}; Lillian Onwuha-Ekpete^{1,2}; Mohammed Refai³; Monika Tokmina-Lukaszewska³; Brian Bothner³; Gregg Fields^{1,2}; ¹Florida Atlantic University, Jupiter, FL; ²The Scripps Research Institute, Jupiter, FL; ³Montana State University, Bozeman, MT
- MP 754 **Proteomic Analysis of Human Glioblastoma Formalin-Fixed Paraffin-Embedded Tissues;** Naomi Uwugiaren¹; Jakub Faktor²; David R Goodlett^{1,3}; Fiona Lickiss^{1,4}; Sofian Al Shboul⁴; Paul M Brennan⁵; Borek Vojtesek²; Theodore R Hupp^{1,4}; Irena Dapic¹; ¹International Centre for Cancer Vaccine Science, University of Gdansk, Gdansk, Poland; ²RECAMO, Brno, Czech Republic; ³University of Maryland, Baltimore, MD; ⁴CRUK, University of Edinburgh, Edinburgh, United Kingdom; ⁵Centre for Clinical Brain Sciences, University of Edinburgh, Edinburgh, United Kingdom
- MP 755 **A Global, Multi-Regional Proteomic Map of the Human Cerebral Cortex;** Zhengguang Guo¹; Chen Shao²; Yang Zhang³; Wenyong Qiu⁴; Wenting Li⁴; Qian Yang⁴; Yin Huang²; Yuepan Dong²; Haidan Sun⁵; Xiaoping Xiao⁵; Wei Sun⁵; Chao Ma⁴; Liwei Zhang³; ¹Peking Union Medicine College, Beijing, China; ²Beijing Proteome Research Center, National Center for Protein Sciences(Beijing), Beijing Institute of Lifeomics, Beijing, China; ³Beijing Tiantan Hospital, Capital Medical University, Beijing, China; ⁴Institute of Basic Medical Sciences, Neuroscience Center, Chinese Academy of Medical Sciences, School of Basic Medicine, Peking Union Medical College, Beijing, China; ⁵Institute of Basic Medical Sciences, Chinese Academy of Medical Sciences/School of Basic Medicine, Peking Union Medical College, Beijing, China
- MP 756 **Identification and Validation of Synapse-Loss Regulating Phosphorylation Events in Schizophrenia;** Megan Garver¹; Ying Ding²; Robert Sweet¹; Nathan A Yates³; Matthew L MacDonald¹; ¹UPMC, Pittsburgh, PA; ²Department of Biostatistics, University of Pittsburgh, Pittsburgh, Pennsylvania; ³BioMS Center, University of Pittsburgh, Pittsburgh, Pennsylvania
- MP 757 **Quantitative proteomics Analysis of Placenta from Zika Virus Infected Women;** Gabriel Borges Vélez¹; Julio Rosado Philipp²; Abiel Roche Lima¹; Kelvin Carrasquillo Carrión¹; Yadira M Cantres Rosario¹; Maria S Correa Rivas³; Loyda M Meléndez⁴; ¹University of Puerto Rico Medical Sciences Campus, San Juan, Puerto Rico; ²University of Puerto Rico Rio Piedras Campus, San Juan, PR; ³University of Puerto Rico Medical Sciences Campus, Quebradillas, PR; ⁴University of Puerto Rico Medical Sciences Campus, San Juan, PR
- MP 758 **Quantitative Proteogenomic Analysis of Inflamed Colon Tissue in Mice Reveals an Increase in Non-Canonical Protein Variants;** Andrew T. Rajczewski¹; Qiyuan Han¹; Subina Mehta¹; Praveen Kumar¹; Pratik D Jagtap¹; Natalia Tretyakova¹; Timothy J. Griffin¹; ¹University of Minnesota, Minneapolis, MN
- MP 759 **Interactome of the PIF Peptide (Preimplantation Factor) in Uterine Environment from Different Mammals – Proteomic Studies;** Anna Fel¹; Paulina Czaplowska¹; Katarzyna Macur¹; Marcel Thiel¹; Stanislaw Oldziej¹; ¹University of Gdansk, Gdansk, Poland
- MP 760 **KIT Restriction of Skin Proteome Analyzed with MALDI-Imaging Mass Spectrometry and Shotgun Proteomics on c-Kitmutant Mice;** Mayuka Kosugi¹; Masaya Ikegawa^{2,3}; Nobuto Kakuda²; Takashi Nirasawa⁴; Ryo Kajita⁴; Kazuo Kinoshita⁵; Yuki Kuzuhara⁵; ¹Doshisha University, Kyotanabe City, Kyoto, Japan; ²Graduate School, Major of Medical Life Systems, Doshisha University, Kyotanabe City, Japan; ³Department of Medical Life Systems, Doshisha University, Kyotanabe City, Japan; ⁴Bruker Japan K.K., Yokohama, Japan; ⁵Shiga Medical Center Research Institute, Moriyama, Japan
- MP 761 **A Label-free Quantification Approach to Identify Differentially Expressed Proteins between Wild Type and Transgenic Alzheimer Rat Brains;** Pritha Bagchi¹; Eric B. Dammer¹; Geng M. Wang¹; Robert M. Cohen²; Nicholas T. Seyfried^{1,3}; ¹Emory Integrated Proteomics Core, Emory University, Atlanta, GA; ²Department of Psychiatry and Behavioral Sciences, Emory University, Atlanta, GA; ³Department of Biochemistry, Emory University, Atlanta, GA
- MP 762 **Fast and Sensitive Quantitative Proteomic Analysis of Formalin-Fixed Paraffin-Embedded Tissue Using a Trapped Ion Mobility Q-TOF;** Matthew Willetts¹; Shourjo Ghose²; Christopher Swift²; Gary Kruppa²; John P Shapiro³; Brad H Rovin³; Matthias Kretzler⁴; Jeff Hodgins⁴; ¹Bruker, Billerica, MA; ²Bruker Scientific, Billerica, MA; ³The Ohio State University, Columbus, OH; ⁴University of Michigan Medical School, Ann Arbor, MI
- MP 763 **Comparison of S-Trap, IST and Conventional Digestion Methods for Serum Proteomics;** Benjamin Neely^{1,2}; Alison Bland^{2,3}; Michael Janech^{2,3}; ¹Marine Biochemical Sciences Group, National Institute of Standards and Technology, NIST Charleston, Charleston, SC; ²Hollings Marine Laboratory, Charleston, SC; ³College of Charleston, Charleston, SC
- MP 764 **Quantitative Proteome and Neuropeptide Profiling in Female Pregnant Mice with Neuropathic Pain by High-Resolution Mass Spectrometry;** Madeleine Parent-Vachon¹; Pascal Vachon¹; Francis Beaudry¹; ¹Université de Montreal, St-Hyacinthe, QC
- MP 765 **Cellular Precision for Infrared Laser Ablation Tissue Microproteomics;** Chao Dong¹; Fabrizio Donnarumma¹; Kelin Wang¹; Kermit K. Murray¹; ¹Louisiana State University, Baton Rouge, LA
- MP 766 **Quantitative Proteomics of Tuberculosis Lung FFPE Tissue by SWATH Analysis;** Amon Suzuki¹; Yasuhiro Hirano¹; Mina Kawamura¹; Akihiro Ishizu²; Susumu Y. Imanishi¹; ¹Meijo University, Nagoya, Japan; ²Hokkaido University, Sapporo, Japan
- MP 767 **MS-Based Strategies Reveal Extracellular Matrix Alterations and N-Glycan Spatial Distribution Changes with the Progression of Ovarian Cancer;** Zihui Li¹; Yatao Shi²; Fengfei Ma²; Kristal L. Gant³; Manish S. Patankar³; Lingjun Li^{1,2}; ¹Department of Chemistry, University of Wisconsin-Madison, Madison, WI; ²School of Pharmacy, University of Wisconsin-Madison, Madison, WI; ³Department of Obstetrics and Gynecology, University of Wisconsin-Madison, Madison, WI
- MP 768 **Latest developments of Liquid Extraction Surface Analysis Mass Spectrometry for Top-Down and Bottom-Up Investigation of Protein Biomarkers in Renal Fibrosis;** Emma K Sisley¹; Francisco Fernandez-Lima²; Tim Johnson³; Peter Hall³; Iain B Styles¹; Helen J Cooper¹; ¹University of Birmingham, Birmingham, United Kingdom; ²Florida International University, Miami, FL; ³UCB Pharma LTD, Slough, United Kingdom

**PROTEOMICS: TOP DOWN ANALYSIS I
769-787**

- MP 769 **Large-Scale Qualitative and Quantitative Top-Down Proteomics Using Capillary Zone Electrophoresis-Electrospray Ionization-Tandem Mass Spectrometry with Nanograms of Proteome Samples;** Rachele Lubeckyi¹; Abdul Rehman Bashara²; Xiaojing Shen³; Xiaowen Liu^{2,4}; Liangliang Sun³; ¹Michigan State University, East Lansing, MI; ²Indiana University-Purdue University Indianapolis, Indianapolis, Indiana; ³Michigan State University, East Lansing; ⁴Indiana University School of Medicine, Indianapolis, Indiana



- MP 770 **Top-down Analysis of β -lactoglobulin Involving Disulfide Bond Cleavages;** Jianzhong Chen; *University of Alabama at Birmingham, Birmingham, AL*
- MP 771 **Valet Parking for Protein Ion Charge State Concentration: Ion/Molecule Reactions in Linear Ion Traps;** David Foreman¹; Jay Bhanot¹; Kenneth W Lee¹; Scott A McLuckey¹; ¹*Purdue University, West Lafayette, IN*
- MP 772 **Single Muscle Fiber Proteomics Enabled by High Sensitivity Top-Down Mass Spectrometry;** Jake A. Melby¹; Yutong Jin¹; Trisha Tucholski¹; Yanlong Zhu¹; Ziqing Lin¹; Gary Diffee¹; Ying Ge¹; ¹*University of Wisconsin, Madison, Madison, WI*
- MP 773 **Improved Top-Down Search Accuracy and Sensitivity using MetaMorpheus and a Novel Algorithm for Monoisotopic Mass Determination;** Robert Millikin¹; Leah V. Schaffer¹; Michael R. Shortreed¹; Lloyd M. Smith¹; ¹*University of Wisconsin Madison, Madison, WI*
- MP 774 **Top-Down Proteomics Applied to Human CSF;** Marina Gay¹; Ester Sánchez-Jiménez¹; Laura Villarreal¹; Mar Vilanova¹; Romain Huguet²; Gianluca Arauz-Garofalo¹; Antonio Lorenzo¹; Mireia Diaz-Lobo¹; Daniel López-Ferrer²; Marta Vilaseca¹; ¹*Institute for Research in Biomedicine (IRB Barcelona), The Barcelona Institute of Science and Technology (BIST), Barcelona, Spain*; ²*ThermoFisher, San Jose, CA*
- MP 775 **Deciphering the Tubulin Code with Top-Down Proteomics;** Mathieu Dupré¹; Thibault Chaze¹; Elise Warter²; Serge Bonnefoy²; Jujimon A.s³; Philippe Bastin²; Carsten Janke³; Mariette Matondo¹; Julia Chamot-Rooke¹; ¹*Mass Spectrometry for Biology Unit, Institut Pasteur, CNRS USR2000, Paris, France*; ²*Trypanosome Cell Biology Unit, Institut Pasteur, INSERM U1201, Paris, France*; ³*Regulation of Microtubule Dynamics and Functions Unit, Institut Curie, CNRS UMR3348, Orsay, France*
- MP 776 **Extending the Mass Range for Native Top-Down Mass Spectrometry by UVPD;** Jean-Francois Greisch^{1, 2}; Sem Tamara^{1, 2}; Albert J.R. Heck^{1, 2}; ¹*Biomolecular Mass Spectrometry and Proteomics, Bijvoet Center for Biomolecular Research and Utrecht Institute of Pharmaceutical Sciences, Utrecht University, Utrecht, Netherlands*; ²*Netherlands Proteomics Center, Utrecht, Netherlands*
- MP 777 **Controlling False-Discovery Rate for Top Down Proteomics Data Using UVPD Fragmentation;** Ken Durbin¹; Luca Fornelli^{2, 3}; Joseph Greer⁴; Ryan Fellers¹; Mick Greer⁵; David Horn⁶; Neil L Kelleher³; ¹*Proteinaceous, Evanston, IL*; ²*University of Oklahoma, Norman, OK*; ³*Northwestern University, Evanston, IL*; ⁴*Proteinaceous, Inc., Evanston, IL*; ⁵*Thermo Fisher Scientific, Austin, TX*; ⁶*Thermo Fisher Scientific, San Jose, CA*
- MP 778 **Precise Characterization and Comparison of KRAS Oncoproteoforms across Three Cancer Contexts;** Lauren Adams¹; Caroline J DeHart¹; Lissa C Anderson²; Luca Fornelli³; Christopher L. Hendrickson²; Neil L Kelleher¹; ¹*Northwestern University, Evanston, IL*; ²*National High Magnetic Field Laboratory, Tallahassee, FL*; ³*University of Oklahoma, Norman, OK*
- MP 779 **Large Scale Informatics for Interrogating Proteoforms in Human Blood Cells with Top Down Proteomics;** Joseph B Greer¹; Ryan T Fellers¹; Richard D Leduc¹; Bryan P Early¹; Josiah E Hutton¹; Rafael D Melani¹; Jacek W Sikora¹; R Vince Gerbasi¹; Jeannie M Camarillo¹; Paul M Thomas¹; Neil L Kelleher¹; ¹*Northwestern University, Evanston, IL*
- MP 780 **High-Field Asymmetric Ion Mobility Spectrometry of Heterogeneous Proteoform Populations from Primary Human Leukocytes;** Robert V Gerbasi¹; Susan E Abbatiello²; Rafael D. Melani¹; Michael W. Belford³; Scott M. Peterman³; Romain Huguet³; Philip D. Compton¹; Paul M Thomas¹; Neil L Kelleher¹; ¹*Northwestern University, Evanston, IL*; ²*Northeastern University, Boston, MA 02115*; ³*Thermo Fisher Scientific, San Jose, CA*
- MP 781 **Identification of Lactobacillus and Saccharomyces at Species Level in Industrial Ethanol Production Using Spectral Signatures by MALDI-TOF MS;** Juliana Guimarões Fonseca; *ESALQ/ USP, Piracicaba, Brazil*
- MP 782 **Middle Down Approach for the Characterization of Monoclonal Antibodies after Ides Digestion and ETD Fragmentation;** John L. Snyder¹; Colin M Wynne¹; Michelle English²; Marshall Bern²; ¹*Eurofins Lancaster Laboratories, Inc., Lancaster, PA*; ²*Protein Metrics Inc., San Carlos, CA*
- MP 783 **Profiling Combinatorial Posttranslational Modifications in Seminal Plasma from Dairy Bulls via Sheathless Capillary Zone Electrophoresis – Top-Down Mass Spectrometry;** Fabio P. Gomes¹; Jolene K. Diedrich¹; Anthony J. Saviola¹; Abdullah Kaya²; Erdogan Memili³; Arlindo A. Moura⁴; John R. Yates, III¹; ¹*The Scripps Research Institute, La Jolla, CA*; ²*Selçuk University, Selçuklu, Turkey*; ³*The Mississippi State University, Starkville, MS*; ⁴*The Federal University of Ceara, Fortaleza, Brazil*
- MP 784 **Dipolar DC Induced Collisional Activation of Non-Dissociated Electron-Transfer Products;** Sarju Adhikari¹; Mack Shih¹; Eric T Dziekonski²; Frank A Londry²; Scott A McLuckey¹; ¹*Purdue University, West Lafayette, IN*; ²*SCIEX, Concord, ON*
- MP 785 **Enhancing Top-Down Proteomics Data Analysis by Combining Deconvolution Results using Ensemble Methods;** Molly Wetzel¹; Daniel Belongia²; Yutong Jin³; Zhijie Wu³; Irene M. Ong^{2, 4, 5}; Sean J. McIlwain^{1, 4}; Ying Ge^{1, 2, 6, 7}; ¹*Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI*; ²*School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI*; ³*Department of Chemistry, University of Wisconsin-Madison, Madison, WI*; ⁴*Department of Biostatistics and Medical Informatics, University of Wisconsin - Madison, Madison, WI*; ⁵*Department of Obstetrics & Gynecology, University of Wisconsin - Madison, Madison, WI*; ⁶*Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706*; ⁷*Human Proteomics Program, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI*
- MP 786 **Charge Deconvolution of Dissociation Spectra of Protein Complexes;** Marshall W. Bern¹; Yong J. Kil¹; Jing Yan²; Zachary L VanAernum²; Vicki H Wysocki²; ¹*Protein Metrics, San Carlos, CA*; ²*The Ohio State University, Columbus, OH*
- MP 787 **Investigation into Data-Independent Acquisition in Orbitrap and TOF platform for Topdown Proteomics Using Intact and Bionic software;** Victoria Sanchez¹; Elisabeth Weyher¹; K. Ilker Sen²; Marshall W. Bern²; Nagarjuna Nagaraj¹; ¹*Max Planck Institute of Biochemistry, Martinsried, Germany*; ²*Protein Metrics Inc., Cupertino, CA*



TUESDAY POSTERS

Set up all Tuesday posters
7:00 - 8:00 am

Odd-numbered posters present
10:30 - 11:30 am PLUS 12:30 - 2:30 pm

Even-numbered posters present
10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

Remove all Tuesday posters
7:00 - 8:00 pm

Antibodies & Antibody Drug Conjugates I	001-022
Art, Archaeology & Paleontology	023-036
Biomarkers: Discovery I	037-068
Biomarkers: Quantitative Analysis II	069-099
Clinical Analysis II	100-123
Disease Biomarkers I	124-141
Energy: Hydrocarbon and Petrochemical	142-159
Environmental: General II	160-191
Environmental: Pharmaceuticals and Pesticides	192-212
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Fundamentals: Ion Structure/Energetics	270-287
Fundamentals: Ionization Mechanisms	288-297
GC/MS: Instrumentation and Applications I	298-318
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Imaging MS: Method Development I	344-364
Imaging MS: Pharmaceutical Applications	365-379
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Metabolomics: Untargeted Metabolite Profiling	550-568
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Protein Therapeutics: Quantitative Analysis II	580-605
Protein Therapeutics: Structural Characterization II	606-625
Proteins: PTMs I	626-646
Proteomics: Infectious Diseases	647-657
Proteomics: Intact Proteins	658-666
Proteomics: New Approaches I	667-694
Proteomics: Quantitative II	695-717
Proteomics: Top Down Analysis II	718-737
Small Molecules: Qualitative Analysis	738-756
Systems Biology	757-780

ANTIBODIES & ANTIBODY DRUG CONJUGATES I 001-022

- TP 001 **Evaluating the Performance of an Orbitrap Tribrid at 8000 m/z**; John P. McGee¹; Rafael Melani¹; Mike Senko²; Vlad Zabrouskov²; Philip Remes²; Graeme McAlister²; Christopher Mullen²; Jesse Canterbury²; Michael Goodwin²; Romain Huguet²; Lee Early²; Neil L. Kelleher¹; Philip D. Compton¹; ¹Northwestern University, Evanston, IL; ²Thermo Fisher Scientific, San Jose, CA
- TP 002 **Analysis of Therapeutic Monoclonal Antibodies Using Volatile pH Gradient Cation Exchange Chromatography Directly Coupled to Native Mass Spectrometry**; Julia Baek¹; Rosa Viner²; Terry Zhang²; James Ngai³; Eugen Damoc⁴; Shanhua Lin⁵; ¹Thermo Fisher Scientific, Sunnyvale, California; ²Thermo Fisher Scientific, San Jose, California; ³Thermo Fisher Scientific, Sunnyvale; ⁴Thermo Fisher Scientific, Bremen, Germany; ⁵Thermo Fisher Scientific, Sunnyvale, CA
- TP 003 **Online IEX-MS Characterization and Monitoring of mAb Charge Heterogeneity Using an Optimized Cation Exchange Resin and Compact TOF Mass Spectrometer**; Samantha Ippoliti¹; Qi Wang¹; Ying Qing Yu¹; Matthew A. Lauber¹; Henry Shion¹; ¹Waters Corporation, Milford, MA
- TP 004 **Optimizing MS/MS Acquisition to Generate a Comprehensive Multi-Attribute Method Data Archive of the NISTmAb**; Michael E. Pettit¹; John E. Schiel¹; ¹National Institute of Standards and Technology, Gaithersburg, MD
- TP 005 **A Novel Approach to Stability Characterization of ADC Payload Related Degradation through Assessment of Capped Drug-Linker ADC Surrogates**; Michael Lesslie¹; Beijing Huang¹; Gilbert Mbah¹; Brittney Mills¹; Jianwen Xu²; ¹AbbVie Inc., North Chicago, IL; ²AbbVie Inc., Worcester, MA
- TP 006 **Improve Sensitivity and Mass Accuracy in IEC-MS Analysis of Antibody Charge Variants**; Kyoung-Soon Choi¹; Zhongping Liao¹; Jason X. Tang¹; ¹Eli Lilly & Company, Indianapolis, IN
- TP 007 **Coupling Mixed-Mode Size Exclusion Chromatography with Native Mass Spectrometry for the Analysis of Intact Monoclonal Antibodies**; Yuetian Yan¹; Tao Xing¹; Shunhai Wang¹; Ning Li¹; Thomas J. Daly¹; ¹Regeneron, Tarrytown, NY
- TP 008 **Development and Qualification of a Difluoroacetic acid (DFA)-Based Subunit LC-MS Method for ADC Characterization**; Jacquelynn Smith¹; Jennifer Nguyen²; Olga Friese¹; Jason Rouse³; Matthew A. Lauber²; ¹Pfizer, Chesterfield, MO; ²Waters Corporation, Milford, MA; ³Pfizer, Andover, MA
- TP 009 **Application of Wildcard Search Approach in Sequence Variant Analysis**; Yutian Gan; ¹Genentech, Inc., South San Francisco, CA
- TP 010 **ETHcD Spectrum with Deep Novo Enables the Discrimination of Leucine and Isoleucine**; Yi Liu¹; Wen Zhang¹; Rui Qiao²; Ngoc Hieu Tran²; Lei Xin¹; ¹Bioinformatics Solutions Inc., Waterloo, ON; ²University of Waterloo, Waterloo, ON
- TP 011 **A Simple Approach for Improved LC-MS Analysis of Protein Biopharmaceuticals via Modification of Desolvation Gas**; Shunhai Wang¹; Tao Xing¹; Anita P Liu¹; Zehong He¹; Yuetian Yan¹; Thomas J Daly¹; Ning Li¹; ¹Regeneron Pharmaceuticals Inc., Tarrytown, NY
- TP 012 **Characterization of Cetuximab using pH Gradient Cation Exchange and Microchip Electrophoresis Coupled to Native Orbitrap Mass Spectrometry**; Florian Fuessl¹; Craig Jakes¹; Sara Carillo¹; Ashley Bell²; Erin A. Redman²; Ken Cook³; Jonathan Bones¹; ¹The National Institute for Bioprocessing Research & Training, Dublin, Ireland; ²908 Devices, Boston, MA; ³Thermo Fisher Scientific, Hemel Hempstead, UK, Hemel Hempstead, United Kingdom



- TP 013 **Analysis of Monoclonal Antibodies using SEC-MS in Native and Denaturing States to Identify Aggregation during DuoBody Formation;** [Elsa Gorre](#)¹; Rajiv Rao²; Rebecca Smith²; Andrew Mahan¹; Harsha Gunawardena¹; Hirsh Nanda¹; ¹Janssen Research and Development, Spring House, PA; ²Janssen Research & Development, Large Molecule Drug Product Development, Malvern, PA
- TP 014 **Structural Characterizations of Intact Monoclonal Antibodies by Native MS;** Angela Criscuolo^{1,2}; Tabiwang N. Arrey²; Eugen Damoc²; Thomas Moehring²; Catharina Crone²; [Markus Kellmann](#)²; ¹Leipzig University, Leipzig, Germany; ²Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany
- TP 015 **Automated Comprehensive Characterization and Quantification of Low-Abundance Sequence Variants in a Standard Monoclonal Antibody;** [Joe Shambaugh](#)¹; Aude Tartiere²; Albert Van Wyk³; John McCarter⁴; Cassandra Wigmore⁵; Peter Haber⁶; ¹Genedata Inc, Lexington, MA; ²Genedata, Inc., San Francisco, CA; ³Genedata Ltd, Cambridge, United Kingdom; ⁴Genedata, Inc., Lexington, MA; ⁵Genedata AG, Basel, Switzerland; ⁶Genedata GmbH, Munich, Germany
- TP 016 **Using Cation Exchange Chromatography and Online Mass Spectrometry (CEX-MS) for Assignment of iCIEF Charge Variants;** [Kevin Ray](#)¹; Ben Cutak¹; Shreya Ahuja¹; ¹MilliporeSigma, St. Louis, MO
- TP 017 **Characterization of BiTE® Antibody Constructs by Hydrophilic Interaction Chromatography Coupled to Mass Spectrometry;** [Yang Stella Song](#)¹; Amy Huang¹; John Harrahy¹; ¹Amgen Inc., Cambridge, MA
- TP 018 **Native Top-Down Analysis of Intact Antibodies Using Multiple Dissociation Techniques on a Tribrid Quadrupole Orbitrap Linear Ion Trap Mass Spectrometer;** [Eugen Damoc](#)¹; Kristina Srzentic²; Romain Huguet³; Graeme McAlister³; Christopher Mullen³; Philip M Remes³; Jesse D Canterbury³; Mike Senko³; Vlad Zabrouskov³; ¹Thermo Fisher Scientific, Bremen, Germany; ²Thermo Fisher Scientific, Cambridge, Massachusetts; ³Thermo Fisher Scientific, San Jose, California
- TP 019 **Process Monitoring of Monoclonal Antibodies at Intact and Subunits Levels using a Single Quadrupole LC/MS for Quality Control;** Linfeng Wu¹; [Lisa Zang](#)¹; Guannan Li¹; ¹Agilent Technologies, Santa Clara, CA
- TP 020 **The Impact of Using Different Protease Combinations for “de novo” Protein Sequencing;** [Thierry Le Bihan](#)¹; Paul Taylor¹; Zac McDonald¹; Qixin Liu¹; Jianqiao Shen¹; Kathleen Gorospe¹; Xin Xu¹; Chris Hosfield²; Bin Ma^{1,3}; ¹Rapid Novor Inc, Kitchener; ²Promega Corporation, Madison, WI; ³University of Waterloo, Waterloo
- TP 021 **Improving Assignment of Sequence Variants Using Machine Learning;** Sibylle Heideberger¹; [Lyle Burton](#)²; Sean L. Seymour³; ¹AB Sciex UK Ltd, Warrington, United Kingdom; ²SCIEX, Concord, ON; ³Seymour Data Science, San Francisco, CA
- TP 022 **Isotope Selection in Label-Free Quantification and its Effects in Biopharmaceutical Characterization;** [David Mahon](#)¹; K. Ilker Sen²; Yong J. Kil²; Promod Mehndiratta¹; ¹Celgene, Summit, NJ; ²Protein Metrics Inc., Cupertino, CA
- ART, ARCHAEOLOGY & PALEONTOLOGY**
023-036
- TP 023 **What Sherlock Sorely Missed: The EVA Technology for Cultural Heritage Exploration;** [Gleb Zilberstein](#)¹; Alfonsina D'Amato²; Piergiorgio Righetti³; ¹Spectrophon Ltd., Rehovot, Israel; ²Università degli Studi di Milano, Dept. Pharmaceutical Sciences, Milano, Italy; ³Politecnico di Milano, Dept. of Chemistry, Milano, Italy
- TP 024 **Multiple Techniques Confirm Collagen Remnants in Fossil Bone;** [Brian Thomas](#)¹; Robert Layfield²; Lynn Smith³; Barry Shaw²; Stephen Taylor⁴; ¹University of Liverpool, Glenn Heights, TX; ²University of Nottingham, Nottingham, United Kingdom; ³Norton Priory, Runcorn, United Kingdom; ⁴Mass Spectrometry Group, University of Liverpool, Liverpool, United Kingdom
- TP 025 **Palaeoproteomics on Paintings: Tandem Mass Spectrometry Unravels the History of Artistic Materials through Post-Translational Modifications;** [Fabiana Di Gianvincenzo](#)¹; Meaghan Mackie^{1,2}; Patrick Rütger²; Diana Samodova²; David Peggie³; Jesper V. Olsen²; Enrico Cappellini¹; ¹Department of Biology, University of Copenhagen, Copenhagen, Denmark; ²NNF Center for Protein Research University of Copenhagen, Copenhagen, Denmark; ³National Gallery of London, London, United Kingdom
- TP 026 **Identification of Animal Species by Mass Spectrometry of Collagen Extracted from Neolithic and Paleolithic Bones and Teeth;** [Takashi Nakazawa](#)¹; Momoko Osawa¹; Kana Matsuo¹; Mako Inuzuka¹; Yuki Ito¹; Kazuki Kawahara²; Yuichi Naito³; Seiji Kadowaki³; Yoshihiro Nishiaki⁴; ¹Nara Women's University, Nara, Japan; ²Osaka University, Suita, Japan; ³Nagoya University, Nagoya, Japan; ⁴The University of Tokyo, Bunkyo, Japan
- TP 027 **Species Identification of Materials Used in Cultural Heritage Objects from Alaska in the British Museum's Collection Using 'ZooMS' Methodology;** [Michael Douglas Nairn](#)¹; Chris Mussell²; Amber Lincoln²; ¹Shimadzu, Manchester, UK, Manchester, United Kingdom; ²The British Museum, London, United Kingdom
- TP 028 **GrandPep, a Novel Software for Computational Reconstruction of Ancient Protein Sequences;** [Petra Gutenbrunner](#)¹; Frido Welker²; Jazmin Ramos Madrigal²; Enrico Cappellini²; Juergen Cox¹; ¹Max-Planck Institute of Biochemistry, Planegg, Germany; ²Department of Biology, University of Copenhagen, Copenhagen, Denmark
- TP 029 **Effects of Preparation Methods, Environmental Factors, and Scientific Analysis on Aging of Historical Silk, Parchment, and Bone at Molecular Levels;** [Mehdi Moini](#); George Washington University, Washington, VA
- TP 030 **Revealing the Past through Non-invasive Metabolomics and Proteomics;** [Elettra Barberis](#)¹; Marcello Manfredi²; Pier Giorgio Righetti³; Gleb Zilberstein⁴; Bianucci Raffaella⁵; Emilio Marengo²; ¹University of Piemonte Orientale - Department of Sciences and Technological Innovation, Alessandria, Italy; ²University of Piemonte Orientale, Alessandria, Italy; ³Politecnico di Milano, Dept. of Chemistry, Milano, Italy; ⁴Spectrophon Ltd., Rehovot, Israel; ⁵University of Turin, Torino, Italy
- TP 031 **Microwave-Assisted Acid Hydrolysis for Whole Bone Proteomics and Paleoproteomics;** [Caitlin Colleary](#)¹; Timothy P Cleland¹; ¹Smithsonian Museum Conservation Institute, Suitland, MD
- TP 032 **Archival Proteins: Biomolecular Evidence of Parchment Production Methods;** [Carla L Soto Quintana](#)¹; Sarah Fiddymment¹; Matthew J Collins^{2,3}; ¹University of York, York, United Kingdom; ²University of Copenhagen, Copenhagen, Denmark; ³University of Cambridge, Cambridge, United Kingdom
- TP 033 **Robust Proteomics Workflow for the Identification and Classification of Paleontological Bones;** [Fabrice Bray](#)¹; Stéphanie Flament¹; Patrick Auguste¹; Christian Rolando¹; ¹Université de Lille, Villeneuve d'Ascq, France
- TP 034 **Digging Deeper into Ancient Proteomes – Improved Sampling and Instrumentation Allow for an Unprecedented View of the Archaeological Protein Record;** [Patrick L. Ruether](#)¹; Alberto J. Taurozzi²; Dorte B. Bekker-Jensen¹; Tanveer S. Batth¹; Tabiwang N. Arrey³; Alexander Harder³; Christian D. Kelstrup¹; Enrico Cappellini²; Jesper V. Olsen¹; ¹NNF Center for Protein



- Research University of Copenhagen, Copenhagen, Denmark; ²Natural History Museum of Denmark, Copenhagen, Denmark; ³Thermo Fisher Scientific, Bremen, Germany
- TP 035 **Multidisciplinary Approach to Understanding Preservation and Decomposition at Vindolanda, Roman Fort, UK;** Gillian Taylor¹; Hrafnhildur Helga Halldórsdóttir¹; Rhys Williams¹; Caroline Orr¹; Andrew Birley²; ¹Teesside University, Middlesbrough, United Kingdom; ²Vindolanda, Bardon Mill, United Kingdom
- TP 036 **Adapting Historic Architecture and Engineering Documentation Protocols to the Virtual Preservation of Historically Important Analytical Instruments;** Frances R. Gale¹; P. Jane Gale²; Michael A Grayson³; ¹University of Texas at Austin School of Architecture (ret), Austin, TX; ²ASMS Archivist/Historian, Southborough, MA; ³ASMS Archivist/Historian (ret), St. Louis, MO
- BIOMARKERS: DISCOVERY I**
037-068
- TP 037 **Coccidioidomycosis Detection Using Targeted Plasma and Urine Metabolic Profiling;** Paniz Jasbi¹; Natalie M. Mitchell¹; Xiaojian Shi¹; Thomas E. Grys²; Yiping Wei¹; Li Liu^{2,4}; Douglas F. Lake²; Haiwei Gu¹; ¹Arizona State University, Phoenix, AZ; ²Arizona State University, Tempe, AZ; ³Mayo Clinic, Phoenix, AZ; ⁴Mayo Clinic, Scottsdale, AZ
- TP 038 **Quantitative Serum Proteomics Uncovers Biomarkers for the Prediction of *Staphylococcus aureus* Bacteremia Patient Outcomes and Highlights Dysregulated Host Defense Networks;** Jacob Wozniak¹; Warren Rose²; George Sakoulas¹; David J Gonzalez¹; ¹UCSD, San Diego, CA; ²University of Wisconsin, Madison, Madison, WI
- TP 039 **Proteomic and Lipidomic Analysis Reveals Altered Fatty Acid Metabolism in the Liver of the Symptomatic Niemann-Pick, Type C1 Mouse Model;** Melissa R. Pergande¹; Jonathon Hanek¹; Estefania Zárate¹; Sheher Banu Mohsin²; Carol Haney-Ball³; Stephanie M Cologna¹; ¹University of Illinois at Chicago, Chicago, IL; ²Agilent Technologies, Wood Dale, IL; ³Agilent Technologies, Cary, NC
- TP 040 **Epitope Structures of Aptamer Complexes of the Multi-domain Protein C-Met Revealed by Proteolytic Affinity-Mass Spectrometry;** Michael Przybylski¹; Loredana Lupu²; Pascal Wiegand²; Nico Hüttmann²; Stephan Rawer²; Wolfgang Kleinekofort^{2,3}; Irina Shchugoreva⁴; Anna S. Kichkailo⁵; Felix N. Tomilin⁶; Alexander Lazarev⁶; Maxim V. Berezovskii⁷; ¹Steinbeis Centre Biopolymer Analysis and Biomedical Mass Spectrometry, Ruesselsheim, Germany; ²Steinbeis Centre Biopolymer Analysis and Biomedical Mass Spectrometry, Ruesselsheim, Germany; ³Rhein Main University, Rüsselsheim, Germany; ⁴Kirensky Institute of Physics, Russian Academy of Sciences, Krasnoyarsk, Russia; ⁵Krasnoyarsk State Medical University, Krasnoyarsk, Russia; ⁶Pressure Biosciences Inc., South Easton, MA; ⁷University of Ottawa, Dept. Chemistry, Ottawa, Quebec
- TP 041 **Novel S-Nitrosylated Proteolytic Peptides Derived from Postsynaptic Proteins for Alzheimer's Disease;** George Anis Sarkis¹; John S. Wishnok¹; Steven R Tannenbaum¹; ¹Massachusetts Institute of Technology, Cambridge, MA
- TP 042 **High-Throughput Screening of Antimicrobial Resistance by MALDI-High Resolution Mass Spectrometry of Bacterial Cell Cultures;** Evan Larson¹; Andrew Petersen¹; Bryan Bellaire¹; Young Jin Lee¹; ¹Iowa State University, Ames, IA
- TP 043 **Targeted Metabolomics Profile Sow Milk Components by LC-MS/MS;** Shen Allison¹; Qisheng Zhong²; ¹Shimadzu Global COE, Shimadzu (China) Co., Ltd., China, Guangzhou, China; ²Shimadzu Global COE, Shimadzu (China) Co., Ltd., China, Guangzhou, China
- TP 044 **Colorectal Cancer Patient-Derived Serum Exosomes Promote Cancer Cell Migration;** Hye Ryeon Jung¹; Yu-Ri Seo¹; Jeehee Park¹; Eugene C. Yi¹; ¹Department of Molecular Medicine and Biopharmaceutical Sciences, Graduate School of Convergence Science and Technology, Seoul National University, Seoul, South Korea
- TP 045 **Identification of Novel Serum Protein Biomarkers for ALS Diagnosis and Progression;** Szymon Filip¹; Tori Sosnowski¹; Halil Idrisoglu²; Hande Ozdinler^{3,4}; Young Ah Goo¹; ¹Proteomics Center of Excellence, Northwestern University, Chicago, IL; ²Istanbul University, Istanbul, Turkey; ³Department of Neurology, Northwestern University, Feinberg School of Medicine, Chicago, IL; ⁴Les Turner ALS Center at Northwestern University, Chicago, IL
- TP 046 **Identifying Peptide Signatures in Longitudinally Collected CSF Associated with Progression of ALS Using DIA Mass Spectrometry;** Allyson L Mellinger¹; Jeffrey R. Enders²; Michael S. Bereman^{1,3,4}; ¹Department of Chemistry, North Carolina State University, Raleigh, NC; ²Molecular Education, Technology, and Research Innovation Center, Raleigh, NC; ³Center for Human Health and the Environment, North Carolina State University, Raleigh, NC; ⁴Department of Biological Sciences, North Carolina State University, Raleigh, NC
- TP 047 **Lipid Biomarker Identification for Preterm Birth and Miscarriage via Deuterium Oxide Labeling for Global Omics Relative Quantification;** Byoungsook Goh¹; Ji-Yeon Park²; Joo-Hee Choi²; Jong-Hwan Park²; Tae-Young Kim^{1,3}; ¹Department of Chemistry, Gwangju Institute of Science and Technology, Gwangju, South Korea; ²Laboratory Animal Medicine, College of Veterinary Medicine and BK 21 PLUS Project Team, Chonnam National University, Gwangju, South Korea; ³School of Earth Sciences and Environmental Engineering, Gwangju Institute of Science and Technology, Gwangju, South Korea
- TP 048 **An Integrated System for Sequential Isolation of Circulating Tumor Cells and Exosomes for Proteomic Analysis from the Same Blood Sample;** Jie Zhang¹; Jianhui Zhu¹; Zhijing Tan¹; Mingrui An¹; Yingfeng Zhang¹; Neehar D. Parikh¹; David M. Lubman¹; ¹University of Michigan Medical Center, Ann Arbor, MI
- TP 049 **Screening of Site-Specific Glycopeptides in Serum Haptoglobin as Novel Biomarkers for Non-Alcoholic Steatohepatitis Using ETHcD-MS/MS;** Jianhui Zhu¹; Jie Zhang¹; Zhengwei Chen²; Gabriela Grigorean³; Lingjun Li²; David M. Lubman¹; ¹University of Michigan Medical Center, Ann Arbor, MI; ²University of Wisconsin-Madison, Madison, WI; ³University of Michigan, Ann Arbor, MI
- TP 050 **Systematic Proteomic Analysis of the interaction between UPR and LPS regulated Phosphorylation Establishes Novel Connections to Innate Immunity;** Min Ma¹; Yatao Shi¹; Yusi Cui¹; Junfeng Huang¹; Yiping Liu¹; Judith A Smith¹; Lingjun Li¹; ¹University of Wisconsin-Madison, WI
- TP 051 **Establishment of Q-markers of Niaoduoqing Granule by High Resolution Mass Spectrum Analysis and Network Pharmacology Study;** Yi-Sheng Xu¹; Yuanyuan Xie²; ¹waters cooperation, Shanghai, China; ²Tsinghua University, Beijing, China
- TP 052 **Effects of Daily Vinegar Ingestion on Insulin Sensitivity, Visceral Fat, Body Weight and the Metabolome in Healthy Adults;** Paniz Jasbi¹; Olivia Baker²; Xiaojian Shi¹; Lisa Gonzalez²; Summer Anderson²; Xinchun Wang¹; Haiwei Gu¹; Carol S. Johnston²; ¹Arizona State University, Scottsdale, AZ; ²Arizona State University, Phoenix, AZ
- TP 053 **Lipidomics of Parkinson's Disease: Towards More Accurate Diagnosis Methods through Omics Technologies;** Adriana Zardini Buzatto¹; Barinder Bajwa¹; Jaspaul Tatlay¹; Roger A Dixon¹; Richard Camicioli¹; Liang Li¹; ¹University of Alberta, Edmonton, AB



- TP 054 **Ovarian Cancer Detection Using Plasma Metabolic Profiling;** Yiping Wei¹; Paniz Jasbi¹; Xiaojian Shi¹; Haiwei Gu¹; ¹Arizona State University, Scottsdale, AZ
- TP 055 **Mapping and Sequencing of Gangliosides in Human Cerebellum at Different Developmental Stages by Orbitrap Multistage Mass Spectrometry;** Raluca Ica¹; Mirela Sarbu¹; Alina Petrut¹; Cristian VA Munteanu²; Andrei J Petrescu²; Radu Albuлесcu³; Alina D. D Zamfir¹; ¹National Institute for Research and Development in Electrochemistry and Condensed Matter, Timisoara, Romania, Timisoara, Romania; ²Institute of Biochemistry of the Romanian Academy, Bucharest, Romania; ³National Institute for Chemical - Pharmaceutical Research and Development, Bucharest, Romania
- TP 056 **Lipidomics of Alzheimer's Disease and Cerebral Amyloid Angiopathy: Identification of Potential Biomarkers in Human Plasma by UHPLC-MS;** Barinder Bajwa¹; Adriana Zardini Buzatto¹; Roger A Dixon¹; Richard Camicioli¹; Eric E Smith²; Liang Li¹; ¹University of Alberta, Edmonton, AB; ²University of Calgary, Calgary, AB
- TP 057 **Tyrosine Aminoacyl-tRNA Synthetase Sensitize Breast Cancer to the Combined Chemotherapeutic Regimen;** Ji hye Moon¹; Dohyun Han¹; Hyeyoon Kim¹; Han Suk Ryu¹; ¹Seoul National University Hospital, Seoul, South Korea
- TP 058 **Development and Technical Validation of a Data-Independent Acquisition Approach for Analysis of Human Alzheimer's Disease Cerebrospinal Fluid;** Shannon N. Leslie¹; Rashawn S. Wilson²; Pia W. Kivisakk³; Savannah E. Kandigian³; Bianca A. Trombetta³; Becky C. Carlyle³; Steven E. Arnold³; Angus C. Nairn¹; ¹Yale University, New Haven; ²Yale University Keck MS & Proteomics Core, New Haven, CT; ³Massachusetts General Hospital, Boston, Massachusetts
- TP 059 **Scalable and Automated Plasma Workflow Based on the Thermo Scientific Q Exactive HF-X MS platform;** Jing Wang¹; Sarah Trusiak¹; Ryan D. Bomgarden²; Sergei Snovida³; Emily I. Chen¹; ¹ThermoFisher Scientific Precision Medicine Science Center, Cambridge, MA; ²ThermoFisher Scientific, Rockford, IL; ³Thermo Fisher Scientific, Rockford, IL
- TP 060 **Proteomic Characterization of the Warburg Effects in Clear Cell Renal Cell Carcinoma;** Yuling Chen¹; Yang Lv²; Songfeng Wu³; Jiatong Xu¹; Di Wu²; Haiteng Deng¹; ¹Tsinghua University, Beijing, China; ²Center of Nephrology, the General Hospital of the PLA, Beijing, China; ³Academy of Military Medical Sciences Countermeasures, Beijing, China
- TP 061 **Development of an LC-MRM-MS assay for Analysis of Prostate-Specific Antigen Including its Major Glyco-Proteofoms;** Yuri E.M. van der Burg¹; Kasper Siliakus¹; Guinevere S.M. Lageveen-Kammeijer¹; Manfred Wuhrer¹; L. Renee Ruhaak¹; Christa M. Cobbaert¹; ¹Leiden University Medical Center, Leiden, Netherlands
- TP 062 **A Highly Sensitive FFPE Tissue Workflow by Coupling the Micro Pillar Array Column (μPACTM) with High Resolution Mass Spectrometry;** Antonius Koller¹; Sarah Trusiak²; Xinyu Zhang²; Alexander R Ivanov¹; Emily I. Chen²; ¹Northeastern University, Boston, MA; ²Thermo Fisher Precision Medicine Science Center, Cambridge, MA
- TP 063 **A Quantitative Proteomics Platform for Identifying Potential Biomarkers for Controlling Krypton Misuse in Horseracing;** Kin-Sing Wong¹; Hiu Wing Cheung¹; Timmy L.S. Choi¹; Wai Him Kwok¹; Terence S.M. Wan¹; Jenny K.Y. Wong¹; Peter Curl²; Stewart C. Mechie²; Anil Prabhu²; Emmie N.M. Ho¹; ¹Racing Laboratory, The Hong Kong Jockey Club, Hong Kong, Hong Kong; ²Department of Veterinary Regulation & Biosecurity Policy, The Hong Kong Jockey Club, Hong Kong, Hong Kong
- TP 064 **Mass Spectrometric Analysis of Sebum Contents for Classification of Parkinson's Disease;** Drupad Trivedi¹; Eleanor Sinclair¹; Depanjan Sarkar¹; Joy Milne¹; Monty Silverdale¹; Tilo Kunath²; Roy Goodacre³; Perdita Barran¹; ¹University of Manchester, Manchester, United Kingdom; ²University of Edinburgh, Edinburgh, United Kingdom; ³University of Liverpool, Liverpool, United Kingdom
- TP 065 **Proteomics Comparative Study of Exosome Subpopulations;** Yingfeng Zhang¹; Jianhui Zhu²; Zhijing Tan²; David M. Lubman³; ¹University of Michigan, ANN ARBOR, MI; ²University of Michigan, Ann Arbor, Michigan; ³University of Michigan, Ann Arbor, MI
- TP 066 **Protein Identification - the Translational Research Study of HBx Genes Related to Hepatocellular Carcinoma;** Ming-Hui Yang¹; Yi-Ming Arthur Chen²; Yi-Chia Lee³; Yu-Chang Tyan³; ¹National Health Research Institutes, Zhunan, Taiwan; ²Taipei Medical University, Taipei, Taiwan; ³Kaohsiung Medical University, Kaohsiung, Taiwan
- TP 067 **Use of untargeted metabolomics approach using label free LC-DIA-MS method to identify putative biomarkers involved in spontaneous pre-term birth (sp-PTB);** Shirish Yakkundi¹; James Langridge²; Lee A Gethings²; ¹INFANT Centre, University College Cork, Cork, Ireland; ²Waters Corporation, Wilmslow, United Kingdom
- TP 068 **Development of a Simple and Robust LC-MS/MS Method for the Quantification of the Renal Failure Biomarker Symmetric Dimethyl Arginine (SDMA);** Brittany J Perley¹; Alyssa Kaba¹; Jem Sibbick¹; Rachel Van Heest¹; Sean Maki¹; Katherine Henry¹; Steven Wiltshire¹; Allysen Meymaris¹; ¹Charles River Laboratories, Worcester, MA

BIOMARKERS: QUANTITATIVE ANALYSIS II 069-099

- TP 069 **Evaluation on LC-MS/MS Assay Using Anti-Peptide Immunocapture to Quantify PD-L1 As a Clinical Biomarker in FFPE Tissues for Immuno-Therapy Development;** Naiyu Zheng¹; Kristin Taylor¹; Huidong Gu¹; Rasa Santockyte¹; Xi-Tao Wang¹; Yan J. Zhang¹; Renuka Pillutla¹; Jianing Zeng¹; ¹Bristol-Myers Squibb Company, Princeton, NJ
- TP 070 **Multiple Reaction Monitoring (MRM) and Parallel Reaction Monitoring (PRM) to Identify Biomarkers Predictive of Clinical Response to Tocilizumab (anti-IL-6) Treatment;** Jin woo Jung¹; Byoung-Kyu Cho¹; Kang Hyun Kim¹; Yeong Wook Song^{1,2}; Eugene C. Yi¹; ¹Department of Molecular Medicine and Biopharmaceutical Sciences, Graduate School of Convergence Science and Technology, Seoul National University, Seoul, South Korea; ²Division of Rheumatology, Department of Internal Medicine, College of Medicine, Seoul National University, Seoul, South Korea
- TP 071 **Simultaneous Quantitation of Epinephrine and Norepinephrine as Cardiovascular Biomarkers in Rodent Species Plasma Utilizing a Non-Derivatized UHPLC-MS/MS Assay;** Craig Titsch¹; Enzo Kandoussi¹; Jianing Zeng¹; Glen Banks²; Gayani Fernando²; Yan J. Zhang¹; Renuka Pillutla¹; Naiyu Zheng¹; ¹Bristol-Myers Squibb Co., Lawrenceville, NJ; ²Bristol-Myers Squibb Co., Hopewell, NJ
- TP 072 **In-Sample Calibration Curve Using Multiple Isotopologue Reaction Monitoring of a SIL-Analyte for Instant LC-MS/MS Analysis of Biomarker and Quantitative Proteomics;** Huidong Gu¹; Yue Zhao¹; Marissa DeMichele¹; Naiyu Zheng¹; Yan J. Zhang¹; Renuka Pillutla¹; Jianing Zeng¹; ¹Bristol-Myers Squibb, Princeton, NJ
- TP 073 **Quantification of Soluble MERTK in Serum Using Affinity Enrichment-Liquid Chromatography Mass Spectrometry;** Yongxin Zhu¹; Petia Shipkova²; Thomas Spires²; Karen Augustine²; Timothy Olah²; ¹Bristol-Myers



- Squibb Company, Princeton, NJ; ²Bristol-Myers Squibb Co., Princeton, NJ
- TP 074 **Optimized high-throughput proteomic sample preparation in 96-well plate format for identifying serum Biomarkers of alpha-Dystroglycanopathy;** Mahmud Hossain¹; Monica Lane¹; Hongge Wang¹; Jun Luo¹; Bailin Zhang¹; ¹Sanofi Genzyme, Framingham, MA
- TP 075 **Urinary Mercapturic Acids of Volatile Organic Compounds and Oxidative/Nitrosative Stress Markers in Workers of the Semiconductor Industry;** Hsin-Chang Chen¹; Chen-Hsien Lee²; Kai-Chieh Yang¹; Wei-Lun Su¹; Tzu-Sheng Fang¹; Yi-Chen Sun¹; ¹Institute of Food Safety and Health, National Taiwan University, Taipei, Taiwan; ²Institute of Labor, Occupational Safety and Health, Ministry of Labor, New Taipei City, Taiwan
- TP 076 **Multiplexed Detection of Biomolecules with High Sensitivity and Specificity Using Surface Mass Spectrometry;** Hee-Kyung Na^{1,2}; Hyun Kyong Shon¹; Sunho Joh^{1,3}; Jeong-Hee Moon⁴; Hye Young Son⁵; Yong-Min Huh⁵; Tae Geol Lee¹; ¹KRISS, Daejeon, South Korea; ²Seoul national university, Seoul, South Korea; ³Department of Nano Science, University of Science and Technology, Daejeon, South Korea; ⁴KRIBB, Daejeon, South Korea; ⁵Department of Radiology, College of Medicine, Yonsei University, Seoul, South Korea
- TP 077 **Resolution and Quantitative Analysis of Human Urinary Isomeric Mercapturic Acids Derived from Crotonaldehyde, 2-Methylacrolein, and Methylvinyl Ketone;** Menglan Chen¹; Steven Carmella²; Stephen S Hecht²; ¹Masonic Cancer Center, U of MN, Minneapolis; ²University of Minnesota, Minneapolis, MN
- TP 078 **Development of an Automated Sample Preparation Platform for cPILOT;** Albert Arul¹; Renā A.S. Robinson¹; ¹Vanderbilt University, Nashville, TN
- TP 079 **Effect of Maternal Urinary and Placenta Melamine Levels during Pregnancy on Neonatal Birth Weight by Isotope Dilution LC-MS/MS;** Sih-Syuan Li¹; Chung-Yi Huang¹; Yung-Hung Chen²; Chia-Fang Wu¹; ¹Research Center for Environmental Medicine, Kaohsiung Medical University, Kaohsiung, Taiwan; ²Department of Gynecology and Obstetrics, Kaohsiung Medical University Hospital, Kaohsiung Medical University, Kaohsiung, Taiwan
- TP 080 **Measurement of Cyclooxygenase Inhibition and Selectivity in Human Whole Blood Assay Using LC-MS/MS;** Yifan Shi¹; Heather Murrey¹; Kay Ahn¹; Naidong Weng¹; Shefali Patel¹; ¹Janssen, Spring House, PA
- TP 081 **Highly Sensitive Immuno-MRM Assay for Quantitation of PTEN in Both FFPE and Fresh Frozen Tissue;** Sahar Ibrahim¹; Rene Zahedi²; Naciba Benlimame³; Adriana Aguilar⁴; Mark Basik^{5,6}; Gerald Batist^{6,7,8,9,10}; Christoph H. Borchers^{2,11,12,13}; ¹Department of Experimental Medicine, McGill University, Montreal, Québec; ²Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; ³Research Pathology Facility, Lady Davis Institute, Jewish General Hospital, McGill University, Montreal, QC; ⁴Cancer Genomics and Translational Research Laboratory, Segal Cancer centre, Lady Davis Institute, McGill university, Montreal, QC; ⁵Department of Medicine, Division of Experimental Medicine, McGill University, Montreal, QC; ⁶Department of Oncology, McGill University, Montreal, QC; ⁷Departments of Medicine and Oncology, McGill University, Montreal, QC; ⁸Dept. of Oncology, Sir Mortimer B. Davis-Jewish General Hospital, Montreal, QC; ⁹Segal Cancer Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; ¹⁰McGill Centre for Translational Research in Cancer, Segal Cancer Centre / Lady Davis Institute, Jewish General Hospital, Montreal, QC; ¹¹University of Victoria-Genome BC Proteomics Centre, Victoria, BC; ¹²Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC; ¹³Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC
- TP 082 **Rapid Profiling and Quantification of 17 Bile Acids in Human Plasma by LC-MS/MS;** Dan Li¹; Frances Carroll¹; Shun-Hsin Liang¹; Ravali Alagandula¹; Justin Steimling¹; Sue Steinike¹; Paul Connolly¹; ¹Restek, Bellefonte, PA
- TP 083 **Immunoaffinity LCMS Assay for Measuring Soluble B-Cell Maturation Antigen in Multiple Myeloma Patients;** Ying Zhang¹; John K Meissen¹; Kyle Wald¹; Angela Stauffer²; Michael Hall²; Matthew Blatnik¹; ¹Pfizer Inc., Groton, CT; ²Pfizer WRD, La Jolla, CA
- TP 084 **Development of LC-MS/MS Assays to Measure Thyroid Hormones in Rat Serum;** Hua Wang¹; Seth R Bell¹; Junhong Guo¹; Jeroen Kooistra¹; Pragati S Coder¹; Liam B Moran¹; Elizabeth A Groeber¹; ¹Charles River Laboratories, Ashland, OH
- TP 085 **Quantification of EDB+FN Levels in PDX Tumor and PDX FFPE Samples Using LC-MS/MS Methods;** Fengping Li¹; Bing Kuang²; Andrea Hooper³; Jonathon Golas³; Chao-Pei Betty Chang³; Mauricio Leal³; Hendrik Neubert¹; Lindsay King¹; ¹Pfizer, Andover, MA; ²Pfizer WRD, La Jolla, California; ³Pfizer WRD, Pearl River, New York
- TP 086 **Determining Isocyanate Exposure in Human Urine by LC-MRM;** Maggy Lepine^{1,2}; Lekha Sleno¹; Jacques Lesage¹; Sebastien Gagne²; ¹UQAM, Montreal, QC; ²IRSST, Montreal, QC
- TP 087 **Multiplexed Quantitative Glycoproteomic and Proteomic Analyses of Cerebrospinal Fluid in Alzheimer's Disease;** Xiaofang Zhong¹; Zhengwei Chen¹; Qinying Yu¹; Henrik Zetterberg²; Cynthia Carlsson¹; Ozioma Okonkwo¹; Lingjun Li¹; ¹University of Wisconsin-Madison, Madison, WI; ²University of Gothenburg, Gothenburg, Sweden
- TP 088 **Quantification of Jag1 Protein in Agarose Inflated Lung Airway Samples by Immuno Affinity Enrichment and LC-MS/MS analysis;** Omar S. Barnaby¹; Joon Nam²; Deanna Mohn¹; Brian Bennet²; Jonathan Phillips²; Christopher A. James¹; ¹Amgen, Inc., Thousand Oaks, CA; ²Amgen, Inc., Thousand Oaks, CA
- TP 089 **LC-MS/MS Analysis of Arachidonic Acid as a Biomarker in Human Plasma for Clinical Studies;** Tian-Sheng Lu¹; Elise Snider¹; Nicole Greer¹; Joshua Froning¹; Yong-Xi Li¹; ¹Medpace Bioanalytical Laboratories, Cincinnati, OH
- TP 090 **Developing Protein Biomarker MRM Methods as an Alternative Indicator of Prohibited Substance Abuse in Equine Athletes;** Sophie Bromilow¹; Heather Knych¹; Ben Moeller¹; Rick Arthur¹; Claudia P.B. Martins²; David Horohov³; Scott Stanley³; ¹K.L. Maddy Equine Analytical Chemistry Laboratory, Davis, CA; ²ThermoFisher, San Jose, CA; ³Gluck Equine Research Centre, Lexington, KY
- TP 091 **Metabolic Reprogramming in Prostate Cancer Cell Lines in Response to Tyrosine Kinase Inhibition;** Robert Sprung¹; Surbhi Chouhan¹; Petra Erdmann-Gilmore¹; Qiang Zhang¹; Rose Connors¹; Yiling Mi¹; Nupam Mahajan¹; Reid Townsend¹; ¹Washington University, School of Medicine, St. Louis, MO
- TP 092 **Quantitative Measurement of 7-Ketocholesterol and Cholestane-3 β ,5 α ,6 β -triol as Biomarkers in Human Serum Using LC-MS/MS;** Aiping Zhu¹; Idana Santiago¹; Yu Zhang¹; Yong-Xi Li¹; ¹Medpace Bioanalytical Laboratories, Cincinnati, OH
- TP 093 **Dried Blood Spots from Frozen Whole Blood Provide an Option to Analyze Parkinson's Disease Cohorts for Activity of Lysosomal Enzymes;** Pavlina Wolf¹; Roy Alcalay²; Karolina Helesicova¹; Ruby Chiang¹; Emma-Jane Turton¹; Michael Pauculo³; William Nichols³; Wendy Chung⁴; Pablo Sardi¹; Kate Zhang¹; Petra Oliva¹; ¹Sanofi, Framingham, MA; ²Columbia University Medical Center, Neurological Institute, New York, NY; ³Division of Human Genetics, Cincinnati Children's Hospital Medical Center



- and the Department of Pediatrics, University of Cincinnati College of Medicine, Cincinnati, OH; ⁴Department of Pediatrics and Medicine, Columbia University Medical Center, New York, NY
- TP 094 **LC-MS/MS Assay for Non-Invasive Detection of Prostaglandins and Leukotrienes in Urine**; Xiongfei Wu¹; Hanjiao Song¹; Weiqun Cao¹; Lili Xing¹; Xin Zhang¹; Yi Tao¹; ¹WuXi AppTec, Shanghai, China
- TP 095 **Multiplexed Quantification of Sepsis Prognosis Candidate Biomarkers Spanning a Wide Dynamic Range of Plasma Concentrations (ng/ml to mg/ml)**; Christelle Dubois¹; Didier Payen²; Stéphanie Simon¹; François Fenaille¹; Christophe Junot¹; Nathalie Morel¹; François Becher¹; ¹CEA Saclay, DRF, Institut Joliot, Service de Pharmacologie et d'Immunoanalyse- CEA-INRA UMR 0496, Laboratoire d'Etude du Métabolisme des Médicaments, Gif-sur-Yvette, France; ²Department of Anesthesiology and Critical Care, Lariboisière Hospital, University of Paris Denis Diderot 7, Paris, France
- TP 096 **Metaproteomics of the Human Intestinal Microbiota in Physiological and Pathological Conditions**; celine Henry¹; Ariane Bassignani^{2,3}; Olivier Langella⁴; Véronique Monnet²; Catherine Juste²; the ProteoCardis Consortium^{1,2,4,5,6,7}; ¹PAPPSO, Micalis Institute, INRA, AgroParisTech, Université Paris-Saclay, Jouy en Josas, France; ²Micalis Institute, INRA, AgroParisTech, Université Paris-Saclay, Jouy en Josas, France; ³US1367 MetaGenoPolis, INRA, Jouy en Josas, France; ⁴PAPPSO, GQE Le Moulon, INRA, Univ. Paris-Sud, CNRS, AgroParisTech, Université Paris-Saclay, Gif Sur Yvette, France; ⁵Institut National de la Recherche Agronomique, MalAGE, INRA, Université, Paris-Saclay, Jouy en Josas, France; ⁶Institute of Cardiometabolism and Nutrition, ICAN, Assistance Publique Hôpitaux de Paris and Inserm/Sorbonne University team NutriOmics, Pitié-Salpêtrière Hospital, Paris, France; ⁷Laboratoire de Spectrométrie de Masse BioOrganique, Université de Strasbourg, CNRS, IPHC, UMR 7178, Strasbourg, France
- TP 097 **Liquid-Chromatography coupled to Tandem Mass Spectrometry for 28 Bile Acids Profiling in Serum or Liver Samples**; Yoshihiro Izumi¹; Mikael Levi²; Jun Watanabe²; Takeshi Bamba¹; ¹National University Corporation Kyushu University, Research Center for Transomics Medecine, Fukuoka, Japan; ²Shimadzu Corporation, Kyoto, Japan
- TP 098 **Characterization of Patient-Derived Colorectal Cancer Cells Using the Proteome and Phosphoproteome Information**; Ryohei Narumi¹; Keiko Kasahara¹; Bo Gong²; Yuki Shimizu²; Ryohei Katayama²; Satoshi Nagayama²; Jun Adachi¹; Takeshi Tomonaga¹; ¹NIBIOHN, Ibaraki-city, Japan; ²JFCR, Koto-ku, Japan
- TP 099 **Plasma Proteome Profiling Discovers Novel Proteins Associated with Non-Alcoholic Fatty Liver Disease**; Lili Niu^{1,2}; Rajat Gupta¹; Philipp E. Geyer^{1,2}; Nicolai J. Wewer Albrechtsen^{1,2}; Lise L. Gluud³; Alberto Santos¹; Sophia Doll^{1,2}; Jens J. Holst³; Filip K. Knop³; Tina Vilsbøll³; Anders Junker³; Stephan Sachs⁴; Kerstin Stemmer⁴; Timo D. Müller⁴; Matthias H. Tschöp⁴; Susanna M. Hofmann⁵; Matthias Mann^{1,2}; ¹The Novo Nordisk Foundation center for Protein Research, Copenhagen, Denmark; ²Max Planck Institute of Biochemistry, Martinsried, Germany; ³Faculty of Health and Medical Sciences, University of Copenhagen, Copenhagen, Denmark; ⁴Helmholtz Diabetes Center at Helmholtz Centre Munich & Division of Metabolic Diseases, munich, Germany; ⁵Helmholtz Diabetes Center at Helmholtz Zentrum München, Munich, Germany
- CLINICAL ANALYSIS II**
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- TP 100 **A LC-MS Method for the Measurement of about 250 Compounds of Interest in Toxicology with a Fully-Automated Sample Preparation**; Tiphaine Robin¹; Alan Barnes²; Neil Loftus²; Sylvain Dulaurent¹; Pierre Marquet¹; Souleiman El Balkhi¹; Franck Saint-Marcoux¹; ¹CHU Limoges, Limoges, France; ²Shimadzu Corporation, Manchester, United Kingdom
- TP 101 **Clinical Diagnosis of Congenital Disorders of Glycosylation (CDGs) by Flow Injection Analysis Electrospray Ionization Time-of-Flight Mass Spectrometry (FIA-ESI-TOF-MS)**; Caroline M. Watson¹; Patricia L. Hall¹; S. Caleb Jerris¹; ¹EGL Genetics, Tucker, GA
- TP 102 **Transition Ratios for the Product-Ion-Poor: Activation Energy Modulation in the Absence of Distinct Neutral Losses**; Brian Rappold; LabCorp, Raleigh, NC
- TP 103 **Induced In-Source Fragmentation for the Quantitation of Inulin by ESI-MS/MS to Assess Renal Function**; Oscar Ekpenyong¹; Ken Lin¹; Lufei Hu¹; Maribel Beaumont¹; ¹Merck & Co., Inc., South San Francisco, CA
- TP 104 **Clinical Diagnostics of Lysosomal Storage Diseases in DBS Using New Substrates by MRM-MS**; Brindusa Alina Petre^{1,2,3}; Laura Ion^{1,2}; Cristina Dimitriu⁴; Stefan Maeser²; Wolfgang Kleinekofort²; Cosmin Bulei¹; Michael Przybylski²; ¹Al. I. Cuza University of Iasi, Iasi, Romania; ²Steinbeis Centre Biopolymer Analysis and Biomedical Mass Spectrometry, Ruesselsheim, Germany; ³TRANSCEND - Regional Institute of Oncology, Iasi, Romania; ⁴Grigore T. Popa University of Medicine and Pharmacy, Department of Biochemistry, Iasi, Romania
- TP 105 **A UHPLC-MS/MS Method for the Separation and Low-Level Determination of Catecholamines and Metanephrines in Urine Using a Novel C18-Based Column**; Geoffrey Faden¹; Alan P Mckeown²; ¹MACMOD Analytical Inc., Chadds Ford, PA; ²Advanced Chromatography Technologies Ltd, Aberdeen, United Kingdom
- TP 106 **Irradiation Sterilization Effects on Clinical Specimens Prior to Mass Spectrometric Analyses**; Samantha L Isenberg¹; Melissa D Carter²; Jonathan L Moon²; Sarah Laughlin²; Marla Petway²; Mike A Mojica²; Cody I Sheppard²; Alexis K Gursky²; Dennis A Bagarozzi Jr.²; James L Pirkle²; Rudolph C. Johnson²; ¹Centers for Disease Control and Prevention, Atlanta, GA; ²Centers for Disease Control and Prevention, Atlanta, Georgia
- TP 107 **Analysis of Drugs in Whole Blood by PaperSpray-FAIMS-MS/MS**; Rae Ana Snyder¹; Cornelia Boeser¹; Neloni Wijeratne¹; Mary L. Blackburn¹; ¹Thermo Fisher Scientific, San Jose, CA
- TP 108 **Rapid, Direct and Quantitative Urine Analysis for Common and Emerging Drugs of Abuse by Paper Spray Mass Spectrometry (PS-MS)**; Scott A. Borden^{1,2}; Jan Palaty³; Erik T. Krogh^{1,2}; Christopher G. Gill^{1,2,4,5}; ¹Appl. Env. Res. Labs. (AERL), Vancouver Island University, Chemistry Department, Nanaimo, BC; ²University of Victoria, Chemistry Department, Victoria, BC; ³Lifelabs Medical Laboratories, Burnaby, BC; ⁴Simon Fraser University, Chemistry Department, Burnaby, BC; ⁵University of Washington, DEOHS, Seattle, WA
- TP 109 **Evaluation and Quantitation of Nineteen Bile Acids in Human Plasma by LC-MS Analyses**; Hongyi Cai¹; Peter J. Walter¹; Mayte Gonzalez^{1,2}; ¹NIH, Bethesda, MD; ²Schreiner University, Kerrville, TX
- TP 110 **Desorption Electrospray Ionization Mass Spectrometry as a Tool for Diagnosis of Thyroid Nodules from Fine Needle Aspiration Biopsies**; Rachel J DeHoog¹; Jialing Zhang¹; Elizabeth Alore²; John Lin¹; Spencer Woody¹; Wendong Yu²; Christopher Almandariz¹; Monica Lin¹; Christopher Pirko²; Anton F Engelsman³; Stan B Sidhu³;



- Robert Tibshirani⁴; James Suliburk²; Livia S Eberlin¹; ¹University of Texas at Austin, Austin, TX; ²Baylor College of Medicine, Houston, TX; ³University of Sydney, Sydney, Australia; ⁴Stanford University, Stanford, CA
- TP 111 **High Throughput Analysis of Serum for PFAS Compounds by Reversed Phase High Performance Liquid Chromatography Tandem Mass Spectrometry;** Jessica M. Morrison¹; Michael C. Stagliano¹; Timothy A. Karrer¹; Matthew J. Geiger¹; ¹MI Dept of Health & Human Services, Lansing, MI
- TP 112 **Molecular Detection of Pancreatic Ductal Adenocarcinoma in Pancreatic and Bile Duct Tissues Using the MasSpec Pen;** Mary King¹; Jialing Zhang¹; John Q. Lin¹; Sadhna Dhingra²; Wendong Yu²; George van Buren²; William E. Fisher³; James Suliburk³; Livia S Eberlin¹; ¹University of Texas at Austin, Department of Chemistry, Austin, TX; ²Department of Pathology and Immunology, Baylor College of Medicine, Houston, TX; ³Department of Surgery, Baylor College of Medicine, Houston, TX
- TP 113 **Application of Mass-Spectrometry for Thalassemia Screening;** Weining Zhao¹; Rong Wang¹; Liang Lin¹; ¹BGI-Shenzhen, Beishan Industrial Zone 11th Building, Yantian District, Shenzhen City, China
- TP 114 **Library Build and Patient Assays from 4- & 15-micron Kidney Biopsies;** Wouter Knol¹; Petra Jansen¹; Jesper Kers^{1,2}; Garry Corthals¹; ¹University of Amsterdam, Amsterdam, Netherlands; ²Amsterdam UMC, Amsterdam, Netherlands
- TP 115 **Revealing Proteomic Subgroups with Clinical Classification and Prognostic Prediction in Pancreatic Ductal Adenocarcinoma Using MRM-MS;** Minsoo Son¹; Yoseop Kim¹; Jinyoung Jang²; Youngsoo Kim¹; ¹Department of Biomedical Engineering, Seoul National University College of Medicine, Jongro-gu, South Korea; ²Department of surgery, Seoul National University College of Medicine, Jongro-gu, South Korea
- TP 116 **Liberate, Equilibrate and Automate; Immunosuppressant Analysis in Whole Blood;** Stacy Dee¹; Julia Hannon¹; Matthew Crawford¹; Russell Grant¹; ¹LabCorp, Burlington, NC
- TP 117 **An integrated Pipeline from SWATH Acquisition to MRMHR Workflow Facilitates Identification and Verification of Prostate Diagnostic Markers;** Rui Sun¹; Christie Hunter²; Chen Chen³; Xue Cai¹; Qiushi Zhang¹; Bo Wang⁴; Xiaoyan Yu⁵; Huanhuan Gao¹; Xiaodong Teng⁴; Lirong Chen⁵; Ruedi Aebersold⁶; Yi Zhu¹; Tiannan Guo¹; ¹School of Life Sciences, Westlake University, Hangzhou, China; ²Sciex, Redwood City, CA; ³Sciex, Shanghai, China; ⁴Department of Pathology, The First Affiliated Hospital of College of Medicine, Zhejiang University, Hangzhou, China; ⁵Department of Pathology, The Second Affiliated Hospital, Zhejiang University School of Medicine, Hangzhou, China; ⁶Department of Biology, Institute of Molecular Systems Biology, ETH Zurich, Switzerland, Switzerland
- TP 118 **Bioanalytical Method for Quantification of Polymyxin B1, Polymyxin B2, Polymyxin B3 and Isoleucine-Polymyxin B1 in Human Plasma;** Peiling Hou¹; Shu Qing Chan²; Jie Xing³; ¹Application Development & Support Centre, Shimadzu (Asia Pacific) Pte Ltd., 79 Science Park Drive #02-01/08, Singapore; ²School of Chemical and Life Sciences, Singapore Polytechnic, 500 Dover Road, Singapore; ³Application Development & Support Centre, Shimadzu (Asia Pacific) Pte Ltd, 79 Science Park Drive #02-01/08, Singapore
- TP 119 **Quantitation of Insulin-Like Growth Factor-1 in Serum by MRM-LC-MS/MS;** Yihan Li¹; Ji Jiang¹; Lei Xiong¹; Xiang He¹; ¹SCIEX, Redwood Shores, CA
- TP 120 **A New Approach without Renal Biopsy for Ankylosing Spondylitis with IgA Nephropathy Diagnosis by Glycan Analysis;** Hui-Ling Chiang^{1,2}; Pai-Chi Syue¹; Ching-Yi Lien¹;

- Ning-Sheng Lai²; Kuo-Lung Ku¹; ¹National Chiayi University, Chiayi City, Taiwan; ²Dalin Buddhist Tzu Chi Hospital, Dalin Town, Taiwan
- TP 121 **Measurement of Free Drug Concentration from Biological Tissue by Solid-phase Microextraction: In-Silico and Experimental Study;** Mohammad Maududul Hug¹; Marcos Tascon²; Emir Nazdrajić¹; Anna Roszkowska³; Janusz Pawliszyn¹; ¹University of Waterloo, Waterloo, ON; ²Instituto de Investigación e Ingeniería Ambiental (3iA), Universidad Nacional de San Martín (UNSAM), Buenos Aires, Argentina; ³Department of Pharmaceutical Chemistry, Medical University of Gdańsk, Gdańsk, Poland
- TP 122 **Identification of Circulating Fragments of Human Pancreatic Polypeptide Following Antibody Capture and Liquid Chromatography High Resolution Accurate Mass-Tandem Mass Spectrometry;** Anthony Maus¹; Robert Taylor¹; Ravinder Singh¹; Stefan Grebe¹; ¹Mayo Clinic, Rochester, MN
- TP 123 **High-Sensitivity Analysis of Aldosterone in Low-Volume Serum Samples Using Micro-Flow LC-MS/MS for Clinical Research;** Mikael Levi¹; Jun Watanabe²; ¹SHIMADZU Corporation, Kyoto, Japan; ²Shimadzu Corporation, Kyoto, Japan

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- TP 124 **Immunoepitope Characterization Enhanced with Positive and Negative Mode 193 nm UVPD;** Eleanor C. Watts¹; Melanie J Patterson²; Gregory K Potts²; Alayna George Thompson²; Damien B Ready²; Jennifer S Brodbelt¹; ¹University of Texas at Austin, Austin, TX; ²AbbVie Inc., North Chicago, IL
- TP 125 **Analysis of Ischemic Brain Proteome in Mice in Identifying Clusterin as a Serum Biomarker for Severity of Acute Ischemic Stroke;** Zezong Gu¹; Hailong Song¹; Chenghan Wu²; Jiankun Cui¹; ¹University of Missouri School of Medicine Patholog, Columbia, MO; ²The Second Affiliated Clinical College, Fujian University of Traditional Chinese Medicine, Fuzhou, China
- TP 126 **Urine from the Patients with Vesicoureteral Reflux Reveals Changes in Host and Bacterial Metabolism after Urinary Tract Infection;** Dijana Vitko¹; Kohei Hasegawa²; Joseph W. McQuaid³; Kylie H. Davis¹; Maggie R. Leary¹; Shannon E. DiMartino¹; Jonathan M. Mansbach¹; Richard S. Lee¹; ¹Boston Children's Hospital, Boston; ²Massachusetts General Hospital, Boston, Massachusetts; ³University of Massachusetts Medical School, Worcester, MA
- TP 127 **Ganglioside Biomarker Discovery and Characterization in Neuro Developmental Diseases by High Resolution Multistage Mass Spectrometry;** Mirela Sarbu¹; Raluca Ica¹; Cristian VA Munteanu²; Alina Petrut¹; Alina D Zamfir¹; ¹National Institute for Research and Development in Electrochemistry and Condensed Matter, Timisoara, Romania; ²Institute of Biochemistry of the Romanian Academy, Bucharest, Romania
- TP 128 **Novel Stationary Phase Aids in the Fight Against Cardiovascular Disease;** Robert Puryear; Imtakt USA, Portland, OR
- TP 129 **Identification, Validation, and Quantitation of a Clinically Relevant PSA Variant in Post-DRE Urines by Targeted Mass Spectrometry;** Joseph J. Otto¹; Vanessa L. Correll¹; Hampus Engstroem¹; Brian P. Main¹; Brandi Weaver²; Teresa Johnson-Pais²; Li Fang Yang^{1,3}; Paul C. Boutros⁴; Thomas Kislinger⁵; Robin J. Leach^{2,6}; O. John Semmes^{1,3}; Julius O. Nyalwidhe^{1,3}; ¹Leroy T. Canoles Jr. Cancer Research Center, Eastern Virginia Medical School, Norfolk, VA; ²Department of Urology, The University of Texas Health San Antonio, San Antonio, TX; ³Department of Microbiology and Molecular Cell Biology, Eastern Virginia Medical School, Norfolk, VA; ⁴University of California Los Angeles,



- Los Angeles, CA; ⁵University of Toronto, Toronto, ON; ⁶Department of Cell Systems and Anatomy, The University of Texas Health San Antonio, San Antonio, TX
- TP 130 **Proteomic Insights into the Molecular Mechanisms of Breast Cancer Metastasis;** Shreya Ahuja¹; Iulia M. Lazar¹; ¹Virginia Tech, Blacksburg, VA
- TP 131 **Proteomic Analysis of the HBP-Induced TIFA Interactome;** Tong-You Wade Wei¹; Chi-Chi Chou¹; Wan-Jyun Lin¹; Pei-Yu Wu¹; Ming-Daw Tsai¹; ¹Academia Sinica, Taipei, Taiwan
- TP 132 **Analysis of Metabolome and Lipidome Reveals the Metabolic Changes in Hypothermia Treatment of Cardiac Arrest Patients;** Daniel Contai¹; Naren Gajenthra Kumar²; Joshua Morriss¹; Dayanjan S Wijesinghe¹; ¹Department of Pharmacotherapy and Outcomes Sciences, Virginia Commonwealth University, Richmond, VA; ²Department of Microbiology and Immunology, Virginia Commonwealth University, Richmond, VA
- TP 133 **Investigation of AD and MCI Associated Changes in Blood Plasma Proteome by High Resolution Mass Spectrometry;** Natalia V. Zakharova^{1,2}; Anna Bugrova¹; Maria Indeykina^{1,2}; Alexander Brzhozovskiy^{3,4}; Yana B. Fedorova⁵; Svetlana I. Gavrilova⁵; Igor Popov²; Alexey Kononikhin^{2,3}; Eugene (evgeny) Nikolaev⁴; ¹Emanuel Institute for Biochemical Physics, Russian Academy of Sciences, Moscow, Russia; ²Moscow Institute of Physics and Technology (State University), Dolgoprudny, Russia; ³V.L. Talrose Institute for Energy Problems of Chemical Physics, Russian Academy of Sciences, Moscow, Russia; ⁴Skolkovo institute of science and technology, Moscow Region, Russian Federation; ⁵Mental Health Research Center, Russian Academy of Science, Moscow, Russia
- TP 134 **Detection of Anthrax Toxins in Terminal Organ Tissues by Mass Spectrometry;** Maribel Gallegos Candela¹; Anne E Boyer¹; Adrian R. Woolfitt¹; Renato C. Lins²; Maria I. Solano¹; John R. Barr¹; ¹Center for Disease Control, Atlanta, GA; ²Battelle Integrated Science Solutions, Atlanta, GA
- TP 135 **Analysis of Human Skin Wound Healing Process Using 2D-TOF-SIMS;** Anthony Castellanos¹; Ivan Jozic²; Francisco A. Fernandez-Lima^{3,4}; ¹Florida International University, Miami, FL; ²Dr. Phillip Frost Department of Dermatology & Cutaneous Surgery, University of Miami Miller School of Medicine, Miami, FL; ³Department of Chemistry and Biochemistry, Florida International University, Miami, FL; ⁴Biomolecular Sciences Institute, Florida International University, Miami, FL
- TP 136 **Global Protein Expression Alterations Linked to TDP-43 Dysregulation of Cryptic Exon Expression;** Shivangi Awasthi¹; Rachel Korn¹; Robert E. Drolet¹; Jonathan P. Ling²; Philip C. Wong²; Sophie P. Bateur¹; Sean M. Smith¹; Nathan G. Hatcher¹; ¹Merck & Co. Inc., Kenilworth, New Jersey; ²Departments of Pathology and Neuroscience, The Johns Hopkins University School of Medicine, Baltimore, MD
- TP 137 **Prediction of ZIKV Infection in Mosquitoes by MS Analysis of RNA Modification Biomarkers;** Rachel Netzband^{1,2}; Will McIntyre^{1,2}; Gaston Bonenfant^{1,2}; Sean Bialosuknia³; Alexander Ciota³; Cara T. Pager^{1,2}; Daniele Fabris^{1,2}; ¹University at Albany, Albany, NY; ²The RNA Institute, University at Albany, Albany, NY; ³Wadsworth Center, Department of Health, Albany, NY
- TP 138 **Quantification of Full Length and Activated Anthrax Protective Antigen by Immunocapture and Isotope Dilution Mass Spectrometry;** Maria I. Solano¹; Adrian R. Woolfitt¹; Anne E. Boyer¹; Renato C. Lins²; Maribel Gallegos-Candela¹; Hercules Moura¹; Carrie L. Pierce¹; John R. Barr¹; ¹Centers for Disease Control and Prevention, Atlanta, GA; ²Battelle Memorial Institute at the Centers for Disease Control and Prevention, Atlanta, GA
- TP 139 **Integrating Spectral Library Search and Database Search to Improve Endogenous Peptide Identification;** Lei Xin¹; Xin Chen¹; Zhewei Liang¹; Wenju Zhang¹; Baozhen Shan¹; ¹Bioinformatics Solutions Inc., Waterloo, ON
- TP 140 **Is NAP Treatment a Solution for Neuroprotection in ADNP Mutation Syndrome?** Ming-Hui Yang¹; Yi-Chia Lee²; Hsin-Yi Wu³; Ko-Chin Chen⁴; Yi-Ming Arthur Chen⁵; Yu-Chang Tyan²; ¹National Health Research Institutes, Zhunan, Taiwan; ²Kaohsiung Medical University, Kaohsiung, Taiwan; ³National Taiwan University, Taipei, Taiwan; ⁴Changhua Christian Hospital, Changhua, Taiwan; ⁵Taipei Medical University, Taipei, Taiwan
- TP 141 **Proteomic Profiling in Hematopoietic Tissues of Jak2 Conditional Knock-Out Mice;** Jin Koh¹; Sung Park¹; Mi-Jeong Yoo¹; Sixue Chen¹; Peter Sayeski¹; ¹University of Florida, Gainesville, FL
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- TP 142 **Novel Fractionation Techniques Applied to Oil-Contaminated Residues Characterized by FT-ICR Mass Spectrometry Reveal the Complexity of Ox Transformation Products;** Cameron C. Davis¹; Amy Mckenna M. Mckenna²; Huan Chen²; Ryan P. Rodgers^{2,3}; Sydney Niles^{2,3}; Martha Chacón-Patiño²; Qianxin Lin⁴; Aixin Hou⁵; ¹National High Magnetic Field Laboratory, Tallahassee, FL; ²National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL; ³Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL; ⁴Department of Oceanography and Coastal Sciences, College of the Coast and Environment, Louisiana State University, Baton Rouge, LA; ⁵Department of Environmental Sciences, College of the Coast and Environment, Louisiana State University, Baton Rouge, LA
- TP 143 **Fourier Transform Ion Cyclotron Resonance Mass Spectrometry Reveals the Role of Heteroatoms in Asphaltene Chemistry;** Martha Liliana Chacón-Patiño¹; Donald F. Smith¹; Sydney F. Niles¹; Jonathan C. Putman¹; Amy M. McKenna¹; Yuri E. Corilo¹; Christopher L. Hendrickson¹; Alan G. Marshall¹; Ryan P. Rodgers¹; ¹National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL
- TP 144 **UPLC-MS/MS Determination of Hexahydro-1,3,5-tris(2-hydroxyethyl)-s-triazine and its Reaction Products in Extra Heavy Crude Oil;** Lun-yi Zang¹; Martin Harper^{2,3}; ¹CDC/NIOSH/HELD, Morgantown, WV; ²Zefon International, Inc., Ocala, FL; ³Department of Environmental Engineering Sciences, University of Florida, Gainesville, FL
- TP 145 **Application of Molecular Characterization for fluorine Polymers Using Thermal Desorption/Pyrolysis DART-MS;** Chikako Takei¹; Kenichi Yoshizawa¹; Derek Gonzales²; Sayaka Nakamura³; Hiroaki Sato³; ¹BioChromato, Inc., Fujisawa, Japan; ²BioChromato USA, San Diego, California; ³National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan
- TP 146 **Speciation of Asphaltenes Using Mass-Deficient Tagging Mass Spectrometry and Metal-Reduced Nuclear Magnetic Resonance Spectroscopy;** Ian Anthony¹; Michael T. Spiegel¹; Annie Arvidson¹; Shubhneet Warar¹; Touradj Solouki¹; ¹Baylor University, Waco, TX
- TP 147 **Inductively Coupled Plasma-Mass Spectrometry Characterization of Asphaltene Metals Pre- and Post-Cleanup for Enhanced Nuclear Magnetic Resonance Spectroscopy Results;** Annie E. Arvidson¹; Ian G. M. Anthony¹; Michael T. Spiegel¹; Shubhneet Warar¹; Patrick J. Farmer¹; Touradj Solouki¹; ¹Baylor University, Waco, TX
- TP 148 **Structural Comparison of Nickel and Vanadyl Porphyrins from Natural Seeps and the 1.1-Billion-Year-Old Shale Oil;** Huan Chen¹; Martha L. Chacón-Patiño¹;



- Chad Weisbrod¹; Gregory T. Blakney¹; Jochen Brocks²; Nur Gueneli²; Nao Ohkouchi³; Chris J. Boreham⁴; Jérémie Beghine⁵; David Valentine⁶; Matthias Kellermann⁶; Ryan P. Rodgers¹; Amy McKenna¹; ¹National High Magnetic Field Laboratory, Tallahassee, FL; ²Australian National University, Canberra, Australia; ³Japan Agency for Marine–Earth Science and Technology, Yokosuka, Japan; ⁴Geoscience Australia, Symonston, Australia; ⁵University of Liège, Liège, Belgium; ⁶University of California, Santa Barbara, CA
- TP 149 **Increasing Analytical Separation of Polycyclic Aromatic Hydrocarbons from Crude Oils Using GC-TIMS-MS**; Clement Ajibade Olanrewaju¹; Cesar E. Ramirez²; Francisco Fernandez-Lima Fernandez Lima³; ¹Department of Chemistry and Biochemistry, Florida International University, Miami, FL; ²Advance Mass Spectrometry Facility, Department of Chemistry and Biochemistry, Florida International University, Miami Florida, Miami, FL; ³Department of Chemistry and Biochemistry, Florida International University, Miami, FL
- TP 150 **CID Fragmentation Studies of Asphaltenes at Different Precipitation Times Using Magnetic Resonance Mass Spectrometry (MRMS)**; Matthias Witt¹; Michael L. Easterling²; Estrella Rogel³; ¹Bruker Daltonik GmbH, Bremen, Germany; ²Bruker Daltonics Inc., Billerica, MA; ³Chevron, Richmond, CA
- TP 151 **Analysis of Jet Fuel Thermal Oxidative Deposits by Pyrolysis Gas Chromatography/Mass Spectrometry**; Krege Matthew Christison^{1,2}; Michael Browne²; Tommy Nguyen²; O. David Sparkman²; ¹Chevron, Richmond, CA; ²University of the Pacific, Stockton
- TP 152 **Evaluation of Time Effects on Precipitated Asphaltene Characteristics Using APPI and LDI coupled to Magnetic Resonance Mass Spectrometry (MRMS)**; Estrella Rogel¹; Matthias Witt²; Michael Moir¹; ¹Chevron, Richmond, CA; ²Bruker Daltonik GmbH, Bremen, Germany
- TP 153 **Electron-Transfer Ionization in MALDI-MS for the Direct Targeted Analysis of Metalloporphyrins in Complex Mixtures**; Juan Ramirez^{1,2}; Cristian Blanco-Tirado¹; Pierre Giusti²; Carlos Afonso³; Marianny Y. Combariza¹; ¹Universidad Industrial de Santander, Bucaramanga, Colombia; ²Total Research & Technology Gonfreville, Harfleur, France; ³University of Rouen, Mont Saint Aignan, France
- TP 154 **New Insights in Crude Oil Using MS, NMR, and EPR**; Michael T. Spiegel¹; Ian G. M. Anthony¹; Shubhneet Warar¹; Annie Arvidson¹; Anish Sasmal¹; Touradj Solouki¹; Patrick J. Farmer¹; ¹Baylor University, Waco, TX
- TP 155 **(+/-) ESI FT MS Analysis of Crude Oils from the Volga-Ural Region**; Vlad Lobodin¹; Dmitrii Mazur²; Roman Borisov³; ¹MAXIKAT, INC, Tallahassee, FL; ²The Department of Chemistry, Moscow State University, Moscow, Russia; ³A.V. Topchiev Institute of Petrochemical Synthesis, Moscow, Russia
- TP 156 **Fast, Robust, 'Dilute and Shoot' Screening of Adulterated Low Taxation Fuels**; G. John Langley^{1,2}; Julie M. Herniman¹; James Barker^{2,3}; ¹University of Southampton, Southampton, United Kingdom; ²Energy Institute, London, United Kingdom; ³Innospec Inc., Ellesmere Port, United Kingdom
- TP 157 **Development of Predictive Methods of Sulfur Content in Hydropyrolysis Oil Products by Elemental Sulfur Analysis of Crude Oil Feedstocks**; Kyle L. Wilhelm¹; Drew Stolpman²; Zhao Wang¹; Bill Hockaday¹; Touradj Solouki¹; ¹Baylor University, Waco, TX; ²Baylor University, Waco, TX
- TP 158 **Hydrocarbons High Mass Profiling of Crude and Commercial Oils Using LDTD-HRMS Technology**; Jonathan Rochon¹; Pier-Luc Plante¹; Serge Auger²; Jean Lacoursière²; Pierre Picard²; ¹Université Laval, Québec, QC; ²Phytronix Technologies, Inc., Québec, QC
- TP 159 **Development of Quantitative Isotope Labeling IC-MS/MS method for Phosphonate Scale Inhibitors Analysis**; Lei (Lyla) Cheng¹; Christopher Durnell¹; Robert Pultz¹; Manojkumar Bhandari¹; Christine Kerr¹; Emerilis Casado-Rivera¹; ¹Nalco Champion, Sugar Land, TX
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- TP 160 **Simultaneous Detection of 12 Microcystins, Nodularin, Cylindrospermopsin, and Anatoxin-a**; Matthew Prescott¹; Yingbo C. Guo¹; Ali Haghani²; Andrew Eaton²; ¹Metropolitan Water District of Southern California, La Verne, CA; ²Eurofins Eaton Analytical, 750 Royal Oaks Drive, Monrovia, CA
- TP 161 **Analysis of Drinking Water for Determination of Volatile Organic Components (VOC's) Using Dynamic Headspace Gas Chromatography Mass Spectrometry**; Sanket Anand Chiplunkar¹; Dheeraj Handique¹; Prashant Hase¹; Durvesh Sawant¹; Nitish Suryawanshi¹; Aseem Wagle¹; Pratap Rasam¹; Jitendra Kelkar¹; Ajit Datar¹; Satyendra Thakur²; Sunil Singh²; ¹Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India; ²Shimadzu Analytical (India) Pvt. Ltd., New Delhi, India
- TP 162 **Trace Analysis of PFAS in Environmental and Serum Samples by Micro-SPE**; Andrew Minetti¹; Mohammad Talebi²; Thomas Lockwood³; ¹EPREP, Mulgrave, Australia; ²EnviroLab, Sydney, Australia; ³University of Technology Sydney, Sydney, Australia
- TP 163 **Structural Elucidation of the Direct Photolysis Transformation Products of a Halogenated Estrogen**; Keeton T. Nance¹; Carolyn P. Hutchinson¹; David R. Griffith¹; ¹Willamette University, Salem, OR
- TP 164 **Developing an Untargeted High-resolution Mass Spectrometry Method for the Detection and Identification of Glucuronide Biotransformation Products in Environmentally Exposed Fish**; Marina Evich¹; Jonathan Mosley²; Ioanna Ntai³; Drew Ekman²; Timothy Collette²; ¹ORISE Fellow, US EPA, Athens, GA; ²US EPA, Athens, GA; ³ThermoFisher Scientific, San Jose, CA
- TP 165 **A Novel Mass Spectrometric Method to Measure Siloxanes**; Eleanor Browne¹; Mitchell Alton¹; ¹University of Colorado Boulder, Boulder, CO
- TP 166 **Improved Non-Target Screening Based Identification of Organic Micropollutants in Water Samples**; Andrea Mizzi Brunner¹; Seema Sharma²; Christian Panse³; Romain Huguet²; Dennis Vughs¹; Vlad Zabrouskov²; Annemieke Kolkman¹; ¹KWR Watercycle Research Institute, Nieuwegein, Netherlands; ²Thermo Fisher Scientific, San Jose, Ca, 95134; ³Functional Genomics Center Zurich, Zurich, Switzerland
- TP 167 **You Can Only See What You Can Ionize: A Comparison of Ionization Techniques for Dissolved Organic Matter Mass Spectrometric Characterization**; Juliana R. Laszakovits¹; Allison A MacKay¹; ¹The Ohio State University, Columbus, OH
- TP 168 **Toxin Identification and Correlation to Biological Endpoints Using Multivariate Data Analysis: An LC-HRMS Top-Down Approach to Discerning Differential Toxicological Responses**; Raegyn B. Taylor¹; Jonathan M. Bobbitt¹; Bridgett N. Hill¹; Amanda S. Hering¹; Bryan W. Brooks¹; Kevin Chambliss¹; ¹Baylor University, Waco, TX
- TP 169 **Gestational Exposure to Benzotriazoles and Benzothiazoles in Relation to Birth Weight: A Repeated Measures Study**; Yanqiu Zhou¹; Zongwei Cai²; ¹Hong Kong Baptist University, Hong Kong, Hong Kong; ²Hong Kong Baptist University, Hong Kong, China
- TP 170 **A Direct Inject Approach for Analysis of Legacy and Emerging Perfluoroalkyl Substances in Environmental Water and Soil Samples**; Kari Organtini¹; Kenneth Rosnack¹; Doug Stevens¹; Aurelie Marcotte¹; ¹Waters Corporation, Milford, MA



- TP 171 **Ultrafast Trace Quantitation of PFAS in Drinking and Environmental Waters Using an Automated Sample Preparation and LC-MS/MS System;** Nigel Grieves¹; David Humberstone¹; Cindy Si Ni Lee²; Atsuhiko Toyama²; ¹Shimadzu Scientific Instruments Oceania, Sydney, Australia; ²Shimadzu (Asia Pacific) Pte Ltd, Singapore, Singapore
- TP 172 **Drinking Water Safety and Sustainability: Using Mass Spectrometry to Identify Chemical Drivers of Toxicity;** Joshua M. Allen¹; Michael J. Plewa²; Jia Ai³; Carrie Guo³; Amy A. Cuthbertson¹; Hannah K. Liberatore¹; Tiffany Lee³; Raha Shirkhani³; Stuart W. Krasner³; Susan D. Richardson¹; ¹University of South Carolina, Columbia, SC; ²University of Illinois at Urbana Champaign, Urbana, IL; ³Metropolitan Water District of Southern California, La Verne, CA
- TP 173 **Fast Semi-Automated Extractable Petroleum Hydrocarbons Fractionation and Cleanup;** Tom Hall¹; Ruud Addink¹; ¹Fluid Management Systems, Watertown, MA
- TP 174 **Understanding the Structural Complexity of Dissolved Organic Matter: Isomeric Diversity;** Dennys Leyva¹; Lilian V. Tose¹; Jacob Porter¹; Jeremy Wolff²; Rudolf Jaffé³; Francisco A. Fernandez-Lima^{1,4}; ¹Department of Chemistry and Biochemistry, Florida International University, Miami, FL; ²Bruker Daltonics Inc., Billerica, MA; ³Southeast Environmental Research Center, Florida International University, Miami, FL; ⁴Biomolecular Sciences Institute, Florida International University, Miami, FL
- TP 175 **Detection and Quantification of Nine Haloacetic Acids with Ion Chromatography Mass Spectrometry;** Phuc Nguyen¹; David Clases¹; David Bishop¹; Philip Doble¹; ¹University of Technology Sydney, Sydney, Australia
- TP 176 **Chemicals in Textiles: A Source of Environmental Pollution and Human Exposure?;** Francesco Iadaresta¹; Carlo Crescenzi²; Conny Ostman³; ¹stockholm university, stockholm, Sweden; ²University of Salerno, Salerno, Italy; ³Stockholm University, Stockholm, Sweden
- TP 177 **Integrated Use of QTOF and Q-Exactive Orbitrap Mass Spectrometry for Suspect and Non-Target Screening of Emerging Pollutants in Wastewater;** Hailemariam A. Assress¹; Hlengilizwe H. Nyoni¹; Bhekie B. Mamba¹; Titus TAM Msagati¹; ¹University Of South Africa (UNISA), Johannesburg, South Africa
- TP 178 **High-Throughput Determination of Seventeen Cyanotoxins and Suspect Screening of Other Cyanopeptides by SPE-UHPLC-HRMS in Canadian Lakes;** Audrey Roy-Lachapelle¹; Sung Vo Duy²; Dinh Quoc Tuc²; Gabriel Munoz²; Sébastien Sauvé²; Christian Gagnon¹; ¹Environment and Climate Change Canada, Montréal, QC; ²University of Montreal, Montreal, QC
- TP 179 **Arsenic and Thioarsenic Speciation Using Ion Chromatography Mass Spectrometry;** Tisa Campbell¹; Jianye Zhang¹; ¹Voorhees College, Denmark, SC
- TP 180 **Direct Photolysis Transformation Products from Brominated Estrogens in Treated Wastewater Effluent;** Carolyn P. Hutchinson¹; Keeton T. Nance¹; David R. Griffith¹; ¹Willamette University, Salem, OR
- TP 181 **Photolysis of Emerging Contaminants Absorbed on Plastic Debris in an Aqueous Environment;** Xiomara Martinez¹; Daryl Giblin²; Angeline Alag¹; Kathryn Renyer¹; Michael L. Gross²; M. Paul Chiarelli¹; ¹Loyola University, Chicago, IL; ²Washington University, St. Louis, MO
- TP 182 **High Throughput Analysis of Deer Tissue for Perfluorinated Compounds by Reversed Phase High Performance Liquid Chromatography Tandem Mass Spectrometry;** Michael C. Stagliano¹; Jessica M. Morrison¹; Timothy A. Karrer¹; Matthew J. Geiger¹; ¹MI Dept of Health & Human Services, Lansing, MI
- TP 183 **A New Method for a Systematic Analysis of Siderophores in Soils;** Vineeta Raj¹; Oliver Baars¹; ¹North Carolina State University, Raleigh, NC
- TP 184 **A Single Analytical Method for the Determination of Legacy and Emerging Per- and Poly Fluoroalkyl Substances (PFAS) in Aqueous Matrices;** Timothy Coggan¹; Tarun Anumol²; Bradley Clarke¹; ¹RMIT University, Melbourne, Australia; ²Agilent Technologies, Wilmington, DE
- TP 185 **Moving Beyond Monitoring Legacy Per and Polyfluoroalkyl Substances (PFAS): Screening Strategies for the Growing List;** James S. Pyke¹; Tarun Anumol²; Jerry A. Zweigenbaum²; ¹Agilent Technologies, Inc., Santa Clara, CA; ²Agilent Technologies, Inc., Wilmington, DE
- TP 186 **Identification and Quantification of Microcystins in Western Lake Erie during 2016 and 2017 Harmful Algal Blooms;** Dilrukshika S W Palagama¹; David Baliu-Rodriguez¹; Brenda K Snyder¹; Jennifer A Thornburg¹; Thomas B Bridgeman¹; Dragan Isailovic¹; ¹University of Toledo, Toledo, OH
- TP 187 **Fast Semivolatiles Method by GC/MS/MS that Meets EPA 8720D/E Requirements;** Melissa Churley¹; Bruce Quimby²; Anastasia Andrianova²; ¹Agilent, Santa Clara, CA; ²Agilent, Wilmington, DE
- TP 188 **Determination of 8 Nitrosamines in Water by Liquid Chromatography Coupled to Tandem Mass Spectrometry;** Wei Du¹; Xiaorong Ran¹; ¹Agilent Technologies(China) Co. Ltd., Beijing, China
- TP 189 **Automated Liquid-Liquid Extraction for Environmental Analysis;** Masoomeh Tehranirokh^{1,2}; Marcel Van de Bronk²; Andrew Gooley^{1,2}; Peter Smith³; Zhengshan Dai³; Kyle Bachus²; Simon Mills⁴; Robert Shellie⁵; ¹ARC Training Centre for Portable Analytical Separation Technologies (ASTech), Hobart, Australia; ²Trajan Scientific and Medical, Ringwood, Australia; ³Trajan Scientific and Medical, Morrisville, NC; ⁴Envirolab, Sydney, Australia; ⁵Centre for Advanced Sensory Science (CASS), School of Exercise and Nutrition Sciences, Deakin University, Melbourne, Australia
- TP 190 **Differential Expression of Inflammatory Proteins in New Male and Female Swine Confinement Workers;** Brooke Thompson¹; Paulos Chumala¹; David Schneberger¹; Shelley Kirychuk¹; George S. Katselis¹; ¹University of Saskatchewan, Saskatoon, SK
- TP 191 **Methods for Metaproteomic Analysis of the Ocean;** Matthew McIlvin¹; Mak Saito²; ¹Woods Hole Oceanographic Inst., Woods Hole, MA; ²Woods Hole Oceanographic Institution, Woods Hole, MA

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- TP 192 **Quantitation and Localization of Endocrine Disruptor Compounds Accumulation in Fathead Minnows by Complementary Mass Spectrometry Analyses;** Rachel Davis¹; Sarah Rizzo¹; Jackson Hoang¹; Bobbi J Potter¹; Kevin R Tucker¹; ¹Southern Illinois University Edwardsville, Edwardsville, IL
- TP 193 **Micropollutant Removal during Wastewater Treatment: Evaluation of the Process Effectiveness Using High Resolution Accurate Mass LC-MS/MS;** Madhuri Damaraju¹; Keerthi Katam¹; Lokesh Kumar Akula¹; Prasanth Joseph²; Saikat Banerjee²; Debraj Bhattacharyya¹; ¹Indian institute of Technology, Hyderabad, India; ²Agilent Technologies, Whitefield, Bengaluru, India
- TP 194 **Quantification of Azithromycin in Sheep Tissue Samples Using LCMSMS;** Chander Mani¹; T.s. Lohith²; Saikat Banerjee¹; Samir Vyas¹; S.m. Byregowda²; K.



- TP 195 Sripad²; ¹Agilent Technologies, Gurgaon, India; ²Institute of Animal Health and Veterinary Biologicals, Bengaluru, India
Developing Methods to Assess the Environmental Impact of Pesticides and Pharmaceuticals on Aquatic Fauna Using Targeted and Untargeted HRAM Q-TOF; Christopher Titman¹; Thomas H Miller²; Keng Tiong Ng²; Nicholas R Bury^{3,4}; Leon P Barron²; Alan Barnes⁵; Neil Loftus⁵; ¹Shimadzu UK Limited, Milton Keynes, United Kingdom; ²Department of Analytical, Environmental & Forensic Sciences, School of Population Health & Environmental Sciences, Faculty of Life Sciences and Medicine, King's College London, United Kingdom; ³School of Science, Technology and Engineering, University of Suffolk, James Hehir Building, University Avenue, Ipswich, United Kingdom; ⁴Division of Diabetes and Nutritional Sciences, Faculty of Life Sciences and Medicine, King's College London, Franklin Wilkins Building, United Kingdom; ⁵Shimadzu Corporation, Manchester, United Kingdom
- TP 196 **An LC-MS/MS Study of the Kinetics of Atrazine Decomposition Catalyzed by Interactions with Soil;** Heather Gamble¹; Donald S Gamble²; Jincun Wu¹; Mitesh Patel³; ¹PerkinElmer Inc., Woodbridge, ON; ²St. Mary's University, Halifax, NS; ³PerkinElmer Inc., Bolton, ON
- TP 197 **ESS-MAT: A New Approach for Simultaneous Analysis of Organophosphate Pesticides and their Degradation Products On Agricultural Products;** noam Kirshenbaum¹; Tamara Polubesova¹; Benny Chefetz¹; ¹Department of Soil and Water Sciences The Robert H. Smith Faculty of Agriculture, Food and Environment The Hebrew University of Jerusalem, Rehovot, Israel
- TP 198 **Identification and Quantification of Degradation Products in Amoxicillin and Sertraline Stored Aboard the International Space Station;** Virginia K James¹; Wendy Cory¹; ¹College of Charleston, Charleston, SC
- TP 199 **Combination of Targeted and Non-Targeted Workflows for the Identification of Pollutants in River Water Using a Passive Sampling Method;** Anthony Gravell¹; Melanie Schumacher¹; Bob Galvin²; Carsten Baessmann³; ¹Natural Resources Wales, Swansea University, Swansea, United Kingdom; ²Bruker UK Ltd., Coventry, United Kingdom; ³Bruker Daltonik GmbH, Bremen, Germany
- TP 200 **Trace determination of Octyl & Nonyl-phenols and Ethoxylates and Bisphenol A Using On-Line SPE and Q Exactive Focus Orbitrap LCMSMS;** Neville Llewellyn¹; James Thomas²; Olaf Scheibner³; Ed George⁴; ¹ThermoFisher Scientific, Hemel Hempstead, United Kingdom; ²Scottish Environment Protection Agency, Glasgow, United Kingdom; ³Thermo Fisher Scientific (Bremen), Bremen, Germany; ⁴Thermo Fisher Scientific, San Jose, CA
- TP 201 **Simultaneous Targeted Quantification and Suspect Screening of Environmental Contaminates in Sewage Sludge by High Resolution LC-QTOF;** James S Pyke¹; Gabrielle Black²; Kai Chen¹; Tarun Anumol³; Thomas M Young²; ¹Agilent Technologies, Inc., Santa Clara, CA; ²University of California, Davis, Davis, CA; ³Agilent Technologies, Inc., Wilmington, DE
- TP 202 **Fast Creatinine Determination in Wastewater by Liquid Chromatography-Mass Spectrometry;** Lisa Wanders¹; Matthew Obusek¹; ¹Thomson Instrument Co, Oceanside, CA
- TP 203 **Use of Triple Quadrupole Mass Spectrometry to Characterize Antibiotics in Cow Manure;** Andrea Yarberr¹; Clifford Rice¹; Carlton Pointexter²; Stephanie Lansing²; ¹United States Department of Agriculture, Beltsville, Maryland; ²University of Maryland, College Park, Maryland
- TP 204 **Estrogen Monitoring in River Waters at Low Part Per Trillion Levels by Online SPE-UHPLC-MS/MS;** Jason Weisenseel¹; Jamie Foss¹; Wilhad Reuter¹; ¹PerkinElmer, Shelton, CT
- TP 205 **Analysis of Pharmaceuticals and Personal Care Products (PPCPs) in Drinking Water at Low Part Per Trillion Levels by Online SPE-UHPLC-MS/MS;** Jamie Foss¹; Wilhad Reuter¹; ¹PerkinElmer, Shelton, CT
- TP 206 **Reliable Determination of Sulfonamides in Environmental Water Matrices Using UHPLC-MS/MS;** Xiulan Zhang¹; Chaofei Zhu¹; Jing Guo¹; Meiling Lu²; Liang Dong¹; Yeru Huang¹; ¹National Center for Environmental Analysis and Measurement, Beijing, China; ²Agilent Technologies (China) Limited, Beijing, China
- TP 207 **Exploring the Physicochemical Properties of Pesticides Using Differential Mobility Spectrometry and Machine Learning-Based Modelling;** J. Larry Campbell¹; J. C. Yves Le Blanc¹; Brendon Seale^{1,2}; Zack Bowman³; Jeff Crouse³; Ce Zhou³; W. Scott Hopkins³; ¹SCIEX, Concord, ON; ²York University, Toronto, ON; ³University of Waterloo, Waterloo, ON
- TP 208 **Orbitrap Assessment of Targeted and Non-Targeted Pharmaceuticals and Personal Care Products in Wastewater Effluents and their Impact on River Water;** Vimbai Mhuka¹; simiso Dube²; Mathew M Nindji¹; ¹UNISA, Florida Park, Roodepoort, South Africa; ²UNISA, Florida Park, Roodepoort, South Africa
- TP 209 **Qualitative and Quantitative in vitro Fish Metabolism Study for Environmental Safety Assessment of Xenobiotics using LC-HRMS;** Vivek Badwaik¹; Mingming Ma¹; Xiao Zhou¹; Mercedes Biven¹; Jeremy McFadden¹; Guomin Shan¹; Yelena A Adelfinskaya¹; ¹Corteva Agriscience, Indianapolis, IN
- TP 210 **Application of UPLC-MS/MS for Determination of Synthetic Organic Dyes and their Metabolites;** Angelika Tkaczyk¹; Kamila Mitrowska¹; Andrzej Posyniak¹; ¹National Veterinary Research Institute (PIWet), Pulawy, Poland
- TP 211 **Ultra-Fast Screening of Glyphosate, Glufosinate and AMPA in Surface Water by LDTD-QqQMS;** Cassandra Guérette¹; Serge Auger²; Pierre Picard²; Pedro A. Segura¹; ¹Université de Sherbrooke, Sherbrooke, Quebec; ²Phytronix Technologies, Inc., Quebec, QC
- TP 212 **Analysis of Semi-Volatile Organics in Drinking Water with Semi-Automated Solid Phase Extraction Using EPA Method 525.3;** Rashid Juma¹; Rudolf Addink¹; ¹Toxic Report, Watertown, MA
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- TP 213 **A High Resolution Mass Spectrometry (HRMS) Method for More 1000 Pesticides and Other Poisons: Methods and Madness;** Marc E. Engel¹; Harrison Ansley¹; Walter Hammack¹; ¹FDACS, Tallahassee, FL
- TP 214 **Investigation of Gluten Protein Degradation throughout Brewing Using N-Terminal Labeling Mass Spectrometry Analysis;** Wanying Cao¹; Joseph Baumert¹; Melanie Downs¹; ¹University of Nebraska, Lincoln, Lincoln, Nebraska
- TP 215 **Determination of Polar Pesticides in Grapes Using a Compact Ion Chromatography System Coupled with Tandem Mass Spectrometry;** Beibei Huang¹; Jeffrey Rohrer¹; ¹Thermo Fisher Scientific, Sunnyvale
- TP 216 **Highly Sensitive Direct Analysis of Glyphosate, Glufosinate and AMPA in the Beverages by LC-MS / MS;** Manami Kobayashi¹; Miho Kawashima²; Yusuke Inohana²; Nozomi Maeshima¹; Junichi Masuda¹; Yoshihiro Hayakawa²; ¹Shimadzu Corporation, Hadano, Japan; ²Shimadzu Corporation, Kyoto, Japan
- TP 217 **Analysis of Benzo[a]pyrene in Tobacco and Related Products by Ultra High-Performance Liquid Chromatography - Tandem Mass Spectrometry;** Xia Geng¹; Jincun Wu²; Lizhong Yang³; Feng Qin²;



- ¹PerkinElmer Management(Shanghai)Co.,Ltd., Shanghai, China; ²PerkinElmer Inc., Woodbridge, Ontario; ³Perkinelmer Management (Shanghai) Co., Ltd., Shanghai, China
- TP 218 **Quantitation of Heterocyclic Amines in Non-Meat Products and their Cancer Risks as Exposed;** Izu-Sheng Fang¹; Wei-Lun Su¹; Yi-Chen Sun¹; Hsin-Chang Cheng¹; ¹Institute of Food Safety and Health, National Taiwan University, Taipei, Taiwan
- TP 219 **Fatty Acid Composition Analysis for Glycerides in Edible Oils Using Thermal Desorption/Pyrolysis DART-QTOFMS;** Kenichi Yoshizawa¹; Chikako Takei¹; Michael Churchill²; ¹BioChromato, Inc., Fujisawa, Japan; ²BioChromato USA, San Diego, California
- TP 220 **Quantitation of Process-Induced Nitrogen Compounds in Foods Using QuEChERS Coupled with UPLC-MS/MS;** Wei Lun Su¹; Hsin-Chang Chen¹; ¹Institute of Food Safety and Health, National Taiwan University, Taipei, Taiwan
- TP 221 **Determination of Pyrrolizidine Alkaloids in Plant Material Using SFC-MS/MS;** Anja Gruening¹; Gesa J. Schad¹; Jan Stenzler²; ¹Shimadzu Europa GmbH, Duisburg, Germany; ²Shimadzu Deutschland GmbH, Duisburg, Germany
- TP 222 **Distribution of Heterocyclic Amines in Fried and Braised Plant Protein Foods;** Kai-Chieh Yang¹; Yi-Chen Sun¹; Wei Lun Su¹; Hsin-Chang Chen¹; ¹Institute of Food Safety and Health, National Taiwan University, Taipei, Taiwan
- TP 223 **Recent Trends in PDE-5 Inhibitors in Consumer Products;** Flavia Morales-garcia¹; Sara E. Kern¹; Valerie M. Toomey¹; Melanie N. Parsons¹; ¹US FDA Forensic Chemistry Center, Cincinnati, OH
- TP 224 **Development of a PRM Assay for Detection of Walnut and Hazelnut in Foods;** Justin Marsh¹; Charles Yang²; Melanie Downs¹; Philip Johnson¹; ¹University of Nebraska Lincoln, Lincoln, NE; ²Thermo Fisher Scientific, San Jose, CA
- TP 225 **Determination of Total Avilamycin Residues in Beef by LC-MS/MS;** Lusha Xu¹; haijuan an¹; ¹Shimadzu (Shanghai) Global Laboratory Consumables Co., Ltd. Beijing Branch, Beijing, China
- TP 226 **The Evaluation of Malachite Green and its Metabolites in Sediments of Aquaculture Environment in Taiwan;** Lai-Chuan Chang¹; Tzong-Shean Chin²; ¹Biotech Total Solutions Co., Ltd., New Taipei City, Taiwan; ²National Chia Yi University Taiwan, Chia Yi City, Taiwan
- TP 227 **Simultaneous Determination of 130 Veterinary Drug in Pork Using Ultra Performance Liquid Chromatography-Tandem Mass Spectrometry;** Zhao Liu; Shimadzu (China) Co.,Ltd., Shanghai, China
- TP 228 **Determination of 113 Pesticide Residues in Tea by LC-MS/MS;** Chenyuan Zhang¹; Haijuan An²; Jian Kang³; ¹Shimadzu (Shanghai) Global Laboratory Consumables Co., Ltd., Shanghai, China; ²Shimadzu (Shanghai) Global Laboratory Consumables Co., Ltd. Beijing Branch, Beijing, China; ³Shimadzu (Shanghai) Global Laboratory Consumables Co., Ltd., Shanghai, China
- TP 229 **Separation and Quantification of N-Acetyl-Cysteine and Glutathione by Isotopic Iodoacetamide Modification and HILIC Coupled with Tandem Mass Spectrometry;** Shih-shin Liang; Kaohsiung Medical University, Kaohsiung, Taiwan
- TP 230 **Rapid Screening and Quantitative Analysis of Pesticides in Vegetables by Liquid Chromatography Tandem Quadrupole Time of Flight Mass Spectrometry;** Biao Ren; Shimadzu(China)Co.,LTD.Beijing Branch, Beijing, China
- TP 231 **Simultaneous Determination of Tebufenozide and Indoxacarb in Animal Products Using Liquid-Liquid Extraction Method Coupled with Liquid Chromatography-Tandem Mass Spectrometry;** Kyung-Hee Yoo¹; Da-Hee Park¹; Seong-Kwan Kim¹; Ho-Chul Shin¹; ¹Konkuk university, Seoul, South Korea
- TP 232 **Simultaneous Detection of Eight Prohibited Flavor Compounds in Foodstuffs Using Gas Chromatography-Tandem Mass Spectrometry;** Feng Zhang¹; Feng Feng¹; ¹Institute of Food Safety, Chinese Academy of Inspection and Quarantine, Beijing, China
- TP 233 **The Best Out of Three Worlds – Pesticide Analysis in Honey by Hyphenation of TLC, HPLC and MS;** Anita Piper¹; Markus Burholt¹; Michaela Oberle¹; Stephan Altmaier¹; Michael Schulz¹; ¹Merck KGaA, Darmstadt, Germany
- TP 234 **Extractables and Leachables Analysis of Common Household Food Storage Products Using a Quadrupole Time-of-Flight (Q-TOF) Mass Spectrometer;** Evelyn H. Wang¹; Helen Hao¹; Gerard Byrne¹; Jennifer Davis¹; Katie Pryor¹; Christopher Gilles¹; ¹Shimadzu Scientific Instruments, Inc., Columbia, MD
- TP 235 **Pesticide Residue Analyses of QuEChERS Extracts of Different Food Matrices Using an Online Robotic SPE Clean-up Procedure Coupled to LC-MS/MS;** Michael Hudson; Thermo Fisher Scientific, San Jose, CA
- TP 236 **Simultaneous Analysis of Multiple Food Allergen and its Detection from Processed Food;** Tairo Ogura¹; Yuka Fujito²; Toshiya Matsubara¹; Ichiro Hirano¹; ¹Shimadzu Corporation, Kyoto, Japan; ²Shimadzu Scientific Instruments, Inc., Columbia, MD
- TP 237 **A Multiresidue Method for Quantitation and Screening of Pesticide Residues in Baby Food Using LC-MS/MS;** Anastasia Kalli¹; Charles Yang¹; Ed George¹; Dipankar Ghosh²; ¹Thermo Fisher Scientific, San Jose, CA; ²Thermo Fisher Scientific, San Jose, CA
- TP 238 **A Multiresidue Method for Pesticide Analysis Using an Orbitrap Tribrid Mass Spectrometer and Automatic Background Exclusion;** Anastasia Kalli¹; Dipankar Ghosh¹; Seema Sharma¹; ¹Thermo Fisher Scientific, San Jose, CA
- TP 239 **Targeted Screening and Quantitation of Pesticide Residues in Green Tea Using a Quadrupole Time-of-Flight Mass Spectrometer;** Toshiya Matsubara¹; Huan Lin¹; Natsuyo Asano¹; Mikie Shima²; ¹Shimadzu Corporation, Kyoto, Japan; ²AiSTI Science Co., Ltd., Wakayama, Japan
- TP 240 **Simultaneous Determination of Pesticide Residues in Vegetable Extract by Liquid Chromatograph Tandem Mass Spectrometry for High Recovery Rate;** Nozomi Maeshima¹; Manami Kobayashi¹; Masuda Junichi¹; ¹Shimadzu Corporation, Hadano, Japan
- TP 241 **New Workflow for Contaminants Screening in Strawberries Using High-Resolution GC/Q-TOF and Expanded Accurate Mass Library of Pesticides and Environmental Pollutants;** Sofia Nieto¹; Anastasia Andrianova²; Jessica Westland²; Kai Chen¹; Vadim Kalmeyer¹; Yoshimasa Tsunoi¹; Li Sun¹; Lei Tao¹; Bruce Quimby²; Courtney Milner¹; ¹Agilent Technologies, Inc., Santa Clara, CA; ²Agilent Technologies, Inc., Wilmington, DE
- TP 242 **Development and Validation of LC-MS/MS Method for Determination of Lipophilic and Hydrophilic Marine Toxins;** Renat Selimov¹; Ayshat Botasheva¹; Elizaveta Goncharova^{1,2}; Denis Nekrasov¹; Pavel Metalnikov¹; Alexandre Komarov¹; ¹VGNKI, Moscow, Russian Federation; ²Moscow State University, Moscow, Russian Federation
- TP 243 **Novel Opioid Trends and Retrospective Datamining for Emerging Opioids Using High Resolution Mass Spectrometry;** Amanda L.A. Mohr¹; Mellissa F. Fogarty¹; Judith Rodriguez Salas¹; Barry K. Logan^{1,2}; ¹CFSRE, Willow Grove, PA; ²NMS Labs, Willow Grove, PA

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- TP 244 **Determination of Bloodstain Deposition Time Using Metabolomic Analysis;** Hyebin Choi¹; Ae Eun Seok²; Jiyeoung Lee²; You-rim Lee¹; Arum Park²; Sora Mun¹; Yoo-jin Lee¹; Hyo-jin Kim¹; Hee-gyoo Kang^{1,2}; ¹Department of Senior Healthcare, BK21 Plus Program, Graduate School, Eulji University, Daejeon, South Korea; ²Department of Biomedical Laboratory Science, College of Health Sciences, Eulji University, Seongnam-si, South Korea
- TP 245 **BAC Analysis Utilizing GCMS and FID Combined with Fully Automated Sample Prep Performed by Robotic Sampler;** Alan Owens¹; Rachel Lieberman²; Francis Welch²; Andy Sandy²; ¹Shimadzu Scientific Instruments, Columbia, MD; ²Shimadzu Scientific Instruments, Inc., Columbia, MD
- TP 246 **Time of Flight Secondary Ion Mass Spectrometry (TOF-SIMS) Imaging of Illicit Narcotics;** Greg Gillen¹; Shin Muramoto²; Jennifer R. Verkouteren²; Edward Sisco²; ¹National Institute of Standards and Technology, Gaithersburg, MD; ²NIST, Gaithersburg, MD
- TP 247 **Identifying Suspect Relevance to a Crime Scene Based on Fingerprint Age Biomarkers Using MALDI Imaging;** Paige Hinners¹; Madison Thomas¹; Young Jin Lee¹; ¹Iowa State University, Ames, IA
- TP 248 **Implementation of an Online μ SPE - The Final Step Towards Fully Automated LC-MS Urine Screening in Forensic Toxicology;** Michaela Schmidt^{1,2}; Marina Schumacher³; Birgit Schneider³; Laura M. Huppertz²; Jürgen Kempf²; ¹Faculty Medical and Life Sciences, Furtwangen University, Schwenningen, Germany; ²Institute of Forensic Medicine, Medical Center – University of Freiburg, Freiburg, Germany; ³Bruker Daltonik GmbH, Bremen, Germany
- TP 249 **Targeted Screening for Drugs of Abuse in Postmortem Blood using LC-MS/MS;** Dina Swanson¹; Theresa Evans-Nguyen¹; ¹University of South Florida, Tampa, FL
- TP 250 **High-Spatial Resolution Matrix Assisted Laser Desorption/Ionization Mass Spectrometry Imaging of Human Hair Cross-Sections;** Emily C King¹; Young-Jin Lee¹; ¹Iowa State University, Ames, IA
- TP 251 **Method Validation of Drugs of Abuse Using Microchip Capillary Electrophoresis/Mass Spectrometry;** Christopher Nicholson¹; Sabra Botch-Jones²; Scott Miller¹; Adi Kulkarni¹; ¹908 Devices, Boston, MA; ²Boston University School of Medicine, Boston, MA
- TP 252 **Novel Platform for Online Sample Preparation and LC-MS/MS Analysis of Drugs in Biological Matrices;** Sarah Olive¹; Joshua Emory¹; Aria McCall²; Ruth Gordillo³; Robert English¹; Rachel Lieberman¹; Brian Feld¹; Benjamin Figard¹; ¹Shimadzu Scientific Instruments, Inc., Columbia, Maryland; ²Tarrant County Medical Examiner's Office, Fort Worth, Texas; ³University of Texas Southwestern Medical School, Dallas, Texas
- TP 253 **A New Method for Species Identification Using Mass Spectrometry and Machine Learning;** Hevi Yang¹; Erin Butler¹; Jennifer Teubl²; Samantha Monier¹; David Fenyó²; Donald Siegel¹; ¹Office of Chief Med Exam, New York, NY; ²NYU Medical Center, New York, NY
- TP 254 **Sensitive and Reliable Method for Identification of Genetically Variant Peptides in Human Hair;** Zheng Zhang¹; Meghan C. Burke¹; William E. Wallace¹; Yuxue Liang¹; Sergey L. Sheetlin¹; Yuri A. Mirokhin¹; Dmitrii V. Tchekhovskoi¹; Stephen E. Stein¹; ¹NIST, Gaithersburg, MD
- TP 255 **Analysis of Drugs and their Metabolites in Human Hair by Online SFE-SFC-MS/MS;** Takahiro Goda¹; Junichi Masuda¹; Manami Kobayashi¹; Maiko Kawamura²; Ruri Kikura-Hanajiri²; ¹Shimadzu Corporation, Hadano, Japan; ²National Institute of Health Sciences, Kawasaki, Japan
- TP 256 **Development of a Screening Method for Illicit Drugs in Hair Using LDTD-MS/MS at 8 Seconds Per Sample;** Sandra Imrazene¹; Serge Auger¹; Pier-Luc Plante²; Jean Lacoursière¹; Pierre Picard¹; ¹Phytronix Technologies, Quebec, QC; ²Université Laval, Quebec, Quebec
- TP 257 **Analysis of Synthetic Fentanyl Opioids in Serum Using Captiva EMR-Lipid Sample Preparation by LC-QTOF;** Julie Cichelli; *Agilent Technologies, West Chester, PA*
- TP 258 **Methamphetamine Impurity Profiling with GC \times GC-TOFMS in Korea;** Beom Jun Ko¹; Jin Young Kim¹; Dong Won Shin¹; ¹Supreme Prosecutors' Office, Seoul, South Korea
- TP 259 **Screening, Quantification and Confirmation of Fentanyl Metabolite, N-[1-(2-phenethyl-4-piperidinyl)maloanilinic Acid, in Equine Urine for Doping Control Analysis by LC-MS/MS;** Youwen You¹; Rachel M Proctor¹; Fuyu Guan¹; Jaclyn R Missanelli¹; Xiaoqing Li¹; Mary A Robinson¹; ¹University of Pennsylvania, Philadelphia, PA
- TP 260 **Mass Spectrometry-Based Detection of Genetically Variable Peptides: An Alternative to DNA Typing;** Andrew J Reed¹; Maryam Baniasad²; Stella M Lai³; Liwen Zhang³; Florian Busch³; Vicki H. Wysocki³; Myles W Gardner⁴; F. Curtis Hewitt⁴; Michael A. Freitas³; ¹Campus Chemical Instrument Center, Ohio State University, Columbus, OH; ²The Ohio State University, Columbus, OH; ³The Ohio State University, Columbus, OH; ⁴Signature Science, LLC, Austin, TX
- TP 261 **Sub-minute Analysis for Samples of Forensic Applications;** Luis Cuadra-Rodriguez¹; Melissa Churley¹; Lakshmi Krishnan¹; Courtney Milner¹; ¹Agilent Technologies, Inc., Santa Clara, CA
- TP 262 **Identification of Genetically Variable Peptides from Human Skin Samples for Human Forensic Investigation;** Myles W. Gardner¹; F. Curtis Hewitt¹; Michael A. Freitas²; August E. Woerner³; Liwen Zhang²; Maryam Baniasad²; Kathleen Q. Schulte¹; Alan R. Smith¹; Danielle S. LeSassier¹; Clifton J. Krueger¹; Nicolette C. Albright¹; Katharina L. Weber¹; Tara E. Manley¹; Leah W. Allen¹; Megan E. Powals¹; Benjamin C. Ludolph¹; ¹Signature Science, LLC, Austin, TX; ²The Ohio State University, Columbus, OH; ³Center for Human Identification, University of North Texas Health Science Center, Fort Worth, TX
- TP 263 **Development of Fiber Spray Ionization Mass Spectrometry (FSI-MS) for Direct Analysis of Drugs in Forensic Samples: A Comparison with PSI-MS;** João Francisco Allochio Filho^{1,2}; Nayara Araujo dos Santos²; Hanna Leijoto de Oliveira³; Keyller Bastos Borges³; Valdemar Lacerda Júnior²; Wanderson Romão^{2,4}; ¹Federal Institute of Espírito Santo, São Mateus, Brazil; ²Petroleomic and Forensic Chemistry Laboratory, Department of Chemistry, Federal University of Espírito Santo, Vitória, Brazil; ³Federal University of São João del-Rei, Department of Natural Sciences, São João del-Rei, Brazil; ⁴Federal Institute of Espírito Santo, Vila Velha, Brazil
- TP 264 **Proteomics Can Infer DNA Genotype from a Single Human Hair in Forensic Science;** Glendon Parker¹; Zachary Goecker²; Jennifer Milan²; Christina De Leon²; Rachel Franklin²; Michelle Salemi²; Bailey Wills³; Brett Phinney²; Susan Walsh³; Robert Rice²; ¹University of California Davis, Davis, CA; ²University of California, Davis, Davis, CA; ³Indiana University-Purdue University Indianapolis, Indianapolis, Indiana
- TP 265 **Determination of Health Status by MALDI-MSI of Latent Fingerprints;** Kelly O'neill¹; Paige Hinners¹; Young-Jin Lee¹; ¹Iowa State University, Ames, IA
- TP 266 **Forensic Sampling Using Nanoparticle Extraction and Capture;** Jamira A Stephenson¹; Fabrizio Donnaruma¹; Kermit K Murray¹; ¹Louisiana State University, Baton Rouge, LA
- TP 267 **Rapid In-Situ Analysis of Volatile Organic Compounds from Biological Samples of Forensic Interest;** Stephanie Rankin-Turner; *Loughborough University, Loughborough, United Kingdom*



- TP 268 **Modelling Retention Behavior on Analysis of Psychoactive Compounds in Hallucinogenic Mushrooms by HILIC-MS;** Wen Jiang¹; Norbert Rác²; Júlia Nagy³; Tibor Veress³; ¹HILICON AB, Umea, Sweden; ²Department of Inorganic and Analytical Chemistry, Budapest University of Technology and Economics, Budapest, Hungary; ³Department of Drug and Arson Investigation, Hungarian Institute for Forensic Sciences, Budapest, Hungary
- TP 269 **Utility of High Resolution Mass Spectrometry (HRMS) for the Discovery of Emerging Synthetic Cannabinoids and their Metabolites in Forensic Casework;** Alex Krotulski¹; Amanda LA Mohr¹; Barry K Logan^{1,2}; ¹Center for Forensic Science Research and Education, Willow Grove, PA; ²NMS Labs, Willow Grove, PA
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- TP 270 **Mechanism and Energetics of the Hydration of Th+ to Form Th(OD)3+: Guided Ion Beam and Theoretical Studies;** Peter B. Armentrout¹; Arjun Kafle¹; Richard M Cox²; ¹University of Utah, Salt Lake City, UT; ²Pacific Northwest National Laboratory, Richland, WA
- TP 271 **“Understanding” Adduct Ion Molecular Structures and Stability in the Gas-Phase, Improving the Separation Power in Ion Mobility Spectrometry; A View;** Maarten Honing¹; Darya Hadavi²; Jonah Norbury¹; Marina Borzova¹; Erik Lange van¹; ¹Maastricht Multimodal Molecular Imaging (M4I) Institute, Division of Imaging Mass Spectrometry, Maastricht, Netherlands; ²Maastricht Multimodal Molecular Imaging (M4I) Institute, Division of Imaging Mass Spectrometry, Maastricht, Netherlands
- TP 272 **Systematic Alteration of Gas-Phase Acidities and Conformations with Insertion of a D-Amino Acid in Oligopeptides;** Yuntao Zhang¹; Joshua S. Ho¹; Jianhua Ren¹; ¹University of the Pacific, Stockton, CA
- TP 273 **Conformations and Energetics of B- and Y-Ions in Peptoid Fragmentation;** Joshua S. Ho¹; Yuntao Zhang¹; Jianhua Ren¹; ¹University of the Pacific, Stockton, CA
- TP 274 **Reaction Rate Acceleration in Microdroplets Calculated Using Quantum Mechanical Modeling;** Namita Narendra¹; Jinying Wang¹; James Charles¹; Tillmann Kubis^{1,2,3}; Xingshuo Chen⁴; R. Graham Cooks⁴; ¹School of Electrical and Computer Engineering, Purdue University, West Lafayette, IN; ²Center for Predictive Materials and Devices, Purdue University, West Lafayette, IN 47906; ³Network for Computational Nanotechnology, Purdue University, West Lafayette, IN; ⁴Department of Chemistry, Purdue University, West Lafayette, IN
- TP 275 **Solely Concentrating on the Negative Aspects of Life;** Jordan Rabus¹; Philippe Maître²; Benjamin J Bythell³; ¹University of Missouri, Saint Louis, MO; ²Laboratoire de Chimie Physique (UMR8000), CNRS, Univ. Paris-Sud, Université Paris-Saclay, Orsay, France; ³University of Missouri, St. Louis, MO
- TP 276 **Characterization of Precursor and Product Ions from Copper (II) Cationized, N-terminally Modified Glycine-Glycine Using Infrared Multiple-Photon Photodissociation Spectroscopy;** Susan Kline¹; Amanda Bubas¹; Luke J. Metzler¹; Connor Graca¹; Theodore Corcovilos²; Jonathan Martens³; Giel Berden³; Jos Oomens³; Michael J. Van Stipdonk¹; ¹Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA; ²Department of Physics, Duquesne University, Pittsburgh, PA; ³Radboud University Nijmegen, Institute for Molecules and Materials, FELIX Facility, Nijmegen, Netherlands
- TP 277 **Spectral Derivatives. Exploring and Exploiting the Collision Energy Dependence of Tandem Mass Spectra;** Yamil Simon; NIST, Gaithersburg, MD
- TP 278 **Computational Analysis of Tandem-Trapped Ion Mobility / Mass Spectrometry Measurements Relates Identity of Proteoforms to their Tertiary and Quaternary Structures;** Christian Bleiholder¹; Fanny C Liu¹; Tyler C Cropley¹; Mengqi Chai¹; ¹Florida State University, Tallahassee, FL
- TP 279 **Dissociation Chemistry In Model Crude Oil Components;** Maha Abutokaikah¹; Giri R Gnowali¹; Joseph W Frye¹; Curtis M Stump¹; John Tschampel¹; Christopher D Spilling¹; Benjamin J Bythell¹; ¹University of Missouri, St. Louis, MO
- TP 280 **Structure and Reactivity of Anionic Uranyl Complexes with Acetate and Halide Ligands;** Anna Iacovino¹; Irena Tatosian¹; Luke Metzler¹; Theodore Corcovilos¹; Giel Berden²; Jonathan Martens²; Jos Oomens²; Michael Van Stipdonk¹; ¹Duquesne University, Pittsburgh, PA; ²Radboud University Nijmegen, Institute for Molecules and Materials, FELIX Facility, Nijmegen, Netherlands
- TP 281 **Experimental and Computational Investigation of the Hydrolysis of Gas-phase [UVIO2(R)]+, R=CH3, CH2CH3, CH=CH2 and C6H5;** Michael J. Van Stipdonk¹; Irena Tatosian¹; Amanda Bubas¹; Anna Iacovino¹; Susan Kline¹; Luke Metzler¹; ¹Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA
- TP 282 **Probing the Intrinsic Conformation of Anionic Uranyl Complexes Using IRMPD Spectroscopy and Quantum Chemical Calculations;** Scott D. Rissler¹; Michael J. Van Stipdonk¹; Luke Metzler¹; Connor J Graca¹; Irena Tatosian¹; Amanda Bubas²; ¹Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA; ²University of Utah, Salt Lake City, UT
- TP 283 **MultiCRAFTI: Relative Collision Cross Sections Through FTICR Methods without Need for Accurate Pressure Measurements or Single-Collision Dephasing Conditions;** Brigham Pope¹; Daniel Joaquin¹; Jacob Hickey¹; David Dearden¹; ¹Brigham Young University, Provo, UT
- TP 284 **Dependence of CRAFTI cross-sections on ion-neutral center-of-mass kinetic energy and ion dissociation energy;** Andrew J. Arslanian¹; Noah Mismash¹; Jacob Shaner¹; Tina H. M. Farzan¹; Jamir Shrestha¹; David V. Dearden¹; ¹Brigham Young University, Provo, UT
- TP 285 **Determining Topologies of Alkylammonium Complexes of Cucurbit[6]uril Using multiCRAFTI Techniques in an FTICR Mass Spectrometer;** Jamir Shrestha¹; Zixuan Feng^{1,2}; Mariah Pay¹; Andrew J. Arslanian¹; Tina H. M. Farzan¹; Brigham Pope¹; Jiewen Shen¹; David V. Dearden¹; ¹Brigham Young University, Provo, UT; ²Colorado State University, Fort Collins, CO
- TP 286 **Structures and Characteristics of Cucurbit[5]uril-Halide Inclusion Complexes Capped by Alkali Metal Cations via CRAFTI Collision Cross Sections;** Jiewen Shen¹; Tina H. M. Farzan¹; David V. Dearden¹; ¹Brigham Young University, Provo, UT
- TP 287 **The Effects of Neutral Guest in Cucurbit[5]uril Complexes Containing Various Metals on Its CRAFTI Collision Cross Sections;** Tina H. M. Farzan¹; Joseph W. Wilson¹; Sam Hickenlooper^{1,2}; Andrew J. Arslanian¹; David V. Dearden¹; ¹Brigham Young University, Provo, UT; ²University of Utah, Salt Lake City, UT
- FUNDAMENTALS: IONIZATION MECHANISMS**
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- TP 288 **Spatial Mapping of Ion Distributions in Pneumatically Assisted Electrosprays;** Patrick Brophy¹; Thomas McDonald¹; Jim Murphy¹; ¹Waters Corporation, Milford, MA
- TP 289 **Elucidating H/D-Exchange Mechanism of Active Hydrogen in PAH Compounds;** Arif Ahmed¹; Syful Islam¹; Sunghwan Kim¹; ¹Kyungpook National University, Daegu, South Korea



- TP 290 **Simulation of Charged Nanodroplets in MS-Transfer-Stage Ion-Guides;** Clara Markert¹; Walter Wissdorf¹; Hendrik Kersten¹; Thorsten Benter¹; ¹*Bergische Universität Wuppertal, Wuppertal, Germany*
- TP 291 **Investigating the Mechanism of Multivalent Cation-Induced Protein Supercharging through MD Simulations and Native MS Experiments;** Leanne Martin¹; Haidy Metwally¹; Lars Konermann¹; ¹*University of Western Ontario, London, ON*
- TP 292 **Insights into Ion Release from VSSI Droplets Obtained with Molecular Dynamics Simulations;** Kinkini Udara Jayasundara¹; Nandhini Ranganathan¹; Chong Li¹; Ahmad Kiani Karanji¹; Peng Li¹; Stephen Valentine¹; ¹*West Virginia University, C. Eugene Bennett Department of Chemistry, Morgantown, WV*
- TP 293 **The Role of Trace Constituents for the Sustained Operation of Corona Discharges in APCI;** Florian Stappert¹; Steffen Braekling¹; Hendrik Kersten¹; Thorsten Benter¹; ¹*University of Wuppertal, Wuppertal, Germany*
- TP 294 **Systematic Investigations of Electron Ionization Fragmentation Patterns of Selected MOCVD Precursors: Source Temperature and Electron Energy Dependence;** Yessica Brachthäuser¹; Joshua Rieger²; Markus Langner²; Alexander Laue¹; Hin Yiu Chung¹; Thorsten Benter²; ¹*Zeiss SMT GmbH, Oberkochen, Germany*; ²*University of Wuppertal, Wuppertal, Germany*
- TP 295 **The Mechanism of Carbohydrate Ionization to Form Metal-Ion Adducts from Nanosized Droplets during Electrospray;** Emvia I Calixte¹; Tara Liyanage¹; H. Jamie Kim¹; Emily D. Ziperman¹; Amanda J Pearson¹; Elyssia S. Gallagher¹; ¹*Baylor University, Waco, TX*
- TP 296 **Characterization of Ion-Molecule Reactions within Quadrupole Ion Trap Mass Analyzers by Chemical Modification of the Collision Gas;** Christine Polaczek¹; Marco Thinius²; Hendrik Kersten²; Thorsten Benter²; ¹*University of Wuppertal, Wuppertal, Germany*; ²*University of Wuppertal, Wuppertal, Germany*
- TP 297 **Numerical Study of Fluid Atomization in a High-Velocity Spray;** Wei Wang^{1,2}; Steve Bajic¹; Benzi John²; David R. Emerson²; ¹*Waters Corporation, Wilmslow, United Kingdom*; ²*Daresbury Laboratory, Science and Technology Facilities Council, Warrington, United Kingdom*
- GC/MS: INSTRUMENTATION AND APPLICATIONS I**
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- TP 298 **Comprehensive Machine Learning Prediction of GC/MS Pesticide Recovery Based on the Molecular Fingerprinting for Food QA/QC;** Takeshi Serino^{1,2}; Sadao Nakamura¹; Yoshizumi Takigawa¹; Norton Kitagawa³; Shigehiko Kanaya²; ¹*Agilent Technologies, Hachioji City, Japan*; ²*Nara Institute of Science and Technology, Ikoma city, Japan*; ³*Agilent Technologies, Santa Clara, CA*
- TP 299 **A Simple VOC Capturing Method Coupled with GC-MS;** Takeshi Furuhashi¹; Shigenori Ota²; ¹*Anicom Specialty Medicinal Institute Inc, Tokyo, Japan*; ²*GL science Inc, Iruma city, Saitama prefecture, Japan*
- TP 300 **Tuning the Molecular Ion Abundance in Electron Ionization Mass Spectra and its Effects on Sample Identification;** Ksenia Kladchenko¹; Alexander B. Fialkov¹; Tal Alon¹; Aviv Amirav¹; ¹*Tel-Aviv University, Tel-Aviv, Israel*
- TP 301 **Complementary Techniques in the Environmental GC-MS Analysis;** Albert T Lebedev¹; Viatcheslav Artaev²; Dmitrii Mazur¹; Georgii Tikhonov²; ¹*Moscow State University, Moscow, Russian Federation*; ²*LECO Corporation, St Joseph, MI*
- TP 302 **Rapid Quantitative Analysis of Melamine in Semi-Solid Food;** Michael D Browne¹; Tommy Nguyen¹; Krege Christison¹; Itsuko Iwai²; O. David Sparkman¹; ¹*University of the Pacific, Stockton, CA*; ²*Diablo Analytical, Antioch, CA*
- TP 303 **Comprehensive Determination of 209 Polychlorinated Biphenyls Using Two-Dimensional Gas Chromatography Triple Quadrupole Mass Spectrometry;** Yun Zou¹; Shizhen Zhao²; Gan Zhang²; Satoshi Yamaki¹; Yuki Hashi³; Naoki Hamada¹; ¹*Shimadzu(China)Co.,LTD.Beijing Branch, Beijing, China*; ²*Guangzhou Institute of Geochemistry, Chinese Academy of Sciences, Guangzhou, China*; ³*Shimadzu (China) Co., LTD., SHANGHAI, China*
- TP 304 **Evaluation of Matrix Effect on Pesticides in Vegetables by GC-MS/MS;** Ge Yin¹; Jun Fan²; ¹*Shimadzu China, Shanghai, China*; ²*Shimadzu (China) Co., LTD., Shanghai, China*
- TP 305 **An Optimization Tool for MS Signal Acquisition in GC Triple Quadrupole Mass Spectrometry;** Anastasia Andrianova¹; Melissa Churley²; ¹*Agilent Technologies, Wilmington, DE*; ²*Agilent Technologies, Santa Clara, CA*
- TP 306 **Volatile Profile Comparison of Flavored and Non-Flavored Vodkas by Purge & Trap Thermal Desorption GC/MS;** Ron Shomo; *Adaptas Solutions, ringoes, NJ*
- TP 307 **Open Characterization of Vaping Liquids (e-liquids);** Ivana Kosarac¹; Xinghua Fan¹; Cariton Kubwabo¹; Wei He¹; Jun Man¹; Trevor K. Mischki¹; ¹*Health Canada, Ottawa, ON*
- TP 308 **Fun modulated GCxGC coupled to TOFMS for Non-Target Profiling of Food, Flavor, and Fragrance Samples;** Elizabeth Humston-Fulmer¹; Lorne Fell¹; Joesph E Binkley¹; ¹*LECO Corporation, St Joseph, MI*
- TP 309 **Tandem Ionisation for Improved Characterisation of Fragranced Products;** Pete Grosshans¹; Laura McGregor¹; Nick Bukowski¹; Gerhard Horner²; ¹*SepSolve Analytical, Peterborough, United Kingdom*; ²*Five Technologies, Munich, Germany*
- TP 310 **Coupling Comprehensive Two-Dimensional Gas Chromatography with an Orbitrap MS for Enhanced Separation and Identification;** Xin Zheng¹; Jason Cole²; ¹*Thermo Fisher Scientific, Austin, TX*; ²*Thermo Fisher Scientific, Ausitn, TX*
- TP 311 **Qualitative and Quantitative Analysis of Electronic Cigarette Liquids Using Gas Chromatography – Orbitrap Mass Spectrometry;** Jane A Cooper¹; Chris Allen²; Cristian I Cojocariu¹; Brody Guckenberger³; ¹*Thermo Fisher Scientific, Runcorn, United Kingdom*; ²*Broughton, Skipton, United Kingdom*; ³*Thermo Fisher Scientific, Austin, TX*
- TP 312 **Non-Targeted Analysis of Natural Waters with GC-QTOFMS – Addressing Critical Methodological and Data-Evaluation Challenges;** Christina Troyer¹; Sebastian Handl¹; Zora Jandric¹; Kaan Kutlucinar¹; Tuba Recber¹; Ernest Mayr¹; Roza Allabashi¹; Reinhard Perfler¹; Stephan Hann¹; ¹*University of Natural Resources and Life Sciences (BOKU), Vienna, Austria*
- TP 313 **Novel GC-MS Ionization Technique to Identify Unknown Compounds;** Riki Kitano¹; Masato Takakura²; Akira Aono²; Kouki Tanaka²; ¹*Shimadzu Scientific Instruments, Inc., Columbia, Maryland*; ²*Shimadzu Corporation, Kyoto, Japan*
- TP 314 **Humans Smell to their Skin Microbiome and Microbes Smell Like What They Eat;** Mabel Cristina Gonzalez¹; Chiara Carazzone¹; Adriana Marcela Celis¹; Jorge Alberto Molina¹; ¹*Universidad de los Andes, Bogota, Colombia*
- TP 315 **Highly Sensitive TOF Mass Spectrometer coupled with a New User Friendly Flow Modulator for GCxGC-MS Analysis of Complex Mixtures;** David Jesse Borton¹; Jonelle Shiel¹; Mark Merrick¹; Viatcheslav Artaev¹; John V Seeley²; ¹*LECO Corporation, Saint Joseph, MI*; ²*Oakland University, Rochester, MI*
- TP 316 **Confident Confirmation of Steroids in Urine by Gas Chromatography-Advanced Electron Ionization (AEI)-Triple Quadrupole Mass Spectrometry;** Gustavo de Albuquerque Cavalcanti¹; Amit C Gujar²; Henrique Marcelo Gualberto Pereira³; Francisco Radler de Aquino Neto⁴;



- Monica Costa Padilha^{5,6}; ¹Federal University of Rio de Janeiro - UFRJ- Brazilian Doping Control Laboratory -LBCD, Rio de Janeiro, Brazil; ²Thermo Fisher Scientific, Austin, TX; ³Federal University of Rio de Janeiro - UFRJ - Brazilian Doping Control Laboratory -LBCD, Rio de Janeiro, Brazil; ⁴Federal University of Rio de Janeiro - UFRJ- Brazilian Doping Control Laboratory - LBCD, LADETEC, Rio de Janeiro, Brazil; ⁵Federal University of Rio de Janeiro - UFRJ- Brazilian Doping Control Laboratory -LBCD,, Rio de Janeiro, Brazil; ⁶Federal University of Rio de Janeiro - UFRJ- Research Laboratory of Anabolic Agents, LAPAA, Rio de Janeiro, Rio de Janeiro, Brazil, Rio de Janeiro, Brazil
- TP 317 **Molecular-Ion Detection and Fragmentation Mechanisms of a Common Extractable 1,4,7-Trioxacyclotridecane-8,13-dione by GC/HRMS in Electron Ionization and Chemical Ionization Modes;** Chongming Liu¹; Dajuan Lu¹; Danny Hower¹; Xiaoteng Gong¹; ¹SGS North America Inc., Fairfield, NJ
- TP 318 **Analysis of Polychlorinated Dibenzo-p-dioxins, Furans and Biphenyls in Drinking Water with Semi-Automated Solid Phase Extraction Using EPA Method 1613;** Rudolf Addink¹; Tom Hall¹; ¹Toxic Report, Watertown, MA
- H/D EXCHANGE: PROTEIN STRUCTURE/FUNCTION**
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- TP 319 **Epitope Mapping of Antibodies against Cobrotoxin and Cardiotoxin III by Hydrogen/Deuterium Exchange Mass Spectrometry;** Wei-Ya Chen¹; Wang-Chou Sung²; Sung-Fang Chen¹; ¹National Taiwan Normal University, Taipei, Taiwan; ²National Health Research Institutes, Zhunan, Taiwan
- TP 320 **Hydrogen Deuterium-Exchange Mass Spectrometry to Measure Nucleosome Dynamics;** Abigail A. Lemmon¹; Geoffrey P. Dann¹; Kelly R. Karch¹; Benjamin A. Garcia¹; ¹University of Pennsylvania, Philadelphia, PA
- TP 321 **Conformational Changes of BtuF upon Binding to Vitamin B12 Revealed by Hydrogen Deuterium Exchange Nanospray Mass Spectrometry;** Lijun Zhou; Nanjing University of science and technology, Nanjing, China
- TP 322 **Active Site Single Point Mutations Modulates the Dynamic Properties of Human Monoacylglycerol Lipase: A Hydrogen Deuterium Exchange Mass Spectrometry Study;** Ioannis Karageorgos¹; Sergiy Tyukhtenko²; Kyle Anderson¹; Girija Rajarshi²; Nikolai Znonok²; Alexandros Makriyannis²; Jeffrey Hudgens¹; ¹NIST, Rockville, MD; ²Northeastern University, Boston, MA
- TP 323 **Integrating HDX-MS and Native MS into Structure-Based Drug Discovery;** Liliana Pedro¹; Dayana Argoti¹; Weiping Jia¹; Patrick Rudewicz¹; ¹Novartis Institutes for Biomedical Research, Emeryville, CA
- TP 324 **Hydrogen-Deuterium eXchange Coupled to Mass Spectrometry Highlights a Reciprocal Crosstalk between the Inner and Outer Rings of the 20S Proteasome;** Jean Lesne¹; Julien Parra¹; Dusan Zivkovic¹; Thomas Menneteau¹; Matthieu Chavent¹; Marie Locard-Paulet¹; Marie-Pierre Bousquet-Dubouch¹; Odile Burlet-Schiltz¹; Julien Marcoux¹; ¹Institut de Pharmacologie et de Biologie Structurale, Université de Toulouse, CNRS, UPS, Toulouse, France
- TP 325 **Temperature and Mutation-Dependent Study of a Model TIM Barrel Domain-Containing Enzyme Performed Using Hydrogen/Deuterium Exchange Mass Spectrometry;** Anthony T. Iavarone¹; Emily J. Thompson¹; Judith P. Klinman¹; ¹UC Berkeley, Berkeley, CA
- TP 326 **Analysis of Oxidatively Damaged Proteins by H/D Exchange Mass Spectrometry;** Vincent A Saullo¹; Lars Konermann²; ¹University of Western Ontario, London, ON; ²University of Western Ontario, London , ON
- TP 327 **Connecting Ligand-Induced Dynamics to Potency: Analyzing Anti-Cancer Retinoids by Hydrogen Deuterium Exchange Mass Spectrometry;** Nathalia Melo¹; Alla Klyuyeva¹; Olga V Beliaeva¹; Natalia Kedishvili¹; Matthew Renfrow¹; Peter Prevelige¹; Venkatram Atigadda¹; Donald Muccio¹; ¹University of Alabama at Birmingham, Birmingham, AL
- TP 328 **HDX-MS Unravels Allosteric Mechanisms that Sequentially Unlock the Sec Translocase for Bacterial Protein Secretion;** Srinath Krishnamurthy¹; Nikolaos Eleftheriadis¹; Malvina Papanastasiou²; Athina Portalou¹; Spyridoula Karamanou¹; Giorgos Gouridis¹; Anastassios Economou¹; ¹Rega Institute, Dept of Microbiology and Immunology, KU Leuven, Leuven, Belgium; ²Broad Institute, Cambridge, MA
- TP 329 **Probing Histone Tail Interactions in Mononucleosomes by HX-ETD-Orbitrap-MS;** Malvina Papanastasiou¹; Terry Zhang²; James Mullahoo¹; Samuel A. Myers¹; Steven A. Carr¹; Jacob D. Jaffe¹; ¹Broad Institute, Cambridge, MA; ²Thermo Fisher Scientific, San Jose, CA
- TP 330 **Pulsed Unfolding, HDX, and Digestion of APOE Proteins by Mass Spectrometry Provides Insight into Forcing the Folded Monomeric Species;** Elizabeth T Schaper Bergman¹; Michael L Gross^{1,2}; ¹Washington University, St. Louis, MO; ²Washington University School of Medicine, St. Louis, MO
- TP 331 **Covariation Analysis Reveals Functional Regions of RORγ with Concerted Motions;** Tim Strutzenberg; The Scripps Research Institute, Palm Beach Gardens, FL
- TP 332 **Conformational Preferences for the Tec-Family Tyrosine Kinase BTK in Binding to the HIV-1 Accessory Protein Nef;** Thomas E. Wales¹; Raji E. Joseph²; Shoucheng Du³; Thomas E. Smithgall³; Amy H. Andreotti²; John R. Engen¹; ¹Northeastern University, Boston, MA; ²Iowa State University, Ames, IA; ³University of Pittsburgh School of Medicine, Pittsburgh, PA
- TP 333 **Uncovering Differential Effects of IgG Subclasses on Whole DENV Particles with Hydrogen-Deuterium Exchange Mass Spectrometry;** Xin-Xiang Lim¹; Ganesh S. Anand¹; ¹National University of Singapore, Singapore, Singapore
- TP 334 **A Bacterial Flavin-Dependent Oxidoreductase that Undergoes Conformational Changes to Capture Carbon Dioxide;** Jenna Mattice¹; Bennett Streit¹; Luke Berry¹; John Peters²; Jennifer DuBois¹; Brian Bothner¹; ¹Montana State University, Bozeman, MT; ²Washington State University, Pullman, WA
- TP 335 **Revealing the Impact of Biological Substrate and Drug Ligands on the Conformational Dynamics of the Human Serotonin Transporter Using HDX-MS;** Ingvar R. Möller¹; Marika Slivacka¹; Anne Kathrine Nielsen²; Søren G.F. Rasmussen³; Ulrik Gether³; Claus J. Loland²; Kasper D. Rand¹; ¹Protein Analysis Group, Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark; ²Laboratory for Membrane Protein Dynamics, Department of Neuroscience, University of Copenhagen, Copenhagen, Denmark; ³Department of Neuroscience, University of Copenhagen, Copenhagen, Denmark
- TP 336 **Probing Protein Ligand Interactions through an Offline MALDI-MS based Hydrogen Deuterium Exchange Study;** Laxmi Sinduri Vuppala¹; Theresa Evans-Nguyen¹; Ioannis Gelis¹; John M. Koomen^{1,2}; ¹University of South Florida, Tampa, FL; ²Moffitt Cancer Center & Research Institute, Tampa, FL
- TP 337 **HDX-MS Reveals Allosteric Changes in Subtilisin Serine Protease Upon Inhibitor Binding;** Daniel W Pedersen^{1,2}; Jeppe C Moubitsen¹; Stuart Pengelley³; Detlev Suckau³; Thomas J D Jørgensen²; Christian I Jørgensen¹; ¹Novozymes A/S, Bagsvaerd, Denmark; ²University of



Southern Denmark, Odense, Denmark; ³Bruker Daltonik GmbH, Bremen, Germany

TP 338 **Probing Copper Binding in Orange Carotenoid Protein by Using H/DX and Native Mass Spectrometry;** Haijun Liu¹; Ming Cheng²; Jing Yan¹; Chunyang Guo¹; Andy Xu¹; Michael L Gross¹; Robert E Blankenship¹; ¹Washington University, St. Louis, MO; ²Washington University, St Louis, MO

TP 339 **Thermodynamic Insight for the Formulation Optimization of a Therapeutic Antibody by HDX-MS Analysis and nanoDSF;** Yoshitomo Hamuro¹; Mehabaw Derebe¹; Jennifer F. Nemeth-Seay¹; ¹Janssen Research and Development, Spring House, PA

TP 340 **Gas-Phase Hydrogen Deuterium Exchange Coupled with Dissociation of Enkephalin Variants to Investigate Exchange Mechanism;** Cynthia M Suarez¹; Rebecca A Jockusch¹; ¹University of Toronto, Toronto, ON

TP 341 **Discovery and Characterization of a Synthetic Antigen Binding Fragment (sFab) Inhibiting Marburg Viral RNA Synthesis Incorporating HDX-MS Analyses;** Nicole D. Wagner¹; Parmeshwar Amaty²; Gang Chen³; Priya Luthra⁴; Liuqing Shi¹; Alevtina Pavlenco³; Dominika Borek⁵; Henry Rohrs¹; Christopher F. Basler⁴; Gaya Amarasinghe²; Sachdev Sidhu³; Michael L Gross¹; Daisy Leung²; ¹Washington University, St. Louis, MO; ²Washington University School of Medicine, St. Louis, MO; ³University of Toronto, Toronto, Ontario; ⁴Georgia State University, Atlanta, GA; ⁵UT Southwestern Medical Center, Dallas, TX

TP 342 **Higher-Order Structural Analysis of Pro-Survival BAG-1S through HDX-MS;** Ozge Tatli^{1,2}; Miray Turk¹; Gizem Dinler Doganay¹; ¹Istanbul Technical University, Istanbul, Turkey; ²Istanbul Medeniyet University, Istanbul, Turkey

TP 343 **Cyclic AMP-PKA Signalosome Dynamics by HDXMS and Fluorescence Polarization Reveals Regulatory AMP Oscillations;** Nikhil K Tulsian^{1,2}; Abhijeet Ghode¹; Ganesh S Anand¹; ¹Dept. of Biological Sciences, National University of Singapore, Singapore, Singapore; ²Dept. of Biochemistry, National University of Singapore, Singapore

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TP 344 **Chemical Imaging of Evolving Flow Patterns Through a Porous Membrane Flow Cell via Liquid Extraction-Mass Spectrometry;** Vilmos Kertesz¹; John F. Cahill¹; Scott T. Retterer¹; ¹Oak Ridge National Laboratory, Oak Ridge, TN

TP 345 **Development and Application of Ambient Mass Spectrometry Images for Dermal Melamine Exposures in Melamine Tableware Manufacturing Workers;** Yu-Ming Hsu¹; Jentaie Shiea^{1,2}; Ming-Tsang Wu^{1,3,4}; ¹Research Center for Environmental Medicine, Kaohsiung Medical University, Kaohsiung, Taiwan; ²Department of Chemistry, National Sun Yat-sen University, Kaohsiung, Taiwan; ³Department of Public Health, College of Health Sciences, Kaohsiung Medical University, Kaohsiung, Taiwan; ⁴Department of Family Medicine, Kaohsiung Medical University Hospital, Kaohsiung Medical University, Kaohsiung, Taiwan

TP 346 **Investigation of Chemical Complexity and Cellular Heterogeneity of Human Pancreatic Islets Using Cross-Platform Mass Spectrometric Approach;** Stanislav Rubakhin¹; Elena V. Romanova²; Jonathan V. Sweedler²; ¹Beckman Institute, UIUC, Urbana, IL; ²University of Illinois at Urbana-Champaign, Urbana, IL

TP 347 **Developing a Drug Screening Platform: MALDI-Mass Spectrometry Imaging of Paper-Based Cultures;** Fernando Tobias¹; Gabriel J. LaBonia²; Julie McIntosh³; Matthew R. Lockett³; Amanda B. Hummon¹; ¹Department of Chemistry and Biochemistry, Comprehensive Cancer Center, The Ohio State University, Columbus, Ohio;

²Department of Chemistry and Biochemistry, University of Notre Dame, Notre Dame, Indiana; ³Department of Chemistry, University of North Carolina at Chapel Hill, Chapel Hill, NC

TP 348 **Optimisation of a Bottom-Up Strategy to Detect Biopharmaceuticals in 3D Tumour Models Using MALDI-MSI;** Lucy E Flint¹; Neil A Cross¹; Laura M Cole¹; David P Smith¹; Malcolm R Clench¹; ¹Sheffield Hallam University, Sheffield, United Kingdom

TP 349 **Utilizing Formalin Fixation for Enhancing Detection of Neuropeptides from the Crustacean Brain by MALDI-MS Imaging;** Nhu Q. Vu¹; Amanda R. Buchberger¹; Jillian Johnson¹; Lingjun Li¹; ¹University of Wisconsin - Madison, Madison, WI

TP 350 **Identifying Biomarkers by High Throughput Screening on FFPE Breast Cancer TMAs Using DESI-MSI;** Ólaf Gerdur Ísberg¹; Dipa Gurung¹; James McKenzie¹; Hiromi Kudo¹; Jon G Jonasson²; Sigrídur Klara Bodvarsdóttir³; Margret Thorsteinsdóttir³; Zoltan Takats¹; ¹Imperial College, London, United Kingdom; ²Landspítali, University Hospital, Reykjavík, Iceland; ³University of Iceland, Reykjavík, Iceland

TP 351 **Click Chemistry Driven Fluorophore Addition Allows for Spatial Identification of Liposomal Drug Delivery System Components by MALDI-MSI and Fluorescence Microscopy;** William Andrews; University of Notre Dame, Notre Dame; The Ohio State University, Columbus, OH

TP 352 **Mass Spectrometry Imaging of the in situ Drug Release from Nanocarriers;** Jinjuan Xue¹; Huihui Liu¹; Suming Chen²; Caiqiao Xiong¹; Lingpeng Zhan¹; Jie Sun¹; Zongxiu Nie¹; ¹Institute of Chemistry, Chinese Academy of Sciences, Beijing, China; ²Wuhan University, Wuhan, China

TP 353 **A Tool to Visualize Soil Microbial Community Dynamics Using Mass Spectrometry Imaging and Confocal Microscopy;** Arunima Bhattacharjee¹; Thomas W Wietsma¹; Dusan Velickovic¹; Sheryl L Bell¹; Janet K Jansson¹; Kirsten S Hofmockel¹; Christopher R Anderton¹; ¹Pacific Northwest National Laboratory, Richland, WA

TP 354 **An Elegant Approach for Broad Molecular Imaging of the Root-Soil Interface via Indirect MALDI-FTICR-MSI;** Dusan Velickovic¹; Vivian Lin¹; Albert Rivas¹; Christopher Anderton¹; James Moran¹; ¹Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA

TP 355 **The Combination of DIUTHAME-IMS/FT-ICR Conserves High Mass Accuracy and Resolution over the DIUTHAME-IMS/TOFMS in the Laser Desorption/Ionization Imaging Mass Spectrometry;** Hasan Md. Mahmudul¹; Yasuhide Naito²; Masahiro Kotani³; Takayuki Ohmura³; Mamun Md. Al¹; Shumpei Sato¹; Ariful Islam¹; A s m Waliullah¹; Takashi K Ito¹; Mitsutoshi Setou^{1,4,5}; ¹International Mass Imaging Center and Department of Cellular and Molecular Anatomy, Hamamatsu University School of Medicine, Hamamatsu, Japan; ²The Graduate School for the Creation of New Photonics Industries, Hamamatsu, Japan; ³Hamamatsu Photonics K.K., Iwata, Japan; ⁴Preeminent Medical Photonics Education & Research Center, Hamamatsu, Japan; ⁵Department of Anatomy, The University of Hong Kong, Pokfulam, China

TP 356 **Combination of the Low Vacuum MALDI-Orbitrap Imaging with the Hydrogen/Deuterium Exchange Approach;** Gleb Vladimirov¹; Yury kostyukevich¹; Eugene (evgeny) Nikolaev²; ¹Skolkovo Institute of Science and Technology, Skolkovo, Russian Federation; ²Skolkovo institute of science and technology, Moscow Region, Russian Federation

TP 357 **Direct Atmospheric Pressure Laser Desorption Ionization for Mass Spectrometry Imaging;** Jing Yang¹; Wenpeng Zhang^{1,2}; Wenbo Cao¹; Xiaoxiao Ma¹; Zheng Ouyang¹; ¹State Key Laboratory of Precision Measurement Technology and Instruments, Department



- of Precision Instruments, Tsinghua University, Beijing, China; ²Department of Chemistry, Purdue University, West Lafayette, IN
- TP 358 **Unsaturated Lipid Isomer Distribution Analysis by MALDI MS Imaging with m-CPBA Epoxidation and CID-MS/MS;** Meng Xu¹; Yu Feng²; Lingjun Li^{1,2}; ¹Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706; ²School of Pharmacy, University of Wisconsin-Madison, Madison, WI
- TP 359 **Development of Blotting Method Using DIUTHAME for Imaging MS;** Masahiro Kotani¹; Takayuki Ohmura¹; Akira Tashiro¹; Hirofumi Enomoto²; Yasuhide Naito³; ¹Hamamatsu Photonics K.K., Iwata, Japan; ²Teikyo University, Utsunomiya, Japan; ³The Graduate School for the Creation of New Photonics Industries, Hamamatsu, Japan
- TP 360 **Brimstone Chemistry under Laser Light Assists Mass Spectrometric Detection and Imaging the Distribution of Arsenic in Minerals;** Zhaoyu Zheng¹; Swapnil Lal²; Athula Attygalle¹; ¹Stevens Institute of Technology, Weehawken, NJ; ²Montgomery High School, Skillman, NJ
- TP 361 **Optimizing the Mass Accuracy for Automated Analysis of MALDI Images;** Sophie Rappe¹; Mathieu Tiquet¹; Raphaël La Rocca¹; Johann Far¹; Loïc Quinton¹; Gauthier Eppe¹; Edwin A De Pauw¹; ¹Mass Spectrometry Laboratory, MoSys Research Unit, University of Liege, Liege, Belgium
- TP 362 **Optimizing Tissue Ablation for Mass Spectrometry Imaging Using Light Scattering;** Achala P Deenamulla Kankanamalage¹; Fabrizio Donnaruma¹; Kermit K Murray¹; ¹Louisiana State University, Baton Rouge, LA
- TP 363 **Pulsed Cold Plasma for Post Ionization in MALDI-MS imaging;** Jens Soltwisch^{1,2}; Ulrich Röhling³; Klaus Dreisewerd^{1,2}; ¹Institute for Hygiene, University of Münster, Münster, Germany; ²Interdisciplinary Center for Clinical Research (IZKF), University of Münster, Münster, Germany; ³Institute of Medical Physics and Biophysics, University of Münster, Münster, Germany
- TP 364 **Improving the Mass Range and Field of View in Ion Microscope Imaging Mass Spectrometry;** Natasha M. Smith¹; Fei Gao¹; Ang Guo¹; Michael Burt¹; Robert Burleigh¹; Mark Brouard¹; ¹University of Oxford, Oxford, United Kingdom
- IMAGING MS: PHARMACEUTICAL APPLICATIONS**
365-379
- TP 365 **Implementing Multi-modal Imaging Platform for Tissue Distribution, Metabolite Profiling and Quantification of Peptide Therapeutics;** Bingming Chen¹; Marissa Vavrek¹; Wendy Zhong²; Richard Gundersdorf¹; Bernard Choi²; Scott Fauty¹; Mark Cancilla¹; ¹Merck & Co., Inc., West Point, PA; ²Merck & Co., Inc., Rahway, NJ
- TP 366 **Quantitative Mass Spectrometry Imaging of Diclofenac and its Metabolites in Tissues Using Nanospray Desorption Electrospray Ionization Mass Spectrometry;** Hilary Brown¹; Bingming Chen²; Mark Cancilla²; Elizabeth Pierson³; Marissa Vavrek²; Wendy Zhong³; Julia Laskin¹; ¹Purdue University, West Lafayette, IN; ²Merck & Co., Inc., West Point, PA; ³Merck & Co., Inc., Rahway, NJ
- TP 367 **Investigation of Drug Localization in the Intestinal Tract Using Imaging Mass Spectrometry;** Kerri Grove¹; Shaila Hoque¹; Suresh Lakshminarayana¹; Ying-Bo Chen¹; Imad Hanna²; Joe Young¹; Ujjini Manjunatha¹; Patrick Rudewicz¹; ¹Novartis Institutes for BioMedical Research, Emeryville, CA; ²Novartis, Cambridge, MA
- TP 368 **Measurement of Temporal Changes in the Distribution of Imiquimod Administered Transdermally to Mouse Skin Tissue Using Imaging Mass Spectrometry;** Yuki Fukui¹; Hisanao Hazama¹; Taiki Yamasaki¹; Sayami Ito¹; Naoki Okada¹; Kunio Awazu¹; ¹Osaka University, Suita, Japan
- TP 369 **The Spheroid Microarray: Pushing *in vitro* Drug Penetration Towards High-Throughput Technologies;** Jillian Johnson¹; Lingjun Li¹; ¹University of Wisconsin-Madison, Madison, WI
- TP 370 **Mouse Brain Drug Exposure by Imaging Mass Spectrometry and its Correlation to Whole Brain Pharmacodynamic Parameters;** John Bowling¹; Alireza Abdolvahabi¹; Xiang Fu¹; Lei Yang¹; Zoran Rankovic¹; ¹St. Jude Children's Research Hospital, Memphis, TN
- TP 371 **Metabolomic Studies of Amyloid Plaques in Mouse Brain with Alzheimer Disease Using Mass Spectrometry Imaging Strengthened by Image Fusion;** Xiang Tian¹; Zhu Zou¹; Boer Xie²; Junmin Peng²; Zhibo Yang¹; ¹University of Oklahoma, Norman, OK; ²St. Jude Children's Research Hospital, Memphis, TN
- TP 372 **Development of a Detection Method for Antisense Oligonucleotides in Mouse Livers and Kidneys by MALDI Imaging Mass Spectrometry;** Hiroyuki Yokoi^{1,2}; Yuuya Kasahara³; Satoshi Obika^{2,3}; Takefumi Doi²; Haruhiko Kamada³; ¹Otsuka Pharmaceutical Co., Ltd, Tokushima, Afghanistan; ²Graduate School and School of Pharmaceutical Sciences, Osaka University, Osaka, Japan; ³National Institute of Biomedical Innovation, Health and Nutrition, Osaka, Japan
- TP 373 **Comparative Study of Pancreatic Insulin and N-Glycans between Lean and Obese Zucker Rats by MALDI Imaging Mass Spectrometry;** Bin Wang¹; Yatao Shi¹; Zihui Li²; Xudong Shi³; Nannan Tao⁴; Lingjun Li^{1,2}; ¹School of Pharmacy, University of Wisconsin-Madison, Madison, WI 53705; ²Department of Chemistry, University of Wisconsin-Madison, Madison, WI; ³Department of Surgery, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI; ⁴Bruker Scientific, LLC, San Jose, CA
- TP 374 **MALDI-Ion Mobility Mass Spectrometry Imaging for Paclitaxel Nanomedicine Distribution in Solid Tumor Tissue;** Bo Wen¹; Hebao Yuan¹; Lipeng Dai¹; Krishani Rajanayake¹; Miao He¹; Manjunath Pai¹; Duxin Sun¹; ¹University of Michigan, Ann Arbor, MI
- TP 375 **Different MALDI Mass Spectrometry Imaging Applications on a Prototype MALDI-Q-TOF Instrument;** Janina Oetjen¹; Alice Ly¹; Arne Fuetterer¹; Juergen Suetering¹; Niels Goedecke¹; Richard R Drake²; Anand Mehta²; Michael Becker³; Rita Casadonte⁴; Jörg Kriegsmann⁴; Jens Fuchser¹; Lucy Woods¹; Oliver Raether¹; Jens Hoehndorf¹; Shannon Cornett⁵; ¹Bruker Daltonik GmbH, Bremen, Germany; ²Medical University of South Carolina, Charleston, SC; ³Boehringer Ingelheim Pharma GmbH & Co. KG, Department of Drug Discovery Sciences, Biberach an der Riss, Germany; ⁴Proteopath, Trier, Germany; ⁵Bruker Daltonics Inc., Billerica, MA
- TP 376 **ToF-SIMS Depth Profiling of Oral Drug Delivery Films for 3D Visualization and Quantification of Active Pharmaceutical Particles;** Shin Muramoto¹; Greg Gillen²; Cayla Collett²; ¹Gaithersburg, MD; ²National Institute of Standards and Technology, Gaithersburg, MD
- TP 377 ***in-situ* Drug Release Monitoring Using Quantitative 3D Mass Spectrometry Imaging for a Drug Delivery Stent Formulation Optimization;** Lauranne Poncelet^{1,2}; Rima Ait-Belkacem¹; Justine Mougine²; Mickael Maton²; Dyhia Kersani²; Bernard Martel²; Stephanie Degoutin²; Feng Chai²; Nicolas Blanchemain²; Jonathan Stauber³; ¹Imabiotech, Loos, France; ²Université de Lille, Lille, France; ³Imabiotech Corp, Boston, MA
- TP 378 **Gadolinium Deposition from MRI Contrast Agents in the Human Body Unraveled by MS Imaging and Speciation Analysis;** Uwe Karst¹; University of Münster, Münster, Germany



TP 379 **MALDI Imaging Studies of Cisplatin Distribution in Mouse Brain Sections;** Hay-Yan J Wang^{1,2}; Yi-Feng Dai²; Hung-Wei Yang³; Chiung-Yin Huang⁴; Kuo-Chen Wei⁴; ¹Department of Biological Sciences, National Sun Yat-sen University, Kaohsiung, Taiwan; ²Doctoral Degree Program in Marine Biotechnology, National Sun Yat-sen University and Academia Sinica, Kaohsiung, Taiwan; ³Institute of Medical Science and Technology, National Sun Yat-sen University, Kaohsiung, Taiwan; ⁴Department of Neurosurgery, Linko Chang Gung Memorial Hospital, Taoyuan City, Taiwan

IMAGING MS: SAMPLE PREPARATION
380-387

TP 380 **Keeping the Shape of Plant Tissue for Visualizing Metabolite Features of Imaging Mass Spectrometry in *Asparagus officinalis*;** Ryo Nakabayashi¹; Kei Hashimoto¹; Kiminori Toyooka¹; Tetsuya Mori¹; Takashi Nirasawa²; Kazuki Saito^{1,3}; ¹RIKEN Center for Sustainable Resource Science, Yokohama, Japan; ²Bruker Japan K. K., Yokohama, Japan; ³Chiba University, Chuo-ku, Japan

TP 381 **Creating Normalcy Classifications in Human Kidney Tissue via LC-MS/MS Proteomic Analysis for 3-D Molecular Imaging;** Jamie Allen^{1,2}; Danielle Gutierrez^{1,2}; Maya Brewer³; Nathan Heath Patterson^{1,2}; Raf Van de Plas^{1,2,4}; Mark Decaestecker³; Raymond C Harris³; Agnes B Fogo⁵; Richard M. Caprioli^{1,2,6}; Jeffrey Spraggins^{1,2,6}; ¹Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; ²Vanderbilt University Department of Biochemistry, Nashville, TN; ³Vanderbilt University Medical Center, Department of Medicine, Nashville, TN; ⁴Delft University of Technology, Delft, Netherlands; ⁵Vanderbilt University Medical Center Department of Pathology, Microbiology and Immunology, Nashville, TN; ⁶Vanderbilt University Department of Chemistry, Nashville, TN

TP 382 **Understanding and Decreasing Visceral Fat Delocalisation in Imaging Mass Spectrometry;** Frédéric Fournelle¹; Ethan Yang¹; Martin Dufresne²; Pierre Chaurand¹; ¹University of Montreal, Montreal, QC; ²Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN

TP 383 **Comprehensive Evaluation of Zinc Oxide Nanoparticles as Matrix for MALDI MS Tissue Imaging of Metabolites;** Chaochao Chen¹; Ken K.-C. Yeung¹; ¹University of Western Ontario, London, ON

TP 384 **Development of Sample Preparation Method to Improve Sensitivity and Reproducibility of Mass Spectrometry Imaging of Endogenous Metabolites;** Tomomi Morikawa-Ichinose¹; Yoshinori Fujimura¹; Fusa Murayama¹; Yuzo Yamazaki²; Takushi Yamamoto²; Hiroyuki Wariishi¹; Daisuke Miura^{1,3}; ¹Kyushu University, Fukuoka, Japan; ²Shimadzu corp., Kyoto, Japan; ³National Institute of Advanced Industrial Science and Technology, Ibaraki, Japan

TP 385 **MALDI Imaging of Ocular Lens Cytoskeletal Proteins;** Zhen Wang¹; Daniel J Ryan¹; Kevin L Schey¹; ¹Vanderbilt University, Nashville, TN

TP 386 **Combining Mass Spectrometry Imaging and Top-Down Proteomics to Predict Immunotherapy Response in Non-Small-Cell Lung Cancer (NSCLC) Patients;** Eline Berghmans^{1,2}; Karin Schildermans^{1,2}; Kurt Boonen^{1,2}; Patrick Pauwels³; Geert Baggerman^{1,2}; ¹Centre for Proteomics (University of Antwerp/VITO (Belgium)), Antwerpen, Belgium; ²Unit Environmental Risk & Health, VITO, Mol, Belgium; ³Department of Pathology, Antwerp University Hospital, Edegem, Belgium

TP 387 **Biomarker Discovery for Radiation-Induced Lung Injury by Matrix Assisted Laser Desorption/Ionization-Mass Spectrometry Imaging (MALDI-MSI) Using Formalin-Fixed Paraffin-Embedded Tissues;** Ning Pan Bernhardt¹; Maureen A Kane¹; ¹University of Maryland Baltimore School of Pharmacy, Baltimore, MD

IMAGING MS: SMALL MOLECULES
388-407

TP 388 **Spatial Lipidomics Reveals Altered Lipid Profiles in Glomeruli of Human Diabetic Kidney;** Guanshi Zhang^{1,2}; Dušan Veličković³; Viktor Drel^{1,2}; Sanjay Jain⁴; Shweta Bansal^{1,2}; Manjeri A. Venkatachalam¹; Hongping Ye¹; Madesh Muniswamy¹; Xianlin Han¹; Ljiljana Paša-Tolić³; Theodore Alexandrov^{5,6}; Christopher Anderton³; Kumar Sharma^{1,2}; ¹University of Texas Health-San Antonio, San Antonio, TX; ²South Texas Veterans Health Care System, San Antonio, TX; ³Pacific Northwest National Laboratory, Richland, WA; ⁴Washington University, St. Louis, MO; ⁵European Molecular Biology Laboratory, Heidelberg, Germany; ⁶University of California San Diego, La Jolla, CA

TP 389 **Development of Bimetallic Nanoparticles for Surface-Assisted Laser Desorption/Ionisation Mass Spectrometry Imaging of Small Molecules;** Alexandre Verdin¹; Cédric Malherbe¹; Virginie Bertrand¹; Edwin De Pauw¹; Gauthier Eppe¹; ¹University of Liege, MS Lab - GIGA, MolSys Research Unit, Liege, Belgium

TP 390 **A Combination of Unroofing and Chemical Fixation Enable TOF-SIMS to Observe the Intracellular Fatty Acid Distribution;** Makoto Horikawa^{1,2}; Shiro Take³; Chi Zhang¹; Setou Mitsutoshi^{1,2}; ¹Department of Cellular & Molecular Anatomy, Hamamatsu University School of Medicine, Hamamatsu, Japan; ²International Mass Imaging Center, Hamamatsu University School of Medicine, Hamamatsu, Japan; ³Department of Environmental Biology, College of Bioscience and Biotechnology, Chubu University, Kasugai, Japan

TP 391 **Subcellular Imaging of Cardiolipin and Phosphatidylethanolamine Using GCIB-ToF-SIMS;** Lj. Sparvero^{1,2}; Hua Tian³; Andrew Amosco^{1,2}; Simon Watkins⁴; Nicholas Winograd³; Valerian Kagan^{1,2,5,6}; Hülya Bayır^{1,2,7}; ¹University of Pittsburgh -- EOH Department, Pittsburgh, PA; ²Center for Free Radical and Antioxidant Health, Pittsburgh, PA; ³Pennsylvania State University -- Chemistry Department, University Park, PA; ⁴University of Pittsburgh -- Departments of Cell Biology and Immunology, Pittsburgh, PA; ⁵University of Pittsburgh, Departments of Chemistry, Pharmacology and Chemical Biology, Radiation Oncology, Pittsburgh, PA; ⁶Lab of Navigational Redox Lipidomics, IM Sechenov Moscow State Medical University, Moscow, Russia; ⁷University of Pittsburgh -- Department of Critical Care Medicine and Safar Center for Resuscitation Research, Pittsburgh, PA

TP 392 **High Speed, High Lateral Resolution Lipid Imaging in a MALDI-Q-TOF;** Janina Oetjen¹; Arne Fuetterer¹; Juergen Suetering¹; Niels Goedecke¹; Sören-Oliver Deininger¹; Lucy Woods¹; Oliver Raether¹; Jens Hoehndorf¹; Shannon Cornett²; Jens Fuchser¹; Nikolas Kessler¹; Heiko Neuweget¹; Alice Ly¹; ¹Bruker Daltonik GmbH, Bremen, Germany; ²Bruker Daltonics Inc., Billerica, MA

TP 393 **Embryo Transfer Change the Spatiotemporal Lipid Signaling during the Early Stage Embryogenesis;** Stefania Gitta¹; Janos Schmidt¹; Laszlo Mark¹; ¹Institute of Biochemistry and Medical Chemistry, University of Pecs, Pecs, Hungary

TP 394 **Mapping Lipids in Whole-Body Zebrafish Sections Using IR-MALDESI;** Whitney L Stutts¹; Megan M Knuth¹; Måns Ekelöf¹; Debabrata Mahapatra¹; Seth W Kullman¹; David C Muddiman¹; ¹North Carolina State University, Raleigh, NC

TP 395 **Analysis of Cuttlefish Skin Chromatophores Using a Combination of High Resolution 3D-LDI-MS-Imaging and LC-UV-MS;** Jakob Meier-Credo^{1,2}; Jessica S. Eberle²; Marcel A. Lauterbach²; Sam Reiter²; Gilles Laurent²; Julian D. Langer^{1,2}; ¹MPI for Biophysics, Frankfurt am Main, Germany; ²Max Planck Institute for Brain Research, Frankfurt am Main, Germany



- TP 396 **Spatial Distribution of Endogenous Molecules in Coffee Bean by Atmospheric Pressure Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry Imaging;** Honggang Nie¹; Chenglong Dong²; Yehua Han²; Huwei Liu¹; ¹Beijing National Laboratory for Molecular Sciences, Peking University, Beijing, China; ²State Key Laboratory of Heavy Oil Processing, China University of Petroleum, Beijing, China
- TP 397 **Mass Spectrometry Imaging of Dichloroacetate for Evaluating the Effects of Thermoembolization *in-vivo* with CT Correlation;** Dodge Baluya¹; Chunxiao Guo¹; Elizabeth Whitley¹; Erik Cressman¹; ¹UT MD Anderson, Houston, TX
- TP 398 **MALDI Imaging of Anti Tuberculosis Drugs with High Mass and Spatial Resolution in Mouse Model Tissue;** Axel Treu¹; Julia Kokesch-Himmelreich¹; Kerstin Walter²; Christoph Hölscher²; Andreas Römpf¹; ¹University of Bayreuth, Bayreuth, Germany; ²Research Center Borstel, Borstel, Germany
- TP 399 **Multimodal Analysis through Mass Spectrometry Imaging and Multi-energy Tomography Using Cesium as an Integrative Marker;** Dodge Baluya¹; Emily A. Thompson¹; Megan C. Jacobsen¹; Rick R. Layman¹; Elizabeth Whitley¹; Erik Cressman¹; ¹MD Anderson Cancer Center, Houston, TX
- TP 400 **High-Resolution Nano-DESI Mass Spectrometry Imaging for Skeletal Muscle Fiber Analysis;** Daisy M Unsihuay Vila¹; Feng Yue²; Jiamin Qiu²; Shihuan Kuang²; Ruichuan Yin¹; Julia Laskin¹; ¹Department of Chemistry, Purdue University, West Lafayette, IN 47907; ²Department of Animal Sciences, Purdue University, 901W State Street, West Lafayette, IN
- TP 401 **Quantitative Mass Spectrometry Imaging of Eicosanoids Provides Novel Biological Insights into Premature Birth;** Kyle D. Duncan¹; Wenbo Deng²; Xiaofei Sun²; Lisa M. Bramer³; Bobbie-jo M. Webb-robertson³; Jennifer Kyle³; Erin S. Baker⁴; Kristin E. Burnum-Johnson³; Sudhansu K. Dey²; Ingela Lanekoff¹; ¹Uppsala University, Uppsala, Sweden; ²Division of Reproductive Sciences, Cincinnati Children's Hospital Medical Center, Cincinnati, OH; ³Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA; ⁴Department of Chemistry, North Carolina State University, Raleigh, NC
- TP 402 **Quantitative Imaging Mass Spectrometry of Endogenous Metabolites Using In-Line Internal Standards and Stable Isotope Labeled Mimetic Model;** Bindesh Shrestha¹; Khaja Muneeruddin²; Scott A Shaffer²; ¹Waters Corp., Beverly, MA; ²University of Massachusetts Medical School, Worcester, MA
- TP 403 **MALDI Imaging Mass Spectrometry as a Tool to Evaluate Levels of ATP and its Metabolites in Mouse Tumor Models;** Stephanie Dale¹; Cristine Quiason-Huynh²; ¹Genentech, South San Francisco, CA; ²Genentech, Inc., South San Francisco, CA
- TP 404 **Prospect of Using Small Molecules Based High-resolution DESI-QTOF-MS Imaging as a Direct Analysis Method of Classifying CNS Tumors in Diagnostics;** Lei Wang¹; Xu Ma¹; Chunyan Lan^{1,2}; Hainan Li³; Linbo Cai³; Xiaofei Jia⁴; Huiqin Zhong⁴; ¹National Center for Human Genetic Resources, National Research Institute for Health and Family Planning, Beijing, China; ²Peking Union Medical College Graduate School, Beijing, China; ³Guang Dong San Jiu Brain Hospital, Guangzhou, China; ⁴Waters Technologies (Shanghai) Co., Ltd, Shanghai, China
- TP 405 **Visualization of the Distribution of Small Molecule in Pig-to-Nonhuman Primate Islet Xenotransplantation Model by MALDI-MRMS Imaging;** Jong Bok Seo¹; Eui-Gil Jung¹; Hee-Jung Kim¹; Shin Kwon Kang²; JinNyoung Choi²; ¹Korea Basic Science Institute, Seoul, South Korea; ²Bruker Korea Co., Ltd, Seongnam-si, South Korea
- TP 406 **Imaging of Neurotransmitters Using AuNPs with Laser-Desorption Ionization Mass Spectrometry;** Nolan K McLaughlin¹; Kate Stumpo¹; ¹University of Scranton, Scranton, PA
- TP 407 **Rearrangement of TMS and t-BDMS of Halogenated Saturated Aliphatic Alcohols in EI Mass Spectra;** Quan-long Pu¹; Yufang Zheng¹; Stephen Stein¹; ¹NIST, Gaithersburg, MD

IMAGING MS: SOFTWARE 408-415

- TP 408 **Next-Generation Software for Visualization and Computational Analysis of High-performance Ion Mobility Molecular Imaging Data;** Lukasz Migas¹; Jeffrey M. Spraggins^{2,3}; Richard M. Caprioli^{2,3}; Perdita E. Barran^{4,5}; Raf Van de Plas^{1,3}; ¹Delft University of Technology, Delft, Netherlands; ²Vanderbilt University, Nashville, TN; ³Vanderbilt Mass Spectrometry Research Center and Department of Biochemistry, Nashville, TN; ⁴University of Manchester, Manchester, United Kingdom; ⁵Manchester Institute of Biotechnology, University of Manchester, United Kingdom
- TP 409 **Automatic Molecular Annotation of Mass Spectrometry Imaging Data;** Jan H. Kobarg¹; Nikolas Kessler²; Wiebke Timm²; Janina Oetjen²; Klaus Steinhorst¹; Stefan Schiffler¹; Shannon Cornett³; Aiko Barsch²; Heiko Neuweger²; Alice Ly²; Dennis Trede¹; ¹SCiLS, Bremen, Germany; ²Bruker Daltonik GmbH, Bremen, Germany; ³Bruker Daltonics Inc., Billerica, MA
- TP 410 **Artificial Intelligence to Support Mass Spectrometry Imaging Analysis in Drug Discovery;** Ait-Belkacem Rima¹; Fabien Pamelard¹; Lauranne Poncelet¹; Beuque Manon¹; Gael Picard de Muller¹; David Bonnel¹; Jonathan Stauber²; ¹Imabiotech, Loos, France; ²ImaBiotech Corp, Boston, MA01821
- TP 411 **R/Python Application Programming Interface for MSI Statistical Analysis: Tumor Micro Environment Case Study;** Rima Ait-Belkacem¹; Fabien Pamelard¹; Gael Picard de Muller¹; Lauranne Poncelet¹; David Bonnel¹; Jonathan Stauber²; ¹Imabiotech, Loos, France; ²ImaBiotech Corp, Boston, MA01821
- TP 412 **Reliable and Common Quantitative Color Scale to Evaluate at the Same Time Different Molecular Images in QMSI;** Rima Ait-Belkacem¹; Fabien Pamelard¹; Jordan Lerach²; Raphael Legouffe¹; David Bonnel¹; Jonathan Stauber²; ¹Imabiotech, Loos, France; ²ImaBiotech Corp, Boston, MA01821
- TP 413 **Longitudinal Quality Study of MSI PLatform for Pre-Clinical and Clinical Studies;** Rima Ait-Belkacem¹; Fabien Pamelard¹; Gael Picard de Muller¹; Lauranne Poncelet¹; David Bonnel¹; Jonathan Stauber²; ¹Imabiotech, Loos, France; ²ImaBiotech Corp, Boston, MA01821
- TP 414 **A Proposed Software Method of Automatic Tissue Region Selection for Mass-Spectrometry Imaging Acquisition and Data Analysis;** Lei Wang¹; Chunyan Lan^{1,2}; Xu Ma¹; ¹National Center for Human Genetic Resources, National Research Institute for Health and Family Planning, Beijing, China; ²Peking Union Medical College Graduate School, Beijing, China
- TP 415 **"Data Station One": An Open Source, Modular Platform for Custom Imaging Mass Spectrometer Systems;** Matthew Brantley¹; Touradj Solouki¹; ¹Baylor University, Waco, TX



INFORMATICS: MULTIOMICS INTEGRATION

416-440

- TP 416 **Mass-Spectrometry-Based Omics Technology to Reveal the Effect of Herbal Decoction in Cultured Osteoblasts;** Kwan Kin Leung¹; Wong Tin Yan²; Yu Xiao Dan¹; Leung Ka Wing¹; Dong Tina Tingxia¹; Lam Henry Hei Ning²; Tsim Karl Wah Keung¹; ¹Division of Life Science, Center for Chinese Medicine, Hong Kong university of science and technology, Sai Kung, China; ²Department of Chemical & Biological Engineering, Hong Kong university of science and technology, Sai Kung, China
- TP 417 **LC-MS Based Multi-Omics Study on the Impact of Cysteine Feed on CHO Bioprocess mAb Titer, Specific Productivity and Product Quality;** Amr S Ali^{1,2}; Alan Gilbert¹; Rashmi Kshirsagar¹; Alexander R Ivanov²; Li Zang¹; Barry L Karger²; ¹Biogen, Cambridge, MA; ²Northeastern University, Boston, MA
- TP 418 **Global High Resolution Mapping of Organellar Proteomic and Transcriptomic Correlation Profiles;** Mohamed A.W. Elzek¹; Eneko Villanueva¹; Tom S Smith¹; Rayner Queiroz¹; Kathryn Lilley¹; ¹University of Cambridge, Cambridge, United Kingdom
- TP 419 **MMCA: A Web-Based Server for Microbiome and Metabolome Correlation Analysis;** Yan Ni¹; Mingming Su²; Yongqiong Deng³; Tianlu Chen⁴; Xiaojiao Zheng⁴; Wei Jia⁵; ¹The Children's Hospital, Zhejiang University School of Medicine, Hangzhou, China; ²Metabo-Profile biotechnology, Shanghai Co., Ltd., Shanghai, China; ³Department of dermatology & STD, the Affiliated Hospital of Southwest Medical University, Luzhou, China; ⁴Shanghai Jiao Tong University Affiliated Sixth People's Hospital, Shanghai, China; ⁵University of Hawaii Cancer Center, Honolulu, Hawaii
- TP 420 **Development of a Fast Open Source Proteogenomics Pipeline – ProteoAnnotator2;** Da Qi¹; Andrew R. Jones²; Jeyan Thiyaalingam²; Fawaz Ghali³; ¹BGI-Shenzhen, Shenzhen, China; ²University of Liverpool, Liverpool, United Kingdom; ³Manchester Metropolitan University, Manchester, United Kingdom
- TP 421 **Multi-omic Dissection of Oncogenically Active Epiproteomes Identifies Drivers of Invasive Breast Tumors;** John A Wrobel¹; Ling Xie¹; Li Wang¹; Jian Jin²; Xian Chen¹; ¹University of North Carolina, Chapel Hill, NC; ²Icahn School of Medicine at Mount Sinai, New York, NY
- TP 422 **PROTEOFORMER: Novel Developments in the Ribosome Profiling-Assisted Proteogenomic Hunt for New Proteoforms;** Steven Verbruggen¹; Wim Van Criekinge¹; Siegfried Gessulat²; Bernhard Kuster²; Mathias Wilhelm²; Petra Van Damme^{3,4}; Gerben Menschaert¹; ¹Ghent University, BioBix, Lab of Bioinformatics and Computational Genomics, Department of Mathematical Modelling, Statistics and Bioinformatics, Ghent, Belgium; ²Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; ³Department of Biochemistry, Faculty of Health Sciences, Ghent University, Ghent, Belgium, Ghent, Belgium; ⁴VIB-UGent Center for Medical Biotechnology, Ghent, Belgium, Ghent, Belgium
- TP 423 **A Mass Spectrometry Approach to Investigate the Role of EZH2 in Chromatin Remodeling, Cell Proliferation and Tumorigenesis;** Miranda L. Gardner¹; Michael A. Freitas¹; ¹The Ohio State University, Columbus, OH
- TP 424 **Omni-MS: A Method for Concurrent LC-MS Analysis of Electrolytes, Small Molecules, Lipids, Proteins, Nucleic Acids, and Polysaccharides;** Austin Quach¹; Brett Lomenick¹; Alex J. Yoon¹; Whitaker Cohn¹; Julian P. Whitelegge¹; Kym F. Faulk¹; ¹University of California Los Angeles, Los Angeles, CA
- TP 425 **Phosphoproteomics Data Combined with Transcriptomics and Epigenomics Helps to Identify New Drug Targets against Methotrexate Resistance of Colon Cancer;** Alexander Kel¹; Philip Stegmaier¹; Olga Kel-Margoulis¹; ¹geneXplain GmbH, Wolfenbuettel, Germany
- TP 426 **Integrative Personalized Omics Profiling in Response to Acute Exercise in Healthy and Prediabetic Individuals;** Kevin Contrepois¹; Kegan Moneghetti²; Si Wu²; Sara Ahadi²; Daniel Hornburg²; Eric Wey²; Ming-Shian Tsai²; Jeffrey W Christle²; Francois Haddad²; Michael Snyder²; ¹Stanford University, Stanford; ²Stanford University, Palo Alto, CA
- TP 427 **An Integrated Experimental and Computational Approach for the Characterization of Proteins of Unknown Function (PUFs) in *Clostridium thermocellum* DSM 1313;** Suresh Poudel¹; Alex Cope^{1,2}; Kaela O'Dell^{1,3}; Adam M Guss²; Robert L. Hettich^{2,4}; ¹University of Tennessee, Knoxville, TN; ²Oak Ridge National Laboratory, Oak Ridge, TN; ³Oak Ridge National Laboratory, Oak Ridge, Tennessee; ⁴University of Tennessee, Knoxville, TN
- TP 428 **Conotoxin Exploitation from *Conus betulinus* Using an Integrated Approach of Transcriptomic and Peptidomics;** He yanbin¹; Lin zhilong¹; Luo Xing¹; Ren zhe¹; Roy Bhaskar¹; Qi Da¹; Liu Siqi¹; ¹BGI-Shenzhen, Shenzhen, China
- TP 429 **Meta-analysis of Public Proteomics Datasets Supports the Evaluation of Cancer Cell Lines as Tumour Models and Improves Drug Sensitivity Prediction;** Andrew F. Jarnuczak¹; Hanna Najgebauer¹; Mitra P Barzine¹; Deepti Jaiswal Kundu¹; Fatemeh Zamanzad Ghavidel²; Yasset Perez-Riverol¹; Irene Papatheodorou¹; Alvis Brazma¹; Juan Antonio Vizcaíno¹; ¹EMBL-EBI, Cambridge, United Kingdom; ²University of Bergen, Bergen, Norway
- TP 430 **DeepRibo: Precise Gene Annotation of Prokaryotes Using Deep Learning and Ribosome Profiling Data, Validated with Mass Spectrometry Data;** Jim Clauwaert¹; Gerben Menschaert²; Willem Waegeman¹; ¹KERMIT, Department of Data Analysis and Mathematical Modelling, Ghent University, Ghent, Belgium; ²BioBix, Lab of Bioinformatics and Computational Genomics, Department of Mathematical Modelling, Statistics and Bioinformatics, Ghent, Belgium
- TP 431 **Proteogenomics Pipeline for Discovery of Genetically Variable Peptides in Humans;** Myles W. Gardner¹; August E. Woerner²; Michael A. Freitas³; Nicolette C. Albright¹; Alan R. Smith¹; F. Curtis Hewitt¹; ¹Signature Science, LLC, Austin, TX; ²Center for Human Identification, University of North Texas Health Science Center, Fort Worth, TX; ³The Ohio State University, Columbus, OH
- TP 432 **A Multi-Omics Approach to Linking Proteomic Profiles and Metabolomic Phenotypes Provides Insight into Colorectal Cancer Cell Metabolism;** Peter Doubleday¹; Ioanna Ntai²; Luca Fornelli³; Emily Boja⁴; Henry Rodriguez⁴; Neil L Kelleher¹; ¹Northwestern University, Evanston; ²Thermo Fisher Scientific, San Jose, CA; ³The University of Oklahoma, Norman, OK; ⁴Office of Cancer Clinical Proteomics Research, NIH, Bethesda, MD
- TP 433 **Non-Ribosomal Peptide Antibiotic Discovery in Microbial Communities via Integration of Computational Metagenomics and Mass Spectrometry;** Bahar Behsaz¹; Alexey Gurevich²; Rob Knight³; Pieter Dorrestein¹; Pavel A. Pevzner³; Hosein Mohimani⁴; ¹University of California San Diego, La Jolla, CA; ²St. Petersburg State University, St. Petersburg, Russia; ³University of California, San Diego, La Jolla, CA; ⁴Carnegie Mellon University, Pittsburgh, PA
- TP 434 **Evaluating Machine Learning Methods Capable of Handling Missing Values for Protein Biomarker Studies;** David Nusinow¹; John Szpyt¹; Steven P Gygi¹; ¹Harvard Medical School, Boston, MA



- TP 435 **imetaQuantome Workflow: An Integrated Metaproteomics Workflow for Interactive, Statistical and Functional Microbiome Analysis**; [Subina Mehta](#)¹; Ray Sajulga¹; Caleb W Easterly¹; Francesco Delogu²; Benoit J Kunath²; Praveen Kumar¹; Marie Crane³; Emma Leith¹; James E. Johnson¹; Thomas McGowan¹; Joel Rudney¹; Phil B Pope²; Magnus Ø Arntzen²; Timothy J. Griffin¹; Pratik D Jagtap¹; ¹University of Minnesota, Minneapolis, MN; ²NMBU - Norwegian University of Life Sciences, Ås, Norway; ³Macalester College, Saint Paul, MN
- TP 436 **Integration of Metabolomic and Lipidomic Workflows for Studying Clinical and Biological Systems**; Adriana Zardini Buzatto¹; Shuang Zhao¹; Ulrike Schweiger Hufnagel²; Aiko Barsch²; [Liang Li](#)¹; ¹University of Alberta, Edmonton, AB; ²Bruker Daltonik GmbH, Bremen, Germany
- TP 437 **pmartR: Software for Quality Control and Statistics Robust to Missing Data for Mass Spectrometry-Based Biological Data**; [Lisa Bramer](#)¹; Kelly G. Stratton¹; Bobbiejo M. Webb-robertson¹; Lee Ann McCue¹; Bryan Stanfill¹; Daniel Claborne¹; Allison M. Thompson¹; Iobani Godinez¹; ¹Pacific Northwest National Laboratory, Richland, WA
- TP 438 **Metaproteomics Powered By Metatranscriptomics: Towards a Multi-Omic Functional Microbiome Analysis**; [Pratik Dilip Jagtap](#)¹; Praveen Kumar¹; Francesco Delogu²; Benoit J Kunath²; Sujun Li³; Marie Crane⁴; Subina Mehta¹; Ray Sajulga¹; Emma Leith¹; James E. Johnson⁵; Yuzhen Ye³; Berenice Batut⁶; Haixu Tang³; Phil B Pope²; Magnus Ø Arntzen²; Timothy Griffin¹; ¹University of Minnesota, Minneapolis, MN; ²Faculty of Chemistry, Biotechnology and Food Science, NMBU, Ås, Norway; ³School of Informatics, Computing, and Engineering, Indiana University, Bloomington, IN; ⁴Macalester College, Saint Paul, MN; ⁵Minnesota Supercomputing Institute, University of Minnesota, Minneapolis, MN; ⁶Bioinformatics Group, University of Freiburg, Freiburg, Germany
- TP 439 **Integrated Omics Analysis Across 32 Human Tissues**; [Lihua Jiang](#)¹; Meng Wang²; Shin Lin³; Ruiqi Jian²; Joanne Chan²; Xiao Li²; Huaying Fang²; Hua Tang²; Michael Snyder²; ¹Stanford University, Stanford, CA; ²Stanford University, Palo Alto, CA; ³University of Washington, Seattle, WA
- TP 440 **SysMet: A Tool for Integrative Systems Metabolomics**; Mohammad R Nezami Ranjbar¹; Ziling Fan¹; Yan Gao¹; [Habtom W Resson](#)¹; ¹OmicsCraft LLC, Washington, DC
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- TP 441 **A Mini Quadrupole Mass Spectrometer with a Continuous Atmospheric Pressure Interface**; [Ranran Liu](#); ¹Institute of Atmospheric Physics, Chinese Academy of Sciences, Beijing, China
- TP 442 **MOMA Mass Spectrometer Laser Desorption Ionization Investigation of Spiked Mineral Samples for ExoMars Mission Planning**; [Friso h.w. Van amerom](#)¹; Marco Castillo²; Xiang Li²; Ryan Danell³; Desmond Kaplan⁴; Eric I. Lyness⁵; Stephanie A. Getty⁶; Andrej Grubisic⁶; William B. Brinckerhoff⁶; Paul R. Mahaffy⁶; ¹Mini-Mass Consulting, Inc, Hyattsville, MD; ²University of Maryland, Baltimore, MD; ³Danell Consulting, Inc., Winterville, NC; ⁴Kapscience, LLC, Tewksbury, MA; ⁵Microtel-LLC, Greenbelt, MD; ⁶NASA Goddard Space Flight Center, Greenbelt, MD
- TP 443 **Development of the Advanced Resolution Organic Molecular Analyzer (AROMA)**; [Adrian Southard](#)¹; Emanuel Hernandez²; Ryan Danell³; Cynthia Gundersen⁴; Lars Hovmand⁵; Andrej Grubisic²; Ricardo Arevalo⁶; ¹Universities Space Research Association, Greenbelt, MD; ²NASA Goddard Space Flight Center, Greenbelt, MD; ³Danell Consulting, Inc., Winterville, NC; ⁴ADNET System, Inc., Bethesda, MD; ⁵Linear labs, Washington, DC; ⁶University of Maryland, College Park, MD
- TP 444 **Calibration Drift and Maintaining Requirements in Harsh Environmental Conditions with the Mars Organic Molecule Analyzer (MOMA) Mass Spectrometer**; [Ryan M. Danell](#)¹; Andrej Grubisic²; Veronica Pinnick²; Desmond A. Kaplan³; Friso Van Amerom⁴; Stephanie A. Getty²; William B. Brinckerhoff²; ¹Danell Consulting, Inc., Winterville, NC; ²NASA Goddard Space Flight Center, Greenbelt, MD; ³KapScience LLC, Tewksbury, MA; ⁴Mini-Mass Consulting, Inc, Hyattsville, MD
- TP 445 **A Handheld Mass Spectrometer for In-Field and POC Analysis**; [Bin Jiao](#)¹; Xinwei Liu¹; Jiexun Bu²; Ningxi Li¹; Zheng Ouyang¹; ¹State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instrument, Tsinghua University, Beijing, China; ²PURSPEC Technologies Inc., Beijing, China
- TP 446 **Development of a Miniature GC-MS Instrument for Fieldable Applications**; [Vladimir M. Doroshenko](#)¹; Victor Laiko¹; Eugene Moskovets¹; Konstantin Novoselov¹; Tzu-Hsuan Chang²; Daniel Struk²; Jean-Marie D. Dimandja²; Milad Navaei²; Peter J. Hesketh²; ¹MassTech, Inc., Columbia, MD; ²Georgia Institute of Technology, Atlanta, GA
- TP 447 **3D Real Time Monitoring of Unintended Concentration of H2/Air in FCV Applications**; [Takashi Nohmi](#)^{1,2}; Toshio Mogi²; ¹HysafeNohmi, Setagaya-Ku, Japan; ²The University of Tokyo, Bunkyo, Japan
- TP 448 **The Development of Miniature MALDI Digital Ion Trap Mass Spectrometer**; Kosuke Hosoi¹; Masaji Furuta¹; Hideharu Shichi¹; Shosei Yamauchi¹; Kiyoshi Watanabe¹; Makoto Hazama¹; Kei Kodera¹; [Shinichi Iwamoto](#)¹; Koichi Tanaka¹; ¹Shimadzu Corporation, Kyoto, Japan
- TP 449 **The Effects of Electrode Misalignment on the Performance of a Linear Wire Ion Trap**; [Radhya W. Gamage](#)¹; Daniel E. Austin¹; ¹Brigham Young University, Provo, UT
- TP 450 **Profiling Agrochemical Residues in Produce via Paper Cone Spray Ionization and Portable Instrumentation**; [Alyssa J. Gasa](#)¹; Makoy R. Overfelt¹; Christopher Mulligan²; ¹Illinois state university, Normal, IL; ²Illinois State University, Normal, IL
- TP 451 **Method to Improve the Higher Pressure Operation Characteristics of Microchannel Plate Detectors, and Its Effect on Performance of Miniature MS**; [Masahiro Hayashi](#); ¹Hamamatsu Photonics K.K., Iwata, Japan
- TP 452 **Microscale Linear Ion Trap Mass Spectrometer**; Trevor Decker¹; Yajun Zheng²; Aaron Ruben¹; Xiao Wang³; Stephen Lammert³; Aaron Hawkins¹; [Daniel Austin](#)¹; ¹Brigham Young University, Provo, UT; ²Xi'an Shiyou University, Xi'an, China; ³PerkinElmer Health Sciences Inc., American Fork, UT
- TP 453 **Development of a Flexible GC Transfer Line for a Field-Deployable GC-EI/MS**; [Steffen Bräkling](#)¹; Kai Kroll¹; Hendrik Kersten¹; Thorsten Benter¹; ¹University of Wuppertal, Wuppertal, Germany
- TP 454 **Development of Micro-Time-of-Flight Mass Spectrometer for in situ Gas Analysis**; [Alex Sonnette](#)¹; Frederic Progent²; Jerome Tupinier²; Pierre-Etienne Buthier²; Jean-Christophe Lictévout²; Sébastien Vigne²; Thomas Alava³; ¹CEA, Arpajon, France; ²CEA, Arpajon, France; ³CEA, Grenoble, France
- TP 455 **A Mixed Computational Fluid Dynamics and Direct Simulation Monte Carlo model of the Intermediate Pressure Regions of a Miniature ESI-MS**; [Edward Crichton](#)¹; Rantej S Kler¹; Richard W Moseley¹; ¹Microsaic Systems, Woking, United Kingdom
- TP 456 **Evaluation of a Portable GC-MS Equipped with a Planar-LTM Column for Chemical and Riot Control Agent Screening Applications**; [Zachary E Lawton](#)¹; Thomas Saul²; Evan Durnal³; Sara Paalhar³; Becky Stille³; Nathan



- TP 457 **Doll³; ¹PerkinElmer, Shelton, CT; ²Smiths Detection, Edgewood, MD; ³MRIGlobal, Kansas City, MO**
Fieldable Atmospheric Pressure Ion Mobility Linear Ion Trap Mass Spectrometer for On-site Chemical Identification; Greg Brabeck¹; Mark Osgood¹; Tomás F Gutierrez¹; Eugenie Hainsworth¹; Marina Loginowski¹; Ching Wu¹; ¹Excellims Corporation, Acton, Massachusetts
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- TP 459 **Development of Lead-Free Channel Electron Multiplier Named CERARION that Achieves Over 100 uA DC Output; Takeshi Endo¹; Hiroshi Kobayashi¹; Kengo Watase¹; hayato inoue¹; ¹HAMAMATSU PHOTONICS K.K., Iwata, Japan**
- TP 460 **Peak Amplitude vs. Peak Area: Which Better Measures Charge in CDMS?; Jiuzhi Gao¹; Daniel E. Austin¹; ¹Brigham Young University, Provo, UT**
- TP 461 **Deconvolution of Complex Protein Mixtures Using Orbitrap-Based Charge Detection Mass Spectrometry; Jared O. Kafader¹; Rafael D. Melani¹; Bryan P. Early¹; Kenneth R. Durbin¹; Benjamin Soye¹; Mike W. Senko²; Vlad Zambouskov²; Alexander A Makarov³; Joshua T. Maze⁴; Deven L. Shinholt⁴; Steven Beu⁵; Neil L Kelleher¹; Philip D. Compton¹; ¹Northwestern University, Evanston, IL; ²Thermo Fisher Scientific, San Jose, CA; ³Thermo Fisher Scientific, Bremen, Germany; ⁴Thermo Fisher Scientific, Austin, TX; ⁵S.C. Beu Consulting, Austin, TX**
- TP 462 **Development of an α -particle and TOF Ion Detector for Precise Measurements of Atomic Mass of Superheavy Nuclei; Toby Shanley¹; Wayne Sheils¹; Michiharu Wada²; Toshitaka Niwase^{2,3}; Yair Benari¹; Hermann Wollnik⁴; Peter Schury²; ¹ETP Ion Detect, Sydney, Australia; ²KEK, High Energy Research Accelerator Organisation, Hirasawa, Japan; ³Kyushu University, Fukuoka, Japan; ⁴New Mexico State University, Las Cruces, NM**
- TP 463 **Sub-Nanosecond, Stable and Long-Lifetime Detector for TOF Applications; Jonathan Garel¹; Semyon Shofman¹; Amit Weingarten¹; Sasha kadyshkevitch¹; Eli Cheifetz¹; ¹El-Mul Technologies, Rehovot, Israel**
- TP 464 **Negative Electron Affinity Material for Increased Ion Detection Sensitivity in Electron Multipliers; Toby Shanley¹; Wayne Sheils¹; ¹ETP Ion Detect, Sydney, Australia**
- TP 465 **Paper Spray Ionization Mass Spectrometry of Sebum Samples: A Step Towards Rapid, Early Diagnosis of Parkinson's Disease; Debanjan Sarkar¹; Drupad Trivedi¹; Caitlin Walton-Doyle¹; Joy Milne¹; Eleanor Sinclair¹; Monty Silverdale¹; Perdita Barran¹; ¹University of Manchester, Manchester, United Kingdom**
- TP 466 **Charge-Sensing Particle Detector (CSPD): A Sensitivity-Enhanced Faraday Cup; Szu-Wei Chou¹; Yi-Kun Lee²; Yi-Teng Hsiao²; Liang-Chun Fan²; Chun-Yen Cheng²; ¹AcroMass technologies, Inc., Taipei, Taiwan; ²AcroMass Technologies, Inc., Hsinchu, Taiwan**
- TP 467 **Enhanced Charge Detection Mass Spectrometry Precision with a Low-Noise Amplifier Without a Feedback Resistor; Aaron R Todd¹; Andrew W Alexander¹; Martin F Jarrold¹; ¹Indiana University, Bloomington, IN**
- TP 468 **Tantalum-Based Superconducting Tunnel Junction Cryodetection Mass Spectrometry; Logan Plath¹; Mohammad A. Halim¹; Stephan Friedrich²; Francisco Ponce³; Jack Harris⁴; Robin Cantor⁵; Mark E. Bier¹; ¹Carnegie Mellon University, Pittsburgh, PA; ²Lawrence Livermore National Laboratory, Livermore, CA; ³Stanford University, Palo Alto, CA; ⁴XIA LLC, Hayward, CA; ⁵STAR Cryoelectronics, Santa Fe, NM**
- TP 469 **Atomic Layer Coating Enabled Performance Improvements of Channel Electron Multipliers (CEM); Matthew Breuer¹; Paula Holmes, Dr. ¹; ¹Photonis USA, Sturbridge, MA**
- TP 470 **Multiplexing in Charge Detection Mass Spectrometry: Rapid Measurement of Large Native Proteins and Macromolecular Complexes; Conner C Harper¹; Andrew G. Elliott¹; Evan R. Williams¹; ¹University of California, Berkeley, Berkeley, CA**
- TP 471 **Generation of Electrospayed Ions for Fundamental Studies Using a Linear Ion Trap Coupled to a Superconducting Tunnel Junction Cryodetector; Mohammad Abdul Halim¹; Logan Plath¹; Jonathan Shulgach¹; Mark E. Bier¹; ¹Carnegie Mellon University, Pittsburgh, PA**
- TP 472 **Distance-of-Flight Mass Spectrometry Using a Semiconductor Ion Detector Array; Steven Ray; ¹University at Buffalo, SUNY, Buffalo, NY**
- TP 473 **High-Pressure Solid-State Ion Detector with 10-uV/e- Gain and 180-e- Noise; Yixin Song¹; Justin Chu¹; Joan Magalhaes¹; Jacob Nowjack¹; Jace Rozsa¹; Eric Swindlehurst¹; Sanjiv Pant¹; Kent Layton^{1,2}; Steve Lammert³; Xiao Wang³; Edgar Lee³; Nathan Porter³; Milton Lee¹; Aaron Hawkins¹; Shih-hua Wood Chiang¹; ¹Brigham Young University, Provo, UT; ²ON Semiconductor, Lindon, UT; ³PerkinElmer Health Sciences Inc., American Fork, UT**
- TP 474 **Electron Ionization LC-MS with Supersonic Molecular Beams - Drug Impurities Analysis and Combination with GC-MS in One System; Svetlana Tszin¹; Tal Alon¹; Alexander B. Fialkov¹; Aviv Amirav¹; ¹Tel-Aviv University, Tel-Aviv, Israel**
- TP 475 **The Use of a Cooled Inlet System to Enable the Measurement of Negatively Charged Compounds Using CIMS; Alan T. Taylor¹; C. Logan Mackay¹; M. J. Cowley¹; N. McKeown¹; ¹University of Edinburgh, Edinburgh, United Kingdom**
- TP 476 **Development of a GC-APCI Interface for an Orbitrap MS; Joshua B Powers¹; Shawn R Campagna¹; ¹University of Tennessee, Knoxville, TN**
- TP 477 **Mechanospray Ionization (MSI) of Macromolecules Produces Lower Average Charge States and Lower Internal Energy Ions than ESI; Liam Dugan¹; Mark E. Bier¹; ¹Carnegie Mellon University, Pittsburgh, PA**
- TP 478 **Combined Atomic and Molecular (CAM) Ionization Source with an Orbitrap 1M: Elemental, Isotopic, and Molecular MS at Resolution of >1.5M; R. Kenneth Marcus¹; Edward D Hoegg²; David W Koppenaar²; Joanna Szpunar³; Simon Godin³; Ryszard Lobinski³; ¹Clemson University, Clemson, SC; ²Pacific Northwest National Laboratory, Richland, WA; ³CNRS, Institute of Analytical Sciences and Physical Chemistry for the Environment and Materials, Pau, France**
- TP 479 **Liquid Sampling – Atmospheric Pressure Glow Discharge (LS-APGD) Interfaced with a Compact (Quadrupole) Mass Spectrometer for Analysis of Diverse Samples; Tyler Williams¹; R. Kenneth Marcus¹; ¹Clemson University, Clemson, SC**
- TP 480 **Direct Analysis of Contaminants in Soil, Aqueous, and Biological Samples Using Membrane Introduction Tandem Mass Spectrometry with Liquid Electron Ionization; Gregory W. Vandergriff^{1,2}; Joseph Monaghan¹; Erik T. Krogh^{1,2,3,4}; Christopher G. Gill^{1,2,3,4}; ¹Appl. Env. Res. Labs. (AERL), Vancouver Island University, Chemistry Department, Nanaimo, BC; ²University of Victoria, Chemistry Department, Victoria, BC; ³Simon Fraser University, Chemistry Department, Burnaby, BC; ⁴University of Washington, DEOHS, Seattle, WA**



- TP 481 **Single-Cell Analysis by Mass Spectrometry Using Electro-Migration and Electroporation;** Zishuai Li¹; Zhengmao Wang^{2,3}; Xiaoxiao Ma⁴; Junmin Pan^{2,3}; Zheng Ouyang^{4,5}; ¹State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instrument, Tsinghua University, Beijing, China; ²Laboratory for Marine Biology and Biotechnology, Qingdao National Laboratory for Marine Science and Technology, Qingdao, China; ³MOE Key Laboratory of Protein Sciences, Tsinghua-Peking Center for Life Sciences, School of Life Sciences, Tsinghua University, Beijing, China; ⁴State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instruments, Tsinghua University, Beijing, China; ⁵Weldon School of Biomedical Engineering, Purdue University, West Lafayette, ILLINOIS
- TP 482 **Microfluidic Open Interface with Liquid Electron Ionization Mass Spectrometry: Rapid Measurement of THC and Other Cannabinoids in Different Matrices;** Pierangela Palma¹; Veronica Termopoli¹; Giorgio Famiglini¹; Greta Giacomelli¹; Achille Cappiello¹; Emir Nazdrajić²; Janusz Pawliszyn²; ¹University of Urbino, Urbino, Italy; ²University of Waterloo, Waterloo, ON
- TP 483 **Static Membrane Extraction Mass Spectrometry for Space Applications;** R. Timothy Short¹; Strawn K. Toler¹; Jennifer C. Stern²; Charles A. Malespin²; Brian M. Leiter³; ¹SRI International, St Petersburg, FL; ²NASA Goddard Space Flight Center, Greenbelt, MD; ³ADNET System, Inc., Bethesda, MD
- TP 484 **Simulation of Isotherm HiKE-IMS – MS Transfer Stage;** Robin Hillen¹; Walter Wissdorf¹; Maria Allers²; Hendrik Kersten¹; Stefan Zimmermann²; Thorsten Benter¹; ¹Bergische Universität Wuppertal, Wuppertal, Germany; ²Leibniz Universität Hannover, Hannover, Germany
- TP 485 **Microflow LC-Nanospray ESI-MS;** Daojing Wang¹; Pan Mao¹; Yuchao Chen¹; ¹Newomics Inc., Berkeley, CA
- TP 486 **A Novel Method for NH₄⁺ Reagent Ion Production in PTR-MS and its Applications;** Christian Lindinger¹; Eugen Hartungen¹; Rene Gutmann¹; Alfons Jordan¹; Lukas Märk¹; Philipp Sulzer¹; ¹IONICON Analytik GmbH., Innsbruck, Austria
- TP 487 **Optimized Nanoflow ESI Source to Eliminate the Need for Tuning;** Yang Kang¹; Bradley B. Schneider¹; Leigh Bedford¹; Thomas R. Covey¹; ¹SCIEX, Concord, ON
- TP 488 **High-Throughput, Low-Cost Reaction Screening Apparatus Using a Modified 3D Printer;** Robert Schrader¹; Stephen T Ayrton¹; R. Graham Cooks¹; ¹Purdue University, West Lafayette, IN
- TP 489 **Development of a Novel Tantalum Cathode for Determining Trace Elements in Soils by Glow Discharge Mass Spectrometry;** Rong Qian¹; Shangjun Zhuo¹; Jiangli Dong¹; ¹Shanghai Institute of Ceramics, Chinese Academy of Sciences, Shanghai, China
- TP 490 **Efficient Ionization of Challenging Pesticides Using Liquid Chromatography/Mass Spectrometry and Dielectric Barrier Discharge Ionization (DBDI);** Juan E Garcia-Reyes¹; Julio César Benítez-Villalba²; Miriam Beneito-Cambra¹; Bienvenida Gilbert-López¹; Antonio Molina-Díaz¹; Sebastian Brandt³; Joachim Franzke³; ¹University of Jaen, Jaen, Spain; ²Universidad Nacional de Asunción, Facultad de Ciencias Exactas y Naturales, San Lorenzo, Paraguay; ³Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Dortmund, Germany
- TP 491 **Microsampling with Cotton Threads and Direct Analysis via Ambient Mass Spectrometry;** Devin Swiner¹; Sierra Jackson¹; George R. Durisek¹; Bridget K. Walsh¹; Yaman Kouatli¹; Abraham K. Badu-Tawiah¹; ¹The Ohio State University, Columbus, OH
- TP 492 **Characterization and Development of a Reagent Cation Source for NETD;** Steven J Kregel¹; Benton J Anderson²; Michael S Westphall¹; Joshua J Coon^{1,2,3,4}; ¹Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI; ²Department of Chemistry, University of Wisconsin-Madison, Madison, WI; ³Morgridge Institute for Research, Madison, WI; ⁴Genome Center of Wisconsin, Madison, WI
- TP 493 **Resolving Elemental Isobaric Interferences with the Liquid Sampling-Atmospheric Pressure Glow Discharge / Orbitrap System for High Precision Isotope Ratio Measurements;** Edward D Hoegg^{1,2}; David W Koppelaar²; Simon Godin³; Joanna Szpunar³; Ryszard Lobinski³; R. Kenneth Marcus¹; ¹Clemson University, Clemson, SC; ²Pacific Northwest National Laboratory, Richland, WA; ³CNRS, Institute of Analytical Sciences and Physical Chemistry for the Environment and Materials, Pau, France
- TP 494 **An Integrated Electrocatalytic nESI-MS Platform for Direct Analysis of C=C Isomers in Fatty Acids Derived from Complex Biofluids;** Kavyasree Chintalapudi¹; Abraham K. Badu-Tawiah¹; ¹The Ohio State University, Columbus, OH
- TP 495 **Quantitative Analysis of Anticancer Drugs in Live Single Suspension Cells: From Cell Lines to Patient Samples;** Shawna Standke¹; Ryan Bensen¹; Devon Colby¹; Anh Le¹; Naga Rama Kothapalli¹; Jonathan E. E. Heinlen²; Anthony Burgett¹; Zhibo Yang¹; ¹University of Oklahoma, Norman, OK; ²University of Oklahoma, Health and Science Center, Oklahoma City, OK
- TP 496 **Direct Analysis of Complex Mixtures by Non-contact Nano-Electrospray Mass Spectrometry Coupled with Simultaneous Atmospheric Pressure Chemical Ionization;** Dmytro S Kulyk¹; Abraham K. Badu-Tawiah¹; ¹OSU, Columbus, OH

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- TP 497 **Probing the Conformational Adaptations of Thermoresponsive Polymers by Ion-Mobility Mass Spectrometry;** Savannah Snyder¹; Megan A Cruz²; Abraham Joy²; Chrys Wesdemiotis¹; ¹The University of Akron Chemistry Department, Akron, OH; ²The University of Akron, Akron
- TP 498 **Ergodic and Non-Ergodic Mobility Selected Fragmentation of Isomeric Model Peptides;** Noa deHaseth¹; Jacob Porter²; Francisco Fernandez-Lima²; ¹University of Florida, Gainesville, FL; ²Florida International University, Miami, FL
- TP 499 **Demonstration of the Unique Capabilities of Cyclic Ion Mobility High Resolution Mass Spectrometry to Resolve Stereoisomeric and Regioisomeric Saponin Ions;** Emmanuel Colson¹; Corentin Decroo¹; Julien De Winter¹; Dale Cooper-Shepherd²; Martin Palmer²; Jan Claereboudt²; Pascal Gerbaux¹; ¹University of Mons, Mons, Belgium; ²Waters Corporation, Cheshire, United Kingdom
- TP 500 **Comparing Solution Phase and Gas Phase Protein Stability Using Collisional Induced Unfolding;** Lucienne Nouchikian^{1,2}; Derek J Wilson^{1,2}; ¹York University, Toronto, ON; ²Center for Research in Mass Spectrometry, Toronto, Ontario
- TP 501 **Analysis of Specific Metal Binding to Alpha-Synuclein with Collisional Induced Unfolding;** Neil R. Quebbemann¹; Joseph A. Loo¹; ¹University of California Los Angeles, Los Angeles, CA
- TP 502 **Utilization of Enhanced Shape Selective Information Obtained from a Cyclic Ion Mobility-Enabled –Mass Spectrometer for the Characterisation of Complex Mixtures;** Javeria Mehboob¹; James Scrivens¹; Gillian Taylor¹; Safwan Akram¹; Martin Palmer²; Jakub Ujma²; Kevin Giles²; Jonathan P Williams²; David Portwood³; Pablo Navarro³; ¹Teesside University, Middlesbrough, United Kingdom; ²Waters Corporation, Cheshire, United Kingdom; ³Syngenta Jealott's Hill International Research Centre, Bracknell, United Kingdom



- TP 503 **Pursuit of Bottom-Up, Middle-Down, and Top-Down Glycoconjugate Analysis Enabled Through Online CE-ESI-IMS; Daniel Delafield¹**; Gongyu Li²; Lingjun Li³; ¹University of Wisconsin Madison, Madison, WI; ²University of Wisconsin - Madison, Madison, WI; ³University of Wisconsin, Madison, Madison, WI
- TP 504 **Following Conformational Changes in Knot Proteins with nESI-TIMS-MS: Solution vs Gas Phase; Jean R. N. Haler¹**; Kevin Jeanne Dit Fouque¹; Juan Camilo Molano-Arevalo¹; Fenfei Leng¹; Francisco A. Fernandez-Lima¹; ¹Florida International University, Miami, FL
- TP 505 **An Investigation into the use of Cyclic Ion Mobility for the Separation of Biopharmaceutical Peptide and Protein Modifications; Jim Langridge¹**; Henry Shion²; Martin Palmer³; Weibin chen²; Dale A Cooper-Shepherd³; ¹Waters Corporation, Wilmslow, United Kingdom; ²Waters Corporation, Milford, MA; ³Waters Corporation, Wilmslow, United Kingdom
- TP 506 **Fast Collision Induced Unfolding Coupled to Droplet Microfluidic-Based Sample Introduction for High-Throughput Protein Structural Analysis and Drug Discovery; Cara I. D'Amico¹**; Daniel A. Polasky¹; Sugyan M. Dixit¹; Robert T. Kennedy¹; Brandon T. Ruotolo¹; ¹University of Michigan, Ann Arbor, MI
- TP 507 **Structural Characterization of Carbohydrates Oligosaccharide using Tandem Trapped Ion Mobility Spectrometry–Mass Spectrometry; Jusung Lee¹**; Christian Bleiholder¹; ¹Florida State University, Tallahassee, FL
- TP 508 **Direct Identification of Endogenous Ligands Bound to Specific Protein Conformations Using Multistage Gas Phase Separation on a Cyclic-Mobility Mass Spectrometer; Idir Liko¹**; Joseph F Gault²; Martin Palmer³; Dale A Cooper-Shepherd³; Jakub Ujma³; Carol V. Robinson²; ¹OMass Therapeutics, Oxford, United Kingdom; ²Oxford University, Oxford, United Kingdom; ³Waters Corporation, Wilmslow, United Kingdom
- TP 509 **Analysis of Lipid Signaling Class Analytes Using a Travelling Wave Cyclic Ion Mobility Separator; Mike McCullagh¹**; Martin Palmer¹; Emma Marsden-Edwards¹; James I Langridge¹; Johannes PC Vissers¹; ¹Waters Corporation, Wilmslow, United Kingdom
- TP 510 **Separation of Asp/IsoAsp Isobaric Peptides Using Trapped Ion Mobility Spectrometry (TIMS); Anjali Alving¹**; Shourjo Ghose¹; Leah (Hanliu) Wang²; Olga Friese²; ¹Bruker Scientific, Billerica, MA; ²Pfizer, Chesterfield, MO
- TP 511 **Fast Identification and Simultaneous Separation of Electrochemically Generated Isomeric Xenobiotic Phase-I Metabolites by means of Trapped Ion Mobility-Mass Spectrometry; Jens Fangmeyer¹**; Simon Gereon Scheeren¹; Robin Schmid¹; Uwe Karst¹; ¹University of Muenster, Institute of Inorganic and Analytical Chemistry, Muenster, Germany
- TP 512 **All Ion Unfolding/Fragmentation (AIU/AIF): A Modified Native Ion Mobility–Mass Spectrometry (IM-MS) Approach for Diagnostic Glycoprotein Analysis; Ashley Phetsanthad¹**; Gongyu Li²; Lingjun Li^{1,2}; ¹Department of Chemistry, University of Wisconsin-Madison, Madison, WI; ²School of Pharmacy, University of Wisconsin-Madison, Madison, WI
- TP 513 **The Performance of a New Ion Mobility Spectrometer Designed to Measure Singly-charged Protein Ions; W Henry Benner¹**; Ben Aguilar¹; ¹Ion Dx, Monterey, CA
- TP 514 **Short nanoLC Gradients Optimize Throughput on a tims Equipped QTOF for Deep Proteome Measurements; Thomas Kosinski¹**; Scarlet Koch¹; Thorsten Ledertheil¹; Christian Meier-Credo¹; Christoph Gebhardt¹; Gary Kruppa²; Heiner Koch¹; ¹Bruker Daltonik GmbH, Bremen, Germany; ²Bruker Daltonics Inc., Billerica, MA
- TP 515 **A Non Targeted Approach to the Development of a Food Additive CCS Screening Library and its Application; Mike McCullagh¹**; Mike Wilson¹; Severine Goscinnny²; Kenneth Rosnack³; ¹Waters Corporation, Wilmslow, United Kingdom; ²Sciensano, Brussels, Belgium; ³Waters Corporation, Milford, MA
- TP 516 **Investigations into Cross-Platform and Long-Term Robustness of a CCS Metric; David Douce¹**; Mike McCullagh²; Michelle Wood²; Nayan Mistry²; Severine Goscinnny³; Petur Dalsgaard⁴; ¹Waters (MS Technologies), Wilmslow, United Kingdom; ²Waters Corporation, Wilmslow, United Kingdom; ³Sciensano, 14, rue Juliette Wytsman,, Belgium; ⁴Department of Forensic Medicine, University of Copenhagen,, Copenhagen, Denmark
- TP 517 **Effects of Osmolytes on Conformations of Model Proteins as Studied by IM-MS; Christopher Mallis¹**; David H. Russell¹; ¹Texas A&M University, College Station, TX
- TP 518 **Ion Mobility-Accelerated Peptide Separation in Time and Space to Unveil Human Proteomes; Yasushi Ishihama¹**; Kosuke Ogata¹; Ryo Kajita²; Heiner Koch³; Koshi Imami¹; Naoyuki Sugiyama¹; ¹Kyoto University, Kyoto, Japan; ²Bruker Japan K.K., Yokohama, Japan; ³Bruker Daltonik GmbH, Bremen, Germany
- TP 519 **“Zero Charge Selection” Ion Mobility-Mass Spectrometry Reveals the Effect of Sialylation on Glycoprotein Structures; Gongyu Li¹**; Lingjun Li²; ¹University of Wisconsin-Madison, Madison, WI; ²University of Wisconsin, Madison, Madison, WI
- ION MOBILITY: FAIMS/DMS
520-529**
- TP 520 **Simplifying uranium isotope ratio (IR) analysis with nanospray differential mobility spectrometry- mass spectrometry (DMS-MS); Ifeoluwa Ayodeji¹**; Theresa Evans-Nguyen²; ¹University of South Florida, Tampa, FL; ²University of Florida, Tampa, FL
- TP 521 **Chemical Kinetics and Ion Transport Simulations: Cluster Dynamics in Differential Ion Mobility Spectrometry; Walter Wissdorff¹**; Duygu Erdogdu¹; Florian Stappert¹; Hendrik Kersten¹; Thorsten Benter¹; ¹University of Wuppertal, Wuppertal, Germany
- TP 522 **Validated FIA-FAIMS SRM MS Approaches for Vicine and Convicine Quantification from Faba Beans and Implications for Molecular Marker Analysis; Haixia Zhang¹**; Randall W Purves¹; Rob Stonehouse¹; Pete M. P. Iannetta²; Jodi Souter³; Thomas D. Warkentin¹; Albert Vandenberg¹; ¹University of Saskatchewan, Saskatoon, SK; ²The James Hutton Institute, Dundee, United Kingdom; ³Hemp Genetics International, Saskatoon, SK
- TP 523 **FAIMS Separation of Fentanyl-Related Compounds Using Vapor Modification; Nathan a Grimes¹**; Ifeoluwa Ayodeji²; Theresa Evans-Nguyen¹; ¹University of South Florida, Tampa; ²University of South Florida, Tampa, FL
- TP 524 **LC-ultra FAIMS-MS Separation of Opioid Isomers Using Solvent Vapor Addition; Kevin Davis¹**; Michael Wei¹; Robin H.J. Kemperman¹; Timothy J. Garrett²; Richard A Yost¹; ¹Department of Chemistry, University of Florida, Gainesville, FL; ²Department of Pathology, Immunology, and Laboratory Medicine, University of Florida, Gainesville, FL
- TP 525 **Affecting FAIMS Separation with Trace Levels of Gas Modifiers; Michael Belford¹**; Michael Wei²; Eloy R. Wouters¹; ¹Thermo Fisher Scientific, San Jose, CA; ²University of Florida, Gainesville, FL
- TP 526 **Developing the Research to Routine Workflows with FAIMS: Automating Large-Scale SRM Method Creation for Routine Plasma Proteomics Screening; Scott Peterman¹**; Kerry Hassell²; Mary L. Blackburn³; Romain Huguet³; Michael Volny³; Michael Belford³; Satendra Prasad³; ¹Thermo Fisher Scientific, Grimes, IA; ²Thermo



- Fisher Scientific, Somerset, NJ; ³Thermo Fisher Scientific, San Jose, CA 95134
- TP 527 **FAIMS Pro™ Interface Coupled to Triple Quadrupole Mass Spectrometry for Quantification of Peptides in Complex Matrices**; [Michael Volny](#)¹; Claudia P.B. Martins¹; Mary L. Blackburn¹; Michael W. Belford¹; ¹Thermo Fisher Scientific, San Jose, CA
- TP 528 **– Lifting the Albumin Curtain to Increase Plasma Proteome Profiling: Incorporating Differential Ion Mobility for Increased Protein Coverage**; [Scott Peterman](#)¹; Romain Huguet²; Michael Belford²; Satendra Prasad²; Susan E. Abbatiello³; ¹Thermo Fisher Scientific, Grimes, IA; ²Thermo Fisher Scientific, San Jose, CA 95134; ³Northeastern University, Boston, MA
- TP 529 **Influence of Electrospray and Nanoelectrospray on Lithiated Monosaccharide Homodimer Structures Monitored by Differential Ion Mobility Spectrometry-Mass Spectrometry**; [Tiffany L Crawford](#)¹; Gary L. Glish¹; ¹University of North Carolina at Chapel Hill, Chapel Hill, NC
- METABOLOMICS: GENERAL I**
530-549
- TP 530 **Development of a Dansyl Labeled Dipeptide Standard Library for Dipeptide Identification Using Dansylation LC-MS Metabolomics Platform**; [Kamran Mammadli](#)¹; Yunong Li¹; Erik Cardona Gomez²; Liang Li¹; ¹University of Alberta, Edmonton, AB
- TP 531 **Analysis of Neurotransmitters during Rodent Nervous System Development Using Capillary Electrophoresis-Mass Spectrometry**; [Shannon Murphy](#)¹; Amanda C Weiss¹; Jennifer W Mitchell¹; Stanislav S Rubakhin¹; Martha U Gillette¹; Jonathan V. Sweedler¹; ¹University of Illinois at Urbana Champaign, Urbana, IL
- TP 532 **MIDAS: A Targeted Approach for the Systematic Discovery of Protein-Metabolite Interactions**; [Kevin G. Hicks](#)¹; Aubrie Blevins¹; Sean R. Hackett²; James E. Cox^{1,3}; Jared Rutter¹; ¹University of Utah School of Medicine, Department of Biochemistry, Salt Lake City, Utah; ²Calico Life Sciences, South San Francisco, CA; ³University of Utah Mass Spectrometry & Proteomics Core, Salt Lake City, UT
- TP 533 **High-Throughput Metabolite Profiling of Cell Media for Improved Antibody Production Utilizing a Dual Separation/Mass Spectrometry System with Intelligent MSn Acquisition**; [Ioanna Ntai](#)¹; Anson Pierce²; Paul Gulde²; Martin Samonig³; John Brann⁴; Christopher Elicone⁴; Amanda Souza¹; Ralf Tautenhahn¹; Daniel Lopez Ferrer¹; Andreas Huhmer¹; ¹Thermo Fisher Scientific, San Jose, CA; ²Thermo Fisher Scientific, Grand Island, NY; ³Thermo Fisher Scientific, Germering, Germany; ⁴Thermo Fisher Scientific, Franklin, MA
- TP 534 **Metabolomics Uncovers Metabolic Pathways Affected by Glyceryl Trinitrate Treatment: Much More than a Prodrug of Nitric Oxide**; [Jan F. Stevens](#)¹; Elizabeth R. Axton¹; Jaewoo Choi²; ¹Department of Pharmaceutical Sciences, Linus Pauling Institute, Oregon State University, Corvallis, Oregon; ²Linus Pauling Institute, Oregon State University, Corvallis, OR
- TP 535 **Unraveling the Effects of Alternaria Toxins on the Rat Metabolome**; Vincent Lüttig¹; Hannes Puntschner¹; Mira Flasch¹; Harald Höger²; Doris Marko¹; [Benedikt Warth](#)^{1,3,4}; ¹University of Vienna, Faculty of Chemistry, Department of Food Chemistry and Toxicology, Vienna, Austria; ²Medical University of Vienna, Core Center of Biomedical Research, Austria, Vienna, Austria; ³Research Network Chemistry Meets Microbiology, University of Vienna, Vienna, Austria; ⁴Vienna Metabolomics Center (VIME), Vienna, Austria
- TP 536 **Age Association Analysis between Tricarboxylic Acid Metabolites and Neurocognitive Impairment in Persons Living with HIV**; [Sausan Azzam](#)¹; Corri Lynn Hileman²; Daniela Schlatzer¹; Mark R. Chance¹; Katherine Tassiopoulos³; Robert Kalayjian²; ¹Case Western Reserve University, Cleveland, OH; ²MetroHealth Med Ctr, Cleveland, OH; ³Harvard T.H. Chan School of Public Health, Boston, MA
- TP 537 **Development of LC-MS/MS Based Genome-wide Metabolomics for Bacteria**; [Vanessa Phelan](#)¹; Manuel Banzhaf²; Alison Waller³; ¹University of Colorado, Denver - Anschutz, Aurora, CO; ²University of Birmingham, Birmingham, United Kingdom; ³Brock University, St. Catharines, ON
- TP 538 **Comprehensive Discrimination of Triterpenoids in Three Momordica Species Using Targeted LC-MS/MS Based Metabolomics**; [Joydeb Chanda](#)¹; Akanksha Singh²; Sayan Biswas¹; Pulok K Mukherjee¹; Dipankar Malakar²; Manoj Pillai²; ¹School of Natural Product Studies, Jadavpur University, Kolkata, India; ²SCIEX, Gurgaon, India
- TP 539 **A New HILIC LC/Q-TOF Metabolomics Method with Biologically Important Isomer Separation and Broad Coverage of Metabolite Classes**; [Yujin Dai](#)¹; Jordy J. Hsiao¹; ¹Agilent Technologies, Santa Clara, CA
- TP 540 **Development of More Reproducible and Sensitive Polar Metabolomics Methods**; Sara Violante¹; Hardik Shah¹; Yujin Dai²; Steven M Fischer²; [Justin R Cross](#)¹; ¹Memorial Sloan Kettering Cancer Center, New York, NY; ²Agilent Technologies, Inc., Santa Clara, CA
- TP 541 **Metabolomics for Environmental Monitoring: Developing Tools for Monitoring the Remediation Activity of Microbial Consortia**; [Shawn R. Campagna](#)¹; Amanda L. May¹; Yongchao Xie¹; Mandy Michaelsen²; Frank Loeffler^{1,3}; ¹University of Tennessee, Knoxville, TN; ²US Army Corps of Engineers, Seattle, Washington; ³Oak Ridge National Laboratory, Oak Ridge, TN
- TP 542 **DNA Adductome and Oxidative Stress-Related Metabolome Changes by the Cooked Meat Carcinogen 2-Amino-1-methyl-6-phenylimidazo[4,5-b]pyridine in Human Prostate Cells**; [Jingshu Guo](#)¹; Medjda Bellamri¹; Scott Walmsley¹; Christina Brown¹; Haoqing Chen¹; Peter W. Villalta¹; Robert Turesky¹; ¹University of Minnesota, Minneapolis, MN
- TP 543 **A Nontargeted Multi-Omics Workflow for Meconium Analysis Using Ultra High-Pressure Liquid Chromatography Coupled to High Resolution Mass Spectrometry (UHPLC-HRMS)**; [Atiye Ahmadireskety](#)¹; Josef Neu²; Richard A Yost^{1,3}; John A. Bowden⁴; ¹University of Florida Department of Chemistry, Gainesville, FL; ²University of Florida, Department of Pediatrics, College of Medicine, Gainesville, FL, United States, Gainesville, FL; ³University of Florida Department of Pathology, Immunology, and Laboratory Medicine, Gainesville, FL; ⁴University of Florida, College of Veterinary Medicine, Department of Physiological Sciences, Gainesville, FL, United States, Gainesville, FL
- TP 544 **Hydrolysis of Sulfated Steroids, Toxic Endobiotics and Xenobiotics Using Purified Arylsulfatase for Quantitation of Sulfated and Unconjugated Compounds**; [Pongkwan Sitasuwan](#)¹; L. Andrew Lee¹; ¹IMCS, Irmo, SC
- TP 545 **Volatile Metabolites Monitoring of Gut Microbiota Using Secondary Electrospray Based Mass Spectrometry Techniques- a Tale of Two Approaches**; Haorong Li¹; Mengyang Xu¹; [Jiangjiang \(Chris\) Zhu](#)²; ¹Miami University, Oxford, OH; ²The Ohio State University, Columbus, OH
- TP 546 **Revealing the Changes in Pulmonary Arterial Smooth Muscle Cells in Patient by Using Multi-Omics Approach**; [Dan Li](#)^{1,2,3}; Songjie Chen⁴; Marlene Rabinovitch^{1,2,3}; Michael Snyder⁴; ¹Department of Pediatrics, Stanford University School of Medicine, Stanford, CA; ²Stanford Cardiovascular Institute, Stanford University, Stanford, CA; ³Vera Moulton



- Wall Center for Pulmonary Vascular Diseases, Stanford University School of Medicine, Stanford, CA; ⁴Department of Genetics, Stanford University School of Medicine, Stanford, CA
- TP 547 **Development and Systematic Evaluation of Orthogonal LC-MS Platforms for Metabolomics Workflows;** Jim Blasberg¹; Kevin Ray¹; Zhiyun Cao¹; Ben Cutak¹; Mark Angeles¹; ¹MilliporeSigma, St Louis, MO
- TP 548 **Investigation of Metabolite Modifications during Sample Preparation in Chemical Isotope Labeling LC-MS;** Yunong Li¹; Kamran Mammadli¹; Erik Cardona Gomez¹; Liang Li¹; ¹University of Alberta, Edmonton, AB
- TP 549 **Metabolomics Approach to Assess Tissue-Specific Metabolic Alterations in Resuscitated Rats after Prolonged Cardiac Arrest;** Muhammad Shoab¹; Jaewoo Choi²; Tai Yin¹; Lance B Becker¹; Junhwan Kim¹; ¹Feinstein Institute for Medical Research, Manhasset, NY; ²Linus Pauling Institute, Oregon State University, Corvallis, OR
- METABOLOMICS: UNTARGETED
METABOLITE PROFILING
550-568**
- TP 550 **Identification of Type 2 Diabetes Metabolic Biomarkers Based on Chemical Isotope Labeling LC-MS;** Xinyun Gu¹; Ahmad Aljada²; Anas Abdel Rahman^{2,3,4}; Liang Li¹; ¹University of Alberta, Edmonton, AB; ²College of Medicine, Al Faisal University, Riyadh, Saudi Arabia; ³King Faisal Specialist Hospital and Research Center, King Faisal Specialist Hospital and Research Center, Saudi Arabia; ⁴Memorial University of Newfoundland, St. John's, NL
- TP 551 **Metabolomics Profiling of 5XFAD Mice Model Using Optimized Label-free Untargeted Metabolomics Pipeline;** Boer Xie¹; Haiyan Tan²; Junmin Peng²; ¹St. Jude Children's Research Hospital, Memphis, TN; ²St. Jude Children's Research Hospital, Memphis, TN
- TP 552 **Fast Detection of Pesticides and Drugs Removed from Waste Water by Plants Using Flow Injection Analysis Magnetic Resonance Mass Spectrometry;** Claire Villette¹; Matthias Witt²; Aiko Barsch²; Louis Maljers³; Dimitri Heintz⁴; ¹University of Strassbourg, Strassbourg, France; ²Bruker Daltonik GmbH, Bremen, Germany; ³Bruker Daltonics Inc., Billerica, MA; ⁴University of Strasbourg, Strasbourg, France
- TP 553 **Identification of Antifungal Natural Products in Scab Resistant Pecan Trees;** Zhentian Lei¹; Clayton D. Kranawetter¹; Barbara Sumner¹; Andrew L. Thomas¹; Santosh Kumar¹; Lloyd W. Sumner¹; ¹University of Missouri, Columbia, MO
- TP 554 **High-resolution Mass Spectrometry for Monitoring Physiological Impacts and Biotransformation Products in Fish Exposed to Wastewater Effluent;** Jonathan Mosley¹; Marina Evich²; Ioanna Ntai³; Drew Ekman¹; Jenna Cavallin⁴; Daniel Villeneuve⁴; Gerald Ankley⁴; Timothy Collette¹; ¹US EPA, Athens, GA; ²ORISE Fellow, US EPA, Athens, GA; ³Thermo Fisher Scientific, San Jose, California; ⁴US EPA, Duluth, MN
- TP 555 **Profiling Weaning Piglet Serum Metabolomic Affected by Acute Exposure of High Concentrations Atmospheric Hydrogen Sulfide;** Zhen Liu¹; Qingshi Meng¹; Qixiang Miao¹; Yanjiao Xie¹; Hongfu Zhang¹; Xiangfang Tang¹; ¹Institute of Animal Science, Chinese Academy of Agricultural Sciences, Beijing, China
- TP 556 **Metabolomic Profiling of Potential Bioactive Minor Compounds in Amazonian Vegetable Oils and Butters by UHPLC-MSE;** Maira Fasciotti¹; Michael Murgu²; Thays V. C. Monteiro¹; Simone C. Chiapetta³; Alessandra Sussulini⁴; Marcos N. Eberlin⁴; Valnei S. Cunha¹; ¹INMETRO, Duque De Caxias, Brazil; ²Waters Corporation, Barueri, Brazil; ³National Institute of Technology, Rio de Janeiro, Brazil; ⁴University of Campinas, Campinas, Brazil
- TP 557 **Ethanol-Induced Metabolomic Differences in Mice Using HRAM Q-TOF Analysis;** Stephane Moreau¹; Georgios Theodoridis²; Helen G. Gika³; Christina Virgiliou²; Olga Deda³; Ian D Wilson⁴; Neil J Loftus⁵; ¹Shimadzu Europa GmbH, Duisburg, Germany; ²Chem and BIOMIC_AUTH, Aristotle University, Thessaloniki, Greece; ³Medicine and BIOMIC_AUTH, Aristotle University, Thessaloniki, Greece; ⁴Imperial College London, Department of Surgery and Cancer, United Kingdom; ⁵Shimadzu MS/BU, Manchester, United Kingdom
- TP 558 **Fast Profiling of Tryptophan Metabolites in a Gut Microbiome Study Using Wide Isolation Strategies for UHPLC-HRMS/MS;** Vanessa Y. Rubio¹; Joy G. Cagmat¹; Gary P. Wang¹; Richard A Yost¹; Timothy J Garrett¹; ¹University of Florida, Gainesville, FL
- TP 559 **Metabolomics of *Fusarium verticillioides* / Maize Interaction;** Mark Busman; USDA, ARS, NCAUR, BFP, Peoria, IL
- TP 560 **Improved Metabolite Identification in a Single Injection with SWATH® Acquisition for Untargeted Metabolomics Workflow;** Robert Proos¹; Khatereh Motamedchaboki²; ¹Sciex, Framingham, MA; ²Sciex, Redwood City, CA
- TP 561 **A Collisional Cross Section Database for Diverse Small Molecules: Improving Annotation of Metabolomics Data;** Corey D Broeckling¹; Jessica E. Prenni¹; Robert S Plumb²; Giorgis Isaac²; Johannes PC Vissers³; ¹Colorado State University, Fort Collins, CO; ²Waters Corporation, Milford, MA; ³Waters Corporation, Wilmslow, United Kingdom
- TP 562 **Volatile Interactions between *Solanum lycopersicum* and *Phytophthora infestans*;** Lida Garzón; Universidad de los Andes, Bogotá D.C, Colombia
- TP 563 **Metabolomics Study of Human Blood Plasma Using 95% ¹³C Internal Standard with Liquid Chromatography and Ion Mobility-Mass Spectrometry;** Robin H.J. Kemperman¹; Chris W.W. Beecher²; Timothy J. Garrett¹; Richard A Yost¹; ¹University of Florida, Gainesville, FL; ²IROA Technologies LLC, Bolton, MA
- TP 564 **Multi-omic Discovery of Metabolic Rewiring in Triple-negative Breast Cancer Following Mitochondrial Folate Transport Ablation: Strategy to Reveal Drug-targetable Synthetic Lethalities;** Qiuying Chen¹; Joshua B Zuk¹; miller A Christine²; Steven M Fischer²; Steven Gross¹; ¹Weill Medical College of Cornell, New York, NY; ²Agilent Technologies, Inc., Santa Clara, CA
- TP 565 **Metabolomics Rosetta Stone: Testing Strategies for Harmonization of Untargeted Metabolomics Data Across Multiple Analytical Platforms;** Ken Liu¹; Vilinh Tran¹; Chunyu Ma¹; Karan Uppal¹; Dean Jones¹; ¹Emory School of Medicine, Atlanta, GA
- TP 566 **High-Performance Chemical Isotope Labeling LC-MS for Discovery of Metabolite Biomarkers of Rheumatoid Arthritis;** Xiaohang Wang¹; Walter P. Maksymowych¹; Liang Li¹; ¹University of Alberta, Edmonton, AB
- TP 567 **Metabolomics Data in the XCMS Cloud: a Resource for Meta Analysis and Systems Biology;** Amelia Palermo¹; Tao Huan²; Duane Rinehart¹; Markus M Rinschen¹; Paul H Benton¹; Eoin Fahy³; Shuzhao Li⁴; Shankar Subramaniam³; Gary Siuzdak^{1,5}; ¹The Scripps Center for Metabolomics, The Scripps Research Institute, La Jolla, CA; ²Department of Chemistry, University of British Columbia, Vancouver, BC; ³Department of Bioengineering, University of California San Diego, La Jolla, CA; ⁴Department of Medicine, School of Medicine, Emory University, Atlanta, GE; ⁵Department of Chemistry, Molecular and Computational Biology, The Scripps Research Institute, La Jolla, CA
- TP 568 **Metabolomics Characterization of Cell Culture Media by Ultra High Resolution LC-QTOF-MS Analysis;** Xuejun Peng¹; Guillaume Tremintin¹; Anjali Alving²; Heiko



Neuweger³; Aiko Barsch³; Nikolas Kessler³; ¹*Bruker Daltonics Inc., San Jose, CA*; ²*Bruker Daltonics Inc., Billerica, MA*; ³*Bruker Daltonik GmbH, Bremen, Germany*

PHOSPHOPEPTIDES: QUANTITATIVE ANALYSIS

569-579

- TP 569 **Global Quantification of Proteome and Phosphoproteome Revealed Novel Cellular Signaling Mechanisms Responsive to Hypoxia and Iron Deficiency**; Luke Erber¹; Yao Gong¹; Maolin Tu¹; Phu Tran¹; Yue Chen¹; ¹*University of Minnesota, Minneapolis, MN*
- TP 570 **Combining the TMT Calibrator Approach and Immunoaffinity Enrichment for Phosphotyrosine Profiling To Reduce Sample Input Requirements**; Bin Fang¹; Victoria Izumi¹; Lily Remsing Rix¹; Eric Haura¹; Uwe Rix¹; Ian Pike²; John Koomen¹; ¹*H. Lee Moffitt Cancer Center, Tampa, FL*; ²*Proteome Sciences plc, London, United Kingdom*
- TP 571 **Analyzing the Neuronal Phosphoproteome: A Systematic Comparison of Fusion Lumos and timsTOF Pro data**; Kristina Desch¹; Thomas Kosinski²; Scarlet Koch²; Heiner Koch²; Erin M. Schuman¹; Julian Langer^{1,3}; ¹*Max Planck Institute for Brain Research, Frankfurt am Main, Germany*; ²*Bruker Daltonik GmbH, Bremen, Germany*; ³*MPI for Biophysics, Frankfurt Am Main, Germany*
- TP 572 **Phosphoproteomics with LC-FAIMS Separations Coupled to a Modified Tribrid Orbitrap Mass Spectrometer**; Alexander S. Hebert¹; Romain Huguet²; Graeme C. McAlister³; Derek J. Bailey³; Michael W. Belford³; Michael S Westphall¹; Joshua J. Coon^{1,4,5,6}; ¹*Genome Center of Wisconsin, Madison, WI*; ²*Thermo Fisher Scientific, San Jose, California*; ³*Thermo Fisher Scientific, San Jose, CA*; ⁴*Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI*; ⁵*Department of Chemistry, University of Wisconsin-Madison, Madison, WI*; ⁶*Morgridge Institute for Research, Madison, WI*
- TP 573 **Quantitative, Comprehensive Multi-Pathway Signaling Analysis Using an Optimized Phosphopeptide Enrichment Method Combined with an Internal Standard Triggered Targeted MS Assay**; Bhavin Patel¹; Penny Jensen¹; Aaron S. Gajadhar²; Sebastien Gallien³; Jae Choi¹; Romain Huguet²; Graeme McAlister²; Derek Bailey²; Shannon Eliuk²; Markus Kellmann⁴; Tabiwang N. Arrey⁴; Alexander Harder⁴; Andreas Huhmer²; Kay Opperman¹; John C Rogers¹; ¹*Thermo Fisher Scientific, Rockford, IL*; ²*Thermo Fisher Scientific, San Jose, CA*; ³*Thermo Fisher Scientific, Precision Medicine Science Center, Cambridge, MA*; ⁴*Thermo Fisher Scientific, Bremen, Germany*
- TP 574 **Optimization and Implementation of a TMT-based Quantitative Phosphoproteomics Workflow to Identify MELK Substrates**; Joshua Beri^{1,2}; Ian M McDonald²; Alex Prevatte^{1,2}; Dennis Goldfarb^{1,3}; Lee M Graves^{1,2,3}; Laura E Herring^{1,2}; ¹*UNC Proteomics Core Facility, Chapel Hill, NC*; ²*UNC Department of Pharmacology, University of North Carolina at Chapel Hill, Chapel Hill, North Carolina*; ³*Lineberger Comprehensive Cancer Center, University of North Carolina at Chapel Hill, Chapel Hill, NC*
- TP 575 **Evaluation of Spatiotemporal Influences of Interleukin Family- IL-1: Interleukin-33 (IL-33) on Cellular Signal Transduction Pathways**; Rex D a b¹; Sneha M Pinto¹; T. S Keshava Prasad¹; ¹*Yenepoya University, Mangalore, India*
- TP 576 **Proteomic and Phosphoproteomic Network Analysis in Alzheimer's Disease**; Lingyan Ping^{1,2}; Eric B Dammer^{1,2}; Duc M Duong^{2,3}; Marla Gearing²; James J. Lah^{2,4}; Allan I. Levey^{2,4}; Nicholas T. Seyfried^{1,2,4}; ¹*Department of Biochemistry, Emory University, Atlanta, GA*; ²*Center for Neurodegenerative Diseases, Emory School of Medicine, Atlanta, GA*; ³*Department of Biochemistry, Emory University, Atlanta, Georgia*; ⁴*Department of Neurology, Emory University, Atlanta, GA*
- TP 577 **Tandem Mass Tags (TMT) in Global Quantitative Phosphorylation Analysis**; Ling Li¹; Dongmei Zhang¹; Belinda Willard¹; ¹*Cleveland Clinic, Cleveland, OH*
- TP 578 **Phosphoproteomics-Based Molecular Subtyping and Kinase Candidate Nomination for Individual Patients of Diffuse-Type Gastric Cancer**; Mengsha Tong¹; Chunyu Yu²; Jinwen Shi¹; Yi Wang¹; Tingting Li²; Jun Qin¹; ¹*State Key Laboratory of Proteomics, Joint Laboratory of Gastrointestinal Oncology, Beijing Proteome Research Center, National Center for Protein Sciences, Beijing, China*; ²*Department of Biomedical Informatics, School of Basic Medical Sciences, Peking University Health Science Center, Beijing, China*
- TP 579 **Real-Time, High Density Monitoring of pTyr Signaling Targets in Human Tumors Using Heavy Peptide Triggered Targeted Quantitation**; Aaron S Gajadhar¹; Lauren E Stopfer²; Cameron T Flower²; Forest M White²; Bhavin Patel³; Sebastien Gallien⁴; Romain Huguet¹; Graeme McAlister¹; Derek Bailey¹; Shannon Eliuk¹; Markus Kellmann⁵; Tabiwang N. Arrey⁵; Alexander Harder⁵; Daniel Lopez Ferrer¹; Andreas Huhmer¹; ¹*Thermo Fisher Scientific, San Jose, CA*; ²*Department of Biological Engineering, Koch Institute for Integrative Cancer Research, Center for Precision Cancer Medicine, Massachusetts Institute of Technology, Cambridge, MA*; ³*Thermo Fisher Scientific, Rockford, IL*; ⁴*Thermo Fisher Scientific, Paris, France*; ⁵*Thermo Fisher Scientific, Bremen, Germany*

PROTEIN THERAPEUTICS: QUANTITATIVE ANALYSIS II

580-605

- TP 580 **Benchmarking Host Cell Protein Quantification: Label-free vs. a Labeled Global Standard**; Harsha Gunawardena¹; Jeffrey Brelsford¹; Melissa Smith¹; Kevin D. Smith²; Hirsh Nanda²; ¹*Janssen Research & Development, Spring House, PA*; ²*Janssen Research and Development, Spring House, PA*
- TP 581 **Quantitation of Host Cell Contaminants in Biotherapeutic IgG using LC-ToF-MRM with SILAC Labeled Reference Standards**; Tyler Fletcher¹; Marla Popov²; Stuart Haslam³; Ron Orlando^{1,2}; ¹*University of Georgia, Athens, GA*; ²*Glycoscientific LLC, Athens, GA*; ³*Imperial College, London, United Kingdom*
- TP 582 **Immunocapture-LC/MS and LBA-Based Assays as Complementary and Orthogonal Tools for Developing Fusion Protein Therapeutics**; Susan Chen; *Takeda Pharmaceuticals, Inc., Cambridge, MA*
- TP 583 **Validation of Amino Acid-Based Isotope Dilution LC-MS/MS Quantification of Insulin Standard Solution Using Sulfur-Based Isotope Dilution ICP/MS**; Hwjin Kim^{1,2}; Ji-Seon Jeong^{1,2}; Thi Thanh Huong Tran^{1,2}; Youngran Lim²; Sung Woo Heo²; Yong-Hyeon Yim^{1,2}; ¹*University of Science and Technology (UST), Daejeon, South Korea*; ²*KRISS, Daejeon, South Korea*
- TP 584 **Impact of Endogenous Biotin on Streptavidin Based Hybrid LBA-LC/MS Assays for Biotherapeutics**; Eric Ma¹; Moucun Yuan¹; William R Mylott Jr¹; ¹*PPD, Richmond, VA*
- TP 585 **Transformation of Challenging New Modalities – Characterization and Quantitation of Antibody Variant Fragmentation using Affinity Capture Coupled to LC-MS or CE-LIF**; Cong Wu¹; William Sawyer¹; Phillip Chu¹; Neha Srikumar²; Nga Tang¹; Pamela Chan¹; Gloria Meng¹; Brian Roper³; Thomas Niedringhaus³; John Tran¹; ¹*Biochemical and Cellular Pharmacology, Genentech, Inc., South San Francisco, CA*; ²*University of Pennsylvania, Philadelphia, PA*; ³*Protein Analytical Chemistry, Genentech, Inc., South San Francisco, CA*
- TP 586 **Multi Attribute Monitoring in Therapeutic Glycoprotein Process Development: Benchmark of Different Sample Preparation, Mass Spectrometry Platform and Data**



- TP 587 **Processing Software; Bertaccini Diego; Merck KGaA Darmstadt, Germany, Corsier-sur-Vevey, Switzerland**
SI-traceable quantification of an anti-CD20 monoclonal antibody by Isotope Dilution Mass Spectrometry (IDMS); Wei Mi¹; Zhishang Hu¹; Yan Chen²; ¹National institute of metrology, China, Beijing, China; ²Hunan normal university, Changsha, China
- TP 588 **Introducing MA-PAT: a Multi Attribute-Process Analytical Technology to Monitor Protein Quality/ Quantity and Process Characteristics during Biopharma Production; Jérôme Haustant¹; Sandrine Fisch¹; Jérémy Peyrol¹; Emilie Navarro¹; Vivien Le Bras¹; Cédric Mesmin¹; ¹Merck Biodevelopment, Martillac, France**
Employing the MS-based Multi-Attribute Method (MAM) for Automated Quality Monitoring of Biotherapeutics; John N McCarter¹; Joe Shambaugh²; Aude Tartiere³; Albert Van Wyk⁴; Cassandra Wigmore⁵; Peter Haber⁶; ¹Genedata, Inc., Lexington, MA; ²Genedata Inc, Lexington, MA, USA, Lexington, Massachusetts; ³Genedata, San Francisco, CA; ⁴Genedata Ltd, Cambridge, UK, Cambridge, United Kingdom; ⁵Genedata AG, Basel, Switzerland, Basel, Switzerland; ⁶Genedata GmbH, Munich, Germany, Munich, Germany
- TP 590 **Ultra-Sensitive Intact Monoclonal Antibody Quantification Using Automated Sample Preparation Platform and High-Resolution Mass Spectrometer; Xi Qiu¹; Wendi Hale¹; David Wong²; ¹Agilent Technologies, Wilmington, DE; ²Agilent Technologies, Santa Clara, CA**
- TP 591 **A High Resolution Accurate Mass Multi-Attribute Method for Critical Quality Attribute Monitoring and New Peak Detection; Haichuan Liu¹; John Rontree¹; ¹Thermo Fisher Scientific, San Jose, CA**
- TP 592 **Monitoring Multiple Attributes of Biotherapeutics at Peptide Level Using a Single Quadrupole LC/MS for Quality Control; Linfeng Wu¹; Lisa Zang¹; Guannan Li¹; ¹Agilent Technologies, Santa Clara, CA**
- TP 593 **Comparison between Magnetic Bead and Membrane Immunoaffinity Purification Methods for the Measurement of Monoclonal Antibody in Rat Serum; Zhiyu Li¹; Zhiren Yu¹; Feifei Cui¹; Weiqun Cao¹; Lili Xing¹; Xin Zhang¹; Yi Tao¹; ¹WuXi AppTec, Shanghai, China**
- TP 594 **Mass Spectrometric Evaluation of Host Cell Protein Patterns in Biopharmaceutical Products; Daniel Michael Waldera-Lupa¹; Thomas Flad¹; Andreas Dittmar¹; Heiner Falkenberg¹; Roland Moussa¹; ¹Protagen Protein Services, Dortmund, Germany**
- TP 595 **Pre-Clinical Estimation of Cetuximab Using Nano-Surface and Molecular Orientation Limited (nSMOL) Proteolysis and LC-MS/MS; Deepti Bhandarkar¹; Rashi Kochhar¹; Shailendra Rane¹; Shailesh Damale¹; Ashutosh Shelar¹; Purushottam Sutar¹; Anant Lohar¹; Bhaumik Trivedi¹; Navin Devadiga¹; Ajit Datar¹; Pratap Rasam¹; Jitendra Kelkar¹; ¹Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India**
- TP 596 **Quantitation of a PEGylated Human Parathyroid Hormone (1-34) Analog in Rat Plasma Using a Hybrid Immunoaffinity Bottom-Up LC-MS/MS Assay; Jean-Nicholas Mess¹; Jean-Francois Dupuis¹; Kevork Mekhssian¹; Erik Wagner²; Amy Wang²; Xin Xu²; Karim Berrada³; Max Moore³; Anahita Keyhani¹; ¹Altasciences, Laval, QC; ²National Center for Advancing Translational Sciences, NIH, Rockville, MD; ³Frederick National Laboratory for Cancer Research - Leidos Biomedical Research, Frederick, MD**
- TP 597 **Investigation of Tissue Distributions of Therapeutic Monoclonal Antibody with Cassette Dosing Strategy and Novel LC/MS Based Method; Jie Pu¹; Shihan Huo¹; Chao Xue¹; Ming Zhang^{1,2}; Jun Qu^{1,2}; ¹SUNY, at Buffalo, Buffalo, NY; ²New York State Center of Excellence in Bioinformatics & Life Sciences, Buffalo, New York**
- TP 598 **Quantitation of CHO Media Nutrients and Metabolites in under 180 seconds by an Integrated CE-MS Analyzer; Kenion H. Blakeman¹; Ji Young Anderson¹; Colin M. Gavin¹; Drew Blouch¹; Christopher D. Brown¹; Glenn A. Harris¹; ¹908 Devices, Inc., Boston, MA**
- TP 599 **Application of Top Down Degradomics to Guide Development of Stable Antibody Variants; Phillip Chu¹; christopher Davies²; Cong Wu²; Tangsheng Yi²; James Koerber²; John C. Tran²; ¹Genentech Inc., South San Francisco, CA; ²Genentech, South San Francisco, CA**
- TP 600 **Rapid, Sensitive, and Routine Intact mAb Quantification using a Compact ToF HRMS Platform; Yun Alelyunas¹; Henry Shion¹; Mark D Wrona¹; Weibin Chen¹; ¹Waters Corporation, Milford, MA**
- TP 601 **Comprehensive Characterization of Antibody Drug Conjugates Enabled by Top-down and Middle-down Mass Spectrometry Strategies; Eli J Larson¹; Bifan Chen¹; Ziqing Lin^{2,3}; Yanlong Zhu^{2,3}; Yutong Jin¹; Qingge Xu^{2,3}; Cexiong Fu⁴; Zhaorui Zhang⁴; Qunying Zhang⁴; Wayne A Pritts⁴; Ying Ge^{1,2,3}; ¹Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706; ²Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI; ³Human Proteomics Program, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI; ⁴Process Analytical Chemistry, AbbVie Inc., North Chicago, IL**
- TP 602 **Evaluating Stability of Human Monoclonal Antibody in Rat Cell Cultures Using a Surrogate Peptide LC-MS/MS Approach; Nadya Galeva¹; Reed Murbach¹; Krystal Gilligan¹; Kevin Westland¹; Seema Muranjan¹; ¹Sekisui XenoTech, LLC, Kansas City, KS**
- TP 603 **An Integrated LC-MS Platform for Monitoring Quality Attributes of Biotherapeutic Products; Chengfeng Ren¹; Frank Macchi²; Monica Sadek²; Benjamin Moore²; ¹Genentech, South San Francisco, CA; ²Genentech Inc., South San Francisco, CA**
- TP 604 **Non-Labeling Approach for Absolute Quantitation of Total Biotherapeutics and Simultaneous Detection of Blood Volume in Tissues Using LC/MS; Miho Ayabe¹; Naoaki Murao²; Masaki Ishigai³; Hiroyuki Tsunoda¹; ¹Chugai Pharmaceutical Co., Ltd., Kamakura, Japan; ²Chugai Pharmaceutical Co., Ltd., Gotemba, Japan; ³Chugai Pharmaceutical Co., Ltd., Chuo-ku, Japan**
- TP 605 **Limited Tryptic Digestion-Isotope Dilution Mass Spectrometry (LTD-IDMS): An Alternative Potency Assay to Single Radial Immunodiffusion (SRID) for Influenza Vaccines; Tracie Williams¹; Hans C Cooper¹; John R Barr¹; ¹Centers for Disease Control and Prevention, Atlanta, GA**

**PROTEIN THERAPEUTICS:
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- TP 606 **Taking Charge Variant Analysis to the Next Level: Targeted and Automated Charge Variant-Coupled Native Mass Spectrometry (CV-MS); Mauro Sassi¹; Mara Rossi¹; Angelo Palmese¹; ¹Merck KGaA, Guidonia Montecelio, Italy**
- TP 607 **NanoFlow LCMS and Dedicated Bioinformatics Software for Rapid Semi-Automated Biotherapeutics PTM Quantitation; Tun Liu¹; Jennifer Nemeth-Seay²; Michael Merriman³; Sean McCarthy³; ¹Janssen Research & Development, Spring House, PA; ²Janssen Research and Development, Spring House, PA; ³Sciex, Framingham, MA**
- TP 608 **Characterization of Protein Therapeutics Using ZipChip Microfluidic Capillary Electrophoresis-Mass Spectrometry; Ekaterina G. Deyanova¹; Richard Huang¹; Pradyot Nandi¹; Priyanka Madia¹; Guodong Chen¹; ¹Bristol-Myers Squibb Company, Princeton, NJ**



- TP 609 **Using Hydrogen Exchange-Mass Spectrometry (HX-MS) to Identify Agitation-Induced Unfolding Events Causing Aggregation in Monoclonal Antibodies (mAbs);** Chamalee D Gamage¹; David D. Weis¹; Benjamin Walters²; ¹University of Kansas, Lawrence, KS; ²Genentech, Inc., South San Francisco, CA
- TP 610 **Analysis of Aggregation-Prone Full-Length Antibodies Using FPOP-LC-MS/MS;** Owen Cornwell¹; Nicholas J Bond²; Sheena E Radford¹; Alison E Ashcroft¹; ¹University of Leeds, Leeds, United Kingdom; ²MedImmune, Cambridge, United Kingdom
- TP 611 **Assessing the Protein A Binding Affinity of Monoclonal Antibody Variants Using Protein A Chromatography Coupled to Native Mass Spectrometry;** Victoria C. Cotham¹; Shunhai Wang¹; Thomas J. Daly¹; Ning Li¹; ¹Regeneron Pharmaceuticals Inc., Tarrytown, NY
- TP 612 **An Efficient LC/MS Workflow for Identification and Monitoring of Host Cell Proteins for Assisting Monoclonal Antibody Purification;** Catalin Doneanu¹; Malcolm Anderson²; Alex Xenopoulos³; Romas Skudas⁴; Ying Qing Yu¹; Asish Chakraborty¹; Weibin Chen¹; ¹Waters Corporation, Milford, MA; ²Waters Corporation, Wilmslow, United Kingdom; ³EMD Millipore Corporation, Bedford, MA; ⁴Merck KGaA, Darmstadt, Germany
- TP 613 **A Specific and Sensitive LC-MS/MS PRM Method to Quantify C-Terminal Lysine Clipping in Monoclonal Antibodies;** Lei Wang¹; Mei M Zhu¹; Charles Nwosu¹; Anne Kowal¹; ¹Takeda Pharmaceuticals, Inc., Cambridge, MA
- TP 614 **A Comprehensive Physicochemical Characterization of an Original and Biosimilar Tenecteplase by Mass Spectrometry Methods;** Maksim Degterev¹; Maxim Smolov¹; Alexander Vishnevskiy¹; Rakhim Shukurov¹; ¹IBC Generium, Vol'ginskiy, Russian Federation
- TP 615 **Primary Structures of Intact DTPA-Coupled Recombinant Epidermal Growth Factors can be Evaluated via MS-Based Chemical Formula Verification;** Yen-chun Huang¹; Yu-Hsuan Lin¹; Ya-Fen Chen²; C Allen Chang³; Yeou-Guang Tsay^{1,4}; ¹Institute of biochemistry and molecular biology, National Yang-Ming University, Taipei, Taiwan; ²Sunjet Co., Ltd., Taipei, Taiwan; ³Department of Biomedical Imaging and Radiological Sciences, National Yang-Ming University, Taipei, Taiwan; ⁴Proteomics Research Center, National Yang-Ming University, Taipei, Taiwan
- TP 616 **Identifying Early Production Truncated Drug Candidates by Top-Down Mass Spectrometry;** Zhe Zhang; Novartis, Cambridge, MA
- TP 617 **Rapid Critical Quality Attribute Assessment of Biotherapeutic Proteins Using an Automated Top-Down Sequencing LC-MS Workflow;** Matthew Maust¹; Li Cui¹; Greg Kilby¹; Juan Aon¹; Keegan Orzechowski¹; Wilfred Tang²; Michelle English²; Marshall Bern²; ¹GlaxoSmithKline, Collegeville, PA; ²Protein Metrics Inc., Cupertino, CA
- TP 618 **Characterization of Peptide with Disulfide Bond Linkage on LC Time Scale with Differential Mobility and ECD Fragmentation;** Suya Liu¹; Yves Le blanc²; Doug Simmons¹; Pavel Ryumin¹; Takashi Baba¹; ¹SCIEX, Concord, ON; ²SCIEX, Concord, On, ON
- TP 619 **Advancements in Native Analysis by Microchip Capillary Electrophoresis-ESI-MS;** J. Scott Mellors¹; Ashley Bell²; Erin A. Redman¹; ¹908 Devices, Inc., Carboro, NC; ²908 Devices, Boston, MA
- TP 620 **Novel Analytical Paradigm for Accurate Characterization and Routine Monitoring of Deamidation and Succinimide Intermediate in Biotherapeutic Proteins;** Sergei Saveliev¹; Mingyan Cao²; Sri Hari Raju Mulagapati²; Bhargavi Vemulapati²; Jihong Wang²; Alan Hunter²; Marjeta Urh¹; Dengfeng Liu²; ¹Promega Corporation, Madison, WI; ²MedImmune, Gaithersburg, MD
- TP 621 **Structural Characterization of Peptide-Loaded Major Histocompatibility Complexes (pMHC) through Top Down Native Mass Spectrometry;** Dhanashri Bagal¹; Songyu Wang¹; Bradford W. Gibson²; ¹Amgen, South San Francisco, CA; ²Amgen, South San Francisco, CA
- TP 622 **Analysis of Antibody Subunits by ETD Parallel Ion Parking on a Chromatographic Timescale;** Joshua D. Hinkle¹; Emily Zahn¹; Robert D'Ippolito¹; Elizabeth Duselis¹; Dina L. Bai¹; Jeffrey Shabanowitz¹; Donald F. Hunt¹; ¹University of Virginia, Charlottesville, VA
- TP 623 **High Resolution Separations for Detailed LC/MS Analysis of mAb Disulfide Variants;** Barry Boyes¹; William E Miles²; Ben Libert¹; ¹Advanced Materials Technology Inc., Wilmington, DE; ²Advanced Materials Technology, Wilmington, DE
- TP 624 **Ultra-Comprehensive Antibody Fc-Fusion Protein Characterization Using a Tribird Orbitrap Mass Spectrometer Modified for PTR and Extended Mass Range Applications;** Aaron O Bailey¹; Yi Zeng¹; Joshua Silveira²; Kristina Srzentic²; Christopher Mullen²; John E. P. Syka²; Romain Huguet²; Siqi Liu³; Guanghui Han¹; ¹BGI Americas, San Jose, CA; ²Thermo Fisher Scientific, San Jose, CA; ³BGI-Shenzhen, Shenzhen, China
- TP 625 **Not All IgG1 Monoclonal Antibody Disulfide Bonds Are Created Equal;** Andrew Dykstra¹; Neeraj Agrawal¹; ¹Amgen, Thousand Oaks, CA

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- TP 626 **Protein Phosphorylation Landscape of Mouse Spermatids During Spermiogenesis;** Yan Li¹; Yiwei Cheng¹; Tianyu Zhu¹; Hao Zhang¹; Hui Zhu¹; Xuejiang Guo¹; ¹Nanjing Medical University, Nanjing, China
- TP 627 **Identification and Validation of Calcineurin Interactors;** Brooke Brauer¹; Sarah Sheftic²; Isha Nasa¹; Thomas Moon²; Rebecca Page²; Wolfgang Peti²; Arminja N Kettenbach¹; ¹Dartmouth College, Hanover, NH; ²University of Arizona, Tucson, AZ
- TP 628 **A Quantitative Chemical Proteomic Analysis of Cysteine Reactivity;** Evan W. McConnell¹; Leslie M. Hicks¹; ¹UNC, Chapel Hill, NC
- TP 629 **Proximity-Dependent Identification of *in vivo* Putative Substrates of Protein Kinases;** Tomoya Niinae¹; Koshi Imami¹; Chia-Feng Tsai²; Naoyuki Sugiyama¹; Yasushi Ishihama¹; ¹Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, Japan; ²PNNL, Richland, WA
- TP 630 **High Sensitivity PTM Characterization in Cell Lysates Using Trapped Ion Mobility;** Matthew Willetts¹; Shourjo Ghose¹; Gary Kruppa¹; Matthew P Stokes²; Charles Farnsworth²; Kimberly Lee²; ¹Bruker Scientific, Billerica, MA; ²Cell Signaling Technology, Danvers, MA
- TP 631 **Phosphoproteomic Analyses of Multiple Species of Snakes Provides Insight into the Regulation of Intestinal Function and Regeneration;** Abu Hena M Kamal¹; Blair Perry¹; Todd Castoe¹; Stephen M. Secor²; Saiful M. Chowdhury¹; ¹University of Texas at Arlington, Arlington, TX; ²University of Alabama, Tuscaloosa, AL
- TP 632 **Proteomics of Diatoms: Discovery of Polyamine Modifications in Biosilica-Associated Proteins;** Alexander Milentyev¹; Christoph Heintze²; Nicole Poulsen²; Nils Kroeger²; Matthias Wilm³; Andrej Shevchenko⁴; ¹Max Planck Institute of Molecular Cell Biology and Genetics (MPI-CBG), Dresden, Germany; ²Center for Molecular and Cellular Bioengineering (CMCB), Dresden, Germany; ³Conway Institute of Biomolecular and Biomedical Research, Dublin, Ireland; ⁴Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany



- TP 633 **Creating a Functional Map of the Human Phospho-Proteome Using a “Big Data” Approach;** David Ochoa¹; Andrew F. Jarnuczak¹; Pedro Beltrao¹; Juan Antonio Vizcaino¹; ¹EMBL-EBI, Hinxton, United Kingdom
- TP 634 **Determining the Phosphorylation Dynamics in Human Spliceosome;** Kuan-Ting Pan¹; Ivan Silbern¹; Majety Naga Leelaram¹; Olexandr Dybkov¹; Reinhard Luehrmann¹; Henning Urlaub^{1,2}; ¹Max-Planck Inst for Biophysical Chemistry, Goettingen, Germany; ²University Medical Center Goettingen (UMG), Goettingen, Germany
- TP 635 **Comprehensive Characterization of Biotherapeutic Degradation *in vivo* Using a Modified Orbitrap Tribrid with Extended Mass Range;** Kristina Srzentic¹; Romain Huguet²; Luca Fornelli³; ¹Thermo Fisher Scientific, Cambridge, MA; ²Thermo Fisher Scientific, San Jose, CA; ³University of Oklahoma, Norman, OK
- TP 636 **Combined GluC-Based Middle-Down and Top-Down Proteomics of Histone H4 in a Single Analysis;** Matthew Holt¹; Tao Wang¹; Nicolas L Young¹; ¹Baylor College of Medicine, Houston, TX
- TP 637 **An Integrated Intact Mass and Bottom-Up Approach to Characterization of New Biologics;** Hirsh Nanda¹; Bo Zhai¹; Andrew D Mahan¹; Harsha P. Gunawardena¹; Andrew C Nichols²; Jing Li²; Yong J. Kil²; Marshall Bern²; Eric Carlson²; ¹Janssen Research & Development, Cell & Developability Sciences, Spring House, PA; ²Protein Metrics Inc., San Carlos, CA
- TP 638 **Characterization of S-Nitrosylation in Aged Rabbit Using Oxidized Cysteine-Selective cPILOT;** Katarena Ford; Vanderbilt University, Nashville, TN
- TP 639 **Bothrops Snake Venoms: Glycoproteomic Analysis and the Role of Sialic Acid in Toxin Function.;** Carolina Brás Costa^{1,2}; Débora Andrade Silva^{1,2}; Daniela Cajado Carvalho¹; Solange Maria de Toledo Serrano¹; ¹Butantan Institute, São Paulo, Brazil; ²Chemistry Institute -USP, São Paulo, Brazil
- TP 640 **Minimizing Deamidation During the Trypsin Digestion of Proteins;** Paul R Collop¹; Ron Orlando²; ¹University of Georgia, Athens; ²University of Georgia, Athens, GA
- TP 641 **A Rapid and Robust Protocol for Disulfide Bond Identification and Validation Using Pepsin/Trypsin Digestion and Spectrum Identification Machine;** Chuanlong Cui¹; Tong Liu¹; Annie Beuve¹; Hong Li¹; ¹Rutgers New Jersey Medical School, Newark, NJ
- TP 642 **Analysis of Histones from HEK293 Cells Using a QTOF with Trapped Ion Mobility and PASEF Workflows;** Shourjo Ghose¹; Matthew Willetts¹; Miranda Gardner²; Michael Freitas²; Gary Kruppa¹; ¹Bruker Scientific, Billerica, MA; ²The Ohio State University, Columbus, OH
- TP 643 **Quantitative Proteomics Reveals Differential Huntingtin Ubiquitination and Global Proteome Changes in a Mice Model for Huntington’s Disease;** Karen A Sap¹; Arzu Tugce Guler¹; Aleksandra Bury¹; Karel Bezstarosti²; Jeroen A.A. Demmers²; Eric A. Reits¹; ¹Amsterdam UMC, Amsterdam, Netherlands; ²Erasmus MC, Rotterdam, Netherlands
- TP 644 **The Invisible Link – Connecting Autophagy and Alzheimer’s Disease;** Tyler R Lambeth¹; Dylan L. Riggs²; Ryan R. Julian²; ¹University of California-Riverside, Riverside, CA; ²University of California, Riverside, Riverside, CA
- TP 645 **Orthogonal Approaches for Released N-Glycan Characterization and Quantification;** Sean McCarthy¹; Zoe Zhang²; Elliott Jones²; ¹SCIEX, Framingham, MA; ²Sciex, Redwood City, CA
- TP 646 **oxSWATH: An Integrative Method for a Comprehensive Redox-Centered Analysis Combined with a Generic Differential Proteomics Screening;** Bruno Manadas¹; Matilde Melo¹; Liliana R Loureiro¹; Mário Grãos¹; Pedro Castanheira²; Sandra I. Anjo¹; ¹Center for Neuroscience and Cell Biology, Cantanhede, Portugal; ²Biocant, Cantanedo, Portugal
- PROTEOMICS: INFECTIOUS DISEASES**
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- TP 647 **Bacterial Identification Using Machine Learning Defined Peptide Signatures and its Validation by a Targeted Proteomics Approach under Routine Conditions;** Clarisse Gotti-Barban¹; Florence Roux-Dalvai¹; Mickael Leclercq¹; Frédéric Fournier¹; Marie-Claude Hélie²; Judith Marcoux¹; Isabelle Kelly¹; Tabiwang N. Arrey³; Cristina C. Jacob⁴; Claire Dauly³; Claudia P.B. Martins⁴; Julie Bestman-Smith⁵; Maurice Boissinot²; Michel G. Bergeron²; Arnaud Droit¹; ¹Proteomics Platform, CHU de Québec Research Centre, Laval University, Québec, QC; ²Infectiology Research Centre, CHU de Québec, Laval University, Québec, QC; ³Thermo Fisher Scientific, Bremen, Germany; ⁴Thermo Fisher Scientific, San Jose, CA; ⁵Enfant-Jésus Hospital, CHU de Québec, Laval University, Québec, QC
- TP 648 **Dynamic Bovine Milk Proteome Alterations during *Staphylococcus aureus* Infection in Subclinical and Clinical Mastitis;** Kiran Ambatipudi¹; Sudipa Maity¹; Debiprasanna Das²; ¹Indian Institute of Technology Roorkee, Roorkee, India; ²College of Veterinary Science and Animal Husbandry, Bhubaneswar, India
- TP 649 **Identifying the Molecular Mechanisms of Sex-Specific Severity of the Middle East Respiratory Syndrome Coronavirus (MERS-CoV) Using Proteomics;** Natarajan Bhanu¹; Simone Sidoli¹; Ranran Wu¹; Neeltje van Doremalen²; Vincent Munster²; Angela Rasmussen³; Benjamin A. Garcia⁴; ¹University of Pennsylvania, Philadelphia, PA; ²National Institutes of Health, Rocky Mountain Laboratories, Hamilton, MT; ³Columbia University Mailman School of Public Health, New York City, NY; ⁴University of Pennsylvania, Philadelphia, PA
- TP 650 **Quantitative Proteomics Analyses of Neuronal Cells Exposed to HIV-1 Infected MDM Supernatants with High Cathepsin B Secretion;** Camille N. Zenon¹; Estheisy Roman²; Abiel Roche Lima³; Kelvin Carrasquillo Carrión¹; Yadira M Cantres Rosario¹; Loyda M. Melendez¹; ¹University of Puerto Rico Medical Sciences Campus, San Juan, PR; ²Universidad del Este, Carolina, Puerto Rico
- TP 651 **Dynamic Proteomic Profiling of the Salmonella-Host Interplay Reveals New Modes of Action for Known and Novel Virulence Factors;** Jennifer Geddes-McAlister¹; Stefanie Vogt²; Jennifer Rowland²; Sarah Woodward²; Baerbel Raupach³; Brett Finlay²; Felix Meissner⁴; ¹University of Guelph, GUELPH, ON; ²University of British Columbia, Vancouver, BC; ³Max Planck Institute for Infectious Biology, Berlin, Germany; ⁴Max Planck Institute of Biochemistry, Martinsried, Germany
- TP 652 **New Insights in Formaldehyde-Induced Detoxification of the Tetanus Toxin: Chemical Modification Stoichiometry and Characterization of Intra- and Inter-Molecular Cross-Links;** Nour AL Turihi^{1,2}; Sébastien Peronin²; Arnaud Salvador¹; Fabien Barbirato³; Vincent Colombie³; Céline Rocca³; Catherine Jourdat³; Thierry Eynard²; Jérôme Lemoine¹; ¹Institut des Sciences Analytiques, UMR 5280 CNRS Université Lyon 1, Université de Lyon, Villeurbanne, France; ²MTech, Sanofi Pasteur, Neuville-sur-Saône, France; ³Sanofi Pasteur, Marcy l’Etoile, France
- TP 653 **Analysis of *Staphylococcus aureus* Infections through Spatially Targeted Micro-Proteomics;** Daniel Ryan^{1,2}; Nathan H. Patterson^{2,3}; James E. Cassat^{4,5,6}; Eric P. Skaar^{4,7,8}; Richard M. Caprioli^{1,2,3,9,10}; Jeffrey M. Spraggins^{1,2,3}; ¹Department of Chemistry, Vanderbilt University, Nashville, TN; ²Mass Spectrometry Research



- Center, Vanderbilt University, Nashville, TN; ³Department of Biochemistry, Vanderbilt University, Nashville, TN; ⁴Department of Pathology, Microbiology and Immunology, Vanderbilt University School of Medicine, Nashville, TN; ⁵Department of Pediatrics, Vanderbilt University Medical Center, Nashville, TN; ⁶Vanderbilt Center for Bone Biology, Vanderbilt University Medical Center, Nashville, TN; ⁷Vanderbilt Institute for Infection, Immunology, and Inflammation, Vanderbilt University Medical Center, Nashville, TN; ⁸United States Department of Veterans Affairs, Tennessee Valley Healthcare System, Nashville, TN; ⁹Department of Pharmacology, Vanderbilt University, Nashville, TN; ¹⁰Department of Medicine, Vanderbilt University, Nashville, TN
- TP 654 **Challenges in Clinical Metaproteomics Highlighted by the Analysis of Acute Leukemia Patients with Gut Colonization by Multidrug-Resistant *Enterobacteriaceae***; Julia Rechenberger¹; Patroklos Samaras¹; Anna Jarzab¹; Juergen Behr²; Martin Frejno¹; Ana Djukovic³; Jaime Sanz^{4,5}; Eva M. González-Barberá⁴; Miguel Salavert⁴; Jose Luis López-Hontangas⁴; Karina B. Xavier⁶; Laurent Debrauwer^{7,8}; Jean-Marc Rolain⁹; Miguel Sanz^{4,5}; Marc Garcia-Garcera¹⁰; Mathias Wilhelm¹; Carles Ubeda^{3,11}; Bernhard Kuster^{1,2}; ¹Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; ²Bavarian Center for Biomolecular Mass Spectrometry, Freising, Germany; ³Centro Superior de Investigación en Salud Pública-FISABIO, Valencia, Spain; ⁴Hospital Universitari i Politècnic La Fe, Valencia, Spain; ⁵CIBERONC, Instituto Carlos III, Madrid, Spain; ⁶Instituto Gulbenkian de Ciência, Oeiras, Portugal; ⁷Toxalim, Université de Toulouse, INRA, INP-ENVT, INP-EI-Purpan, Université de Toulouse 3 Paul Sabatier, Toulouse, France; ⁸Axiom Platform, UMR 1331 Toxalim, MetaToul-MetaboHUB, National Infrastructure of Metabolomics and Fluxomics, Toulouse, France; ⁹Aix Marseille Univ, IRD, APHM, MEPHI, IHU-Méditerranée Infection, Marseille, France; ¹⁰Department of Fundamental Microbiology, University of Lausanne, Lausanne, Switzerland; ¹¹Centers of Biomedical Research Network (CIBER) in Epidemiology and Public Health, Madrid, Spain
- TP 655 **Analysis of Zika Viral Polyprotein N- and O-glycosylation Using a Novel Lectin-chemoenzymatic Enrichment**; Shuang Yang¹; Felipe Assis¹; Wells W. Wu¹; Johnathan Sjogren²; Lisa Parsons¹; Helén Nyhlén²; Philip Onigman³; Rong-Fong Shen¹; Maria Rios¹; John F. Cipollo¹; ¹CBER, FDA, Silver Springs, MD; ²Genovis AB, Lund, Sweden; ³Genovis Inc., Cambridge, MA
- TP 656 **Comprehensive Analysis of the Human Cytomegalovirus Interactome to Identify Key Hubs of Protein Degradation**; Luis Nobre¹; Katie Nightingale¹; Benjamin J Ravenhill¹; Robin Antrobus¹; Gavin W.G. Wilkinson²; Richard J Stanton²; Edward L Huttlin³; Michael Weekes¹; ¹University of Cambridge, Cambridge, United Kingdom; ²University of Cardiff, Cardiff, United Kingdom; ³Harvard Medical School, Boston, MA
- TP 657 **Scalable Proteomic Analysis of Microbes (SPAM): A New Weapon in the Global Fight Against Antimicrobial Resistance**; Annegret Ulke-Lemee¹; Thomas Rydzak¹; Laurent Brechenmacher¹; Soren Wacker¹; Troy Feener¹; Mario E. Valdes-Tresanco¹; Tara Winstone²; Sergei Y. Noskov¹; Deirdre Church²; Ian A. Lewis¹; ¹University of Calgary, Calgary, AB; ²Calgary Laboratory Services, Calgary, AB
- TP 658 **Multiple Ion Chromatogram (MIC) for Direct Quantification of Intact Proteins Using Q-TOF Mass Spectrometry**; Yonghai Lu¹; Jie Xing¹; Djohan Kesuma¹; Zhaoqi Zhan¹; ¹Shimadzu Asia Pacific, Singapore, Singapore
- TP 659 **Impaired Degradation Dynamics of Synaptic Vesicle Machinery in APPKI Mice**; Nalini R Rao¹; Ewa Bomba-warczak¹; Timothy Hark¹; Jeffrey N. Savas¹; ¹Northwestern University, Chicago, IL
- TP 660 **Mass Spectrometry in the Development of Better Coagulation Tests: Quantitation and Proteoform Characterization of Antithrombin**; Renee Ruhaak¹; Fred P.H.T.M. Romijn¹; Mervin Pieterse¹; Jan Nouta¹; Nico Smit¹; Elena Dominguez-Vega¹; Yuri E.M. van der Burgt¹; Manfred Wuhrer¹; Christa M. Cobbaert¹; ¹LUMC, Leiden, Netherlands
- TP 661 **The Strange Case of “Picket Fence” Peaks: A Study in the Complexity of MS/MS Spectra of Protein Ions**; John E. P. Syka¹; Joshua D. Hinkle²; Christopher Mullen¹; Robert D’Ippolito²; Romain Huguet¹; Lissa C. Anderson³; Jeffrey Shabanowitz²; Donald F. Hunt²; ¹Thermo Fisher Scientific, San Jose, CA; ²University of Virginia, Charlottesville, VA; ³NHMFL, Florida State Univ., Tallahassee, FL
- TP 662 **A Direct Computational Approach to the Analysis of Multiply Charged Biomolecules and Their Modifications with Electrospray Mass Spectrometry**; Ning Zhang¹; Shundi Shi²; Shenglong Zhang¹; David Good³; Don Kuehl⁴; Yongdong Wang⁴; ¹Department of Life Sciences, New York Institute of Technology, New York, NY; ²Department of Chemical Engineering, Columbia University, New York, NY; ³Covance Laboratories Inc., Madison, WI; ⁴Cerno Bioscience, Norwalk, CT
- TP 663 **Top-down Proteomics and Metabolomics based Profiling and Characterization of Collagen by LC-QTOF-MS**; Tao Jiang¹; Todd Osiek¹; Xuejun Peng²; ¹Mallinckrodt, Hazelwood, MO; ²Bruker Daltonics Inc., San Jose, CA
- TP 664 **Liquid Chromatography – Triple Quadrupole Mass Spectrometry for Top-Down Quantitative Analysis of Low Abundance Intact Proteins from Biological Samples**; Katarina Marakova¹; Joshua Lee Isaacs²; Alex J Rai³; Kevin A Schug²; ¹Comenius University in Bratislava, Bratislava, Slovakia; ²The University of Texas at Arlington, Arlington, TX; ³Columbia University, New York, NY
- TP 665 **1400 Proteoforms Identified from Five Micrograms of Escherichia coli Proteins Using Online 2D pH RP/RPLC Top-Down Mass Spectrometry**; Zhe Wang¹; Dahang Yu¹; Xiaowen Liu²; Kenneth Smith³; Si Wu¹; ¹University of Oklahoma, Norman, OK; ²IUPUI, Indianapolis, IN; ³Oklahoma Medical Research Foundation, Oklahoma City, OK
- TP 666 **“Intact Proteomictrum” from Intact-Protein List between 10kDa to 200kDa in Eukaryotic Cell with in Trap-MALDI Mass Spectrometer**; Shih-Chieh Yang¹; Szu-Wei Chou¹; Yi-Teng Hsiao¹; pin-duo lee¹; ¹AcroMass technologies, Inc., Taipei, Taiwan
- PROTEOMICS: NEW APPROACHES I**
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- TP 667 **Toward Robust and High-Throughput Single Cell Proteomics Based on TMT Based Nanodroplet Sample Processing and Ultrasensitive LC-MS**; Maowei Dou¹; Jeremy C. Clair¹; William B. Chrisler¹; Kerui Xu¹; Ryan L. Sontag¹; Rui Zhao¹; Ronald J. Moore¹; Derek Bailey²; Greg A. Foster²; Daniel Lopez-Ferrer²; Richard D. Smith¹; Wei-Jun Qian¹; Ryan T. Kelly^{1,3}; Charles K. Ansong¹; Ying Zhu¹; ¹Pacific Northwest National Laboratory, Richland, WA; ²Thermo Fisher Scientific, San Jose, CA; ³Brigham Young University, Provo, UT
- TP 668 **Application of Probabilistic Information Retrieval for Ultra Rapid Peptide Sequencing Utilizing Comprehensive Protein Isoform Databases**; Jeffrey J. Jones¹; Ryan Benz¹; ¹SoCal Bioinformatics Inc., Montrose, CA
- TP 669 **Extremely Long-Lived Mitochondrial Proteins in Neuronal Health and Aging**; Ewa Bomba-warczak¹; Jeffrey N. Savas¹; ¹Northwestern University, Chicago, IL

PROTEOMICS: INTACT PROTEINS
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- TP 658 **Multiple Ion Chromatogram (MIC) for Direct Quantification of Intact Proteins Using Q-TOF Mass Spectrometry**; Yonghai Lu¹; Jie Xing¹; Djohan Kesuma¹; Zhaoqi Zhan¹; ¹Shimadzu Asia Pacific, Singapore, Singapore



- TP 670 **Single Cell Proteomic Analysis Using PASEF**; Catherine C L Wong; *Center for Precision Medicine Multiomics Research, Peking University, Beijing, China*
- TP 671 **Enriching Low Abundance APEX2 Biotin Modifications from Complex Mixtures**; Morgan Hepburn¹; Frances Snider¹; James D McGhee¹; David C Schriemer¹; ¹*University of Calgary, Calgary, AB*
- TP 672 **Spatiotemporally-Precise Proximity Proteomics Reveals Nuclear Lamina-Peripheral Chromatin Interactome in vivo**; Xi Zhang¹; Kanishk Abhinav²; Tess Branon³; Alice Ting³; John R. Yates, III²; Larry Gerace²; ¹*Scripps, La Jolla*; ²*Scripps Research, La Jolla, CA*; ³*Stanford University, Stanford, CA*
- TP 673 **Ultra-Fast Proteomics Enabled by Scanning SWATH and High-Flow Chromatography**; Christoph B Messner¹; Vadim Demichev^{2,3}; Spyros Vernardis³; Nic Bloomfield⁴; Gordana Ivosev⁴; Fras Wasim⁴; Stephen Tate⁴; Kathryn Lilley²; Markus Ralser^{3,5}; ¹*Francis Crick Institute, London, United Kingdom*; ²*Department of Biochemistry, University of Cambridge, Cambridge, United Kingdom*; ³*The Francis Crick Institute, London, United Kingdom*; ⁴*SCIEX, Concord, ON*; ⁵*Charité, Berlin, Germany*
- TP 674 **Proteomic Analysis of *Rhizopus microsporus* IOC4686 Fungus Isolated from Mining Environment: Screening for Protein Biomarkers Induced by Copper**; Meriellen Dias¹; Thalles Jocelino Gomes de Lacerda²; Lidiane Maria Andrade¹; Claudio Augusto Oller do Nascimento¹; Enrique Eduardo Rozas Sanchez¹; Maria Anita Mendes¹; ¹*Dempster MS Lab- Poli-USP, Sao Paulo, Brazil*; ²*Federal University of São Paulo, Sao Paulo-SP, Brazil*
- TP 675 ***Chlorella vulgaris* Microalgae: Proteomic Changes Due to Copper**; Lidiane Maria de Andrade¹; Meriellen Dias²; Cristiano José de Andrade^{3,5}; Maria Anita Mendes²; Jorge Alberto Soares Tenório⁴; Claudio Augusto Oller Nascimento²; ¹*Dempster MS Lab- Poli-USP, São Paulo, Brazil*; ²*Dempster MS Lab- Poli-USP, Sao Paulo, Brazil*; ³*LiEB – Integrated Laboratory of Biological Engineering - Department of Chemical Engineering and Food Engineering - Federal University of Santa Catarina (UFSC), Florianópolis, Brazil*; ⁴*LAREX-Laboratory of Recycling, Waste Treatment and Extraction-Poli-USP, São Paulo, Brazil*
- TP 676 **Novel Functional Proteomic Approach to Dissect G9a Interactomes Associated with Breast Tumorigenesis**; Adil Muneer¹; Ling Xie¹; Li Wang¹; Jin Jian²; Xian Chen^{1,3}; ¹*Department of Biochemistry & Biophysics, University of North Carolina at Chapel Hill, Chapel Hill, NC*; ²*Department of Pharmacological Sciences and Oncological Sciences, Icahn School of Medicine at Mount Sinai, New York City, NY*; ³*Lineberger Comprehensive Cancer Center, University of North Carolina at Chapel Hill, Chapel Hill, NC*
- TP 677 **Comparison and Optimization of Exosome Digestion and Fractionation Methods for Discovery Proteomic Analysis**; Elizabeth Nunn¹; Nancy Sharkawy¹; Amy-Joan L. Ham¹; ¹*Belmont University, Nashville, TN*
- TP 678 **Moving Towards Single-Cell Proteomics on a TIMS-qTOF Mass Spectrometer with PASEF**; Andreas-David Brunner¹; Florian Meier¹; Markus Lubeck²; Niels Goedecke²; Heiner Koch²; Scarlet Koch²; Oliver Raether²; Matthias Mann¹; ¹*Max-Planck Institute of Biochemistry, Planegg, Germany*; ²*Bruker Daltonik GmbH, Bremen, Germany*
- TP 679 **Cysteine Directed Proteolysis for Middle Down Proteomics**; Joe R. Cannon¹; J. Wade Harper²; Mark Cancilla¹; ¹*Merck & Co., Inc., West Point, PA*; ²*Harvard Medical School, Boston, MA*
- TP 680 **Proteomic Characterization of RAS-Signaling**; German Monogarov¹; Audrey Bettoun²; Yael Aylon²; Moshe Oren²; Jeroen Krijgsveld¹; ¹*German Cancer Research Center (DKFZ), Heidelberg, Germany*; ²*Weizmann Institute of Science, Rehovot, Israel*
- TP 681 **Microflow DIA Using 15min Gradients Analyzes 40 Tumor Proteomes per Day and Effectively Detects Promising Protein Biomarkers**; Rui Sun¹; Christie Hunter²; Chen Chen³; Huanhuan Gao¹; Xue Cai¹; Qiushi Zhang¹; Bo Wang⁴; Xiaoyan Yu⁵; Xiaodong Teng⁴; Lirong Chen⁵; Ruedi Aebersold⁶; Yi Zhu¹; Tiannan Guo¹; ¹*School of Life Sciences, Westlake University, 18 Shilongshan Road, Hangzhou 310024, Zhejiang Province, China, Hang Zhou, China*; ²*Sciex, Redwood City, CA*; ³*Sciex, Shanghai, China*; ⁴*Department of Pathology, The First Affiliated Hospital of College of Medicine, Zhejiang University, Hangzhou, China*; ⁵*Department of Pathology, The Second Affiliated Hospital, Zhejiang University School of Medicine, Hangzhou, China*; ⁶*Department of Biology, Institute of Molecular Systems Biology, ETH Zurich, Switzerland, Switzerland*
- TP 682 **A Novel Strategy Enabled by a Photo-Cleavable Surfactant for Extracellular Matrix Proteomics**; Samantha J Knott¹; Kyle Brown¹; Bifan Chen¹; Ying Ge^{1,2,3}; ¹*The University of Wisconsin Madison's Department of Chemistry, Madison, WI*; ²*The University of Wisconsin Madison's Department of Cell and Regenerative Biology, Madison, WI*; ³*The University of Wisconsin Madison's Human Proteomics Training Program, Madison, WI*
- TP 683 **Comprehensive Evaluation of Shotgun Proteomics Using Thermo Scientific Orbitrap Fusion Lumos Mass Spectrometer with FAIMS Pro Interface**; Yue Zhou¹; Min Huang¹; Xiangyun Yang¹; Mo Hu¹; Jing Li¹; ¹*Thermo Fisher Scientific, Shanghai, China*
- TP 684 **New Insights on Marfan Syndrome from Comparative N-Terminomics of Human Marfan and Non-Diseased Aortas**; Daniel Martin¹; Frank Cikach¹; Emidio Germano¹; Eric Roselli¹; Suneel Apte¹; ¹*Cleveland Clinic, Cleveland, OH*
- TP 685 **Enhancing the Isolation of DNA-Binding Protein from Yeast for High Confidence Interactome Analysis**; Ali Shariat-Panahi¹; Aditya Mojumdar¹; Jennifer A. Cobb¹; David C. Schriemer¹; ¹*Department of Biochemistry and Molecular Biology, University of Calgary, Calgary, AB*
- TP 686 **Effects of Different Tissue Preserving Methods on Proteomic Results**; Ruiqi Jian¹; Lihua Jiang¹; Huaying Fang¹; Meng Wang¹; Joanne Chan¹; Hua Tang¹; Mike Snyder¹; ¹*Stanford University School of Medicine, Palo Alto, CA*
- TP 687 **Plasma Proteomics Goes High Throughput**; Raphael A Heilig¹; Thomas Kosinski²; Yuxin Mi³; Katie L Burnham³; Julian C Knight³; Heiner Koch²; Roman Fischer¹; ¹*Target Discovery Institute, Nuffield Department of Medicine, University of Oxford, Oxford, United Kingdom*; ²*Bruker Daltonik GmbH, Bremen, Germany*; ³*Wellcome Centre for Human Genetics, University of Oxford, Oxford, United Kingdom*
- TP 688 **Large Scale Un-Depleted Human Serum Proteome Profiling and Targeted LC-MS/MS Evaluation toward Biomarker Discovery for Alzheimer's Disease**; Kaushik Kumar Dey¹; Hong Wang²; Mingming Niu²; Xusheng Wang²; yuxin Li²; Ji-Hoon cho²; Haiyan Tan²; Ashutosh Mishra²; Anthony High²; Thomas G Beach³; Junmin Peng²; ¹*St Jude Children's Research Hospital, Memphis, TN*; ²*St Jude Children's Research Hospital, Memphis, TN*; ³*Banner Sun Health Research Institute, Sun City, AZ*
- TP 689 **The Ultra-Soft Picosecond-Infrared Laser - Multi-Tool for Sampling Tissues for Mass Spectrometric Omics**; Hartmut Schluter¹; Marcel Kwiatkowski²; Marcus Wurlitzer¹; Andrey Krutilin^{1,3}; Frederik Busse³; Sascha Epp³; Nils-Owe Hansen³; Wesley Robertson^{3,4}; Dwayne R.J. Miller³; ¹*UKE - Mass Spec Proteomics, Hamburg, Germany*; ²*University of Groningen Faculty of Mathematics & Natural Sciences Pharmacokinetics, Toxicology and Targeting, Groningen, Netherlands*; ³*Max Planck Institute for the Structure & Dynamics of Matter, Atomically Resolved*



- Dynamics Division, Hamburg, Germany; ⁴Georgia Institute of Technology, Georgia Tech Research Institute, Quantum Systems Division, Atlanta, GA 30318*
- TP 690 **A Novel, Small Molecule-Based Method for Tunable Cell-Surface Proximity Labeling to Enable Mapping of Immunomodulatory Receptor Protein Interactions;** Rob Oslund¹; Niyi Fadeyi¹; Tamara Reyes Robles¹; Cory White¹; Jake Tomlinson¹; Kelly Crotty¹; David H. Perlman¹; Lee Roberts¹; Grazia Piizzi¹; Erik Hettl¹; ¹Merck Exploratory Sciences Center, Cambridge, MA
- TP 691 **A Labeling Enrichment Method Based on Synergistic and Reversible Covalent Interactions for Seleno Protein Analysis;** Qingshi Meng¹; Hongfu zhang¹; Xiaohui feng¹; ¹Institute of Animal Sciences, CAAS, Beijing, China
- TP 692 **Enhancing the Sensitivity of Microflow-Based Bottom-Up Proteomic Analyses by the Post-Column Addition of Organic Solvent Modifiers;** Ute Distler¹; Mateusz Krzysztof Łącki¹; Markus Wanninger²; Stefan Tenzer¹; ¹University Medical Center Mainz, Mainz, Germany; ²Waters Corporation, Milford, MA
- TP 693 **Combined Use of SAXS and LC-QTOF-MS in Structural Elucidation of Complex Biomolecules;** Hlengilizwe Nyoni¹; Bhekia B. Mamba¹; Titus TAM Msagati¹; ¹University of South Africa, Johannesburg, South Africa
- TP 694 **Utilizing Metabolic Isotope Labels to monitor protein and Lipid Metabolism to Integrate Alzheimer's Risk Factors into a Cohesive Model;** Joseph Creery¹; Russell Denton¹; Isabella James¹; Kyle J Cutler¹; John Price²; ¹Brigham Young University, Provo, UT; ², Provo, UT
- PROTEOMICS: QUANTITATIVE II**
695-717
- TP 695 **Understanding the Underlying Biological Pathways Affected by Treatment of Triple Negative Breast Cancer with Novel Natural Product Derivatives;** Alisha Birk¹; Catherine C. Going¹; Dhanir Tailor²; Vineet Kumar²; Abel Bermudez¹; Fernando García-Marqués¹; Malleš Pandrala²; Angel Resendez²; Meghan A. Rice¹; Tanya Stoyanova^{1,3}; Sanjay V. Malhotra^{1,2,3}; Sharon J. Pitteri^{1,3}; ¹Department of Radiology, Canary Center at Stanford for Cancer Early Detection, Stanford University School of Medicine, Palo Alto, CA; ²Department of Radiation Oncology, Stanford University School of Medicine, Palo Alto, CA; ³Stanford Cancer Institute, Stanford University School of Medicine, Stanford, CA
- TP 696 **Block Design Enables Highly Reproducible Label-Free Quantitative Proteomics to Profile Cell Responses to Engineered Nanomaterials;** Tong Zhang¹; Matthew J Gaffrey¹; Becky M Hess¹; Karl K Weitz¹; Ronald J. Moore¹; Brian D Thrall¹; Wei-Jun Qian¹; ¹Pacific Northwest National Laboratory, Richland, WA
- TP 697 **Arc-Negative Extracellular Vesicles Promote Bidirectional Synaptic Communication through CaMKII;** Yi-Zhi Wang¹; Samuel N. Smukowski¹; Claire Piochon¹; Ewa Bomba-warczak¹; Qionger He¹; Stacy A. Marshall¹; Elizabeth T. Bartom¹; Ali Shilatifard¹; Anis Contractor¹; Jeffrey N. Savas¹; ¹Northwestern University, Chicago, IL
- TP 698 **Multiplex TMT Based Protein Quantification on timsTOF Pro with Parallel Accumulation and Serial Fragmentation Method;** Pei Liu¹; Brian P. Mooney¹; Michael Sussman²; C. Michael Greenlief¹; ¹University of Missouri, Columbia, MO; ²University of Wisconsin-Madison, Madison, WI
- TP 699 **Quantitative Proteomics: A New Tool for Understanding the Complexity of a Fermentation Media and the Upstream Process of Bacterial Vaccine;** Sébastien Peronin¹; Julia Novion-Ducassou¹; Thierry Eynard¹; ¹Sanofi Pasteur, Neuville-sur-Saône, France
- TP 700 **Dawn to Sunset Fasting for Four Weeks Has A Unique Proteomic Signature in Healthy Subjects;** Antrix Jain¹; Sung Yun Jung¹; Mustafa Abdulsada¹; Antone Opekun¹; Anna Malovannaya¹; Prasun Jalal¹; Ayse Mindikoglu¹; ¹Baylor College of Medicine, Houston, TX
- TP 701 **Determining and Characterizing Substrates of Impaired Protein Degradation in Models of Alzheimer's Disease;** Timothy Hark¹; Ewa Bomba-Warczak¹; Samuel N. Smukowski¹; Laith Ali¹; Jeffrey N. Savas¹; ¹Northwestern University, Chicago, IL
- TP 702 **Bayesian Confidence Intervals for Multiplexed Proteomics Integrate Ion Statistics with Peptide Quantification Concordance;** Leonid Peshkin¹; Meera Gupta²; Lillia Ryazanova²; Martin Wuhr²; ¹Harvard Medical School, Boston, MA; ²Princeton University, Princeton, NJ
- TP 703 **A Super-Silac Method to Assess Myogenesis in Healthy vs Dystrophin-Deficient Muscle Cells;** Mansi V. Goswami¹; Emily Canessa¹; Yetrib Hathout¹; ¹School of Pharmacy and pharmaceutical Sciences, University of Binghamton, Binghamton, NEW YORK
- TP 704 **Molecular Phenotypes Identification by Proteomic Profiling in Nematode Myopathy Using timsTOF Pro Mass Spectrometer;** Liwen Zhang¹; Sophie R. Harvey¹; Rebecca A. Slick^{2,3,4}; Jennifer A. Tinklenberg^{2,3,4}; Federica Montanaro⁵; Michael W. Lawlor^{2,3}; ¹The Ohio State University, Columbus, OH; ²Department of Physiology, Medical College of Wisconsin, Milwaukee, WI; ³Division of Pediatric Pathology, Department of Pathology and Laboratory Medicine and Neuroscience Research Center Medical College of Wisconsin, Milwaukee, WI; ⁴Clinical and Translational Science Institute of Southeast Wisconsin, Medical College of Wisconsin, Milwaukee, WI; ⁵Institute of Child Health, University College London, London, United Kingdom
- TP 705 **Spatially-Resolved Neuroproteomics with IonStar Reveals Differential Landscapes of Signal Transduction Dysregulation in a Rat Ischemic Stroke Model;** Shichen Shen¹; Min Ma²; Ming Zhang¹; David Poulsen¹; Jun Qu¹; ¹University at Buffalo, Buffalo, NY; ²Roswell Park Comprehensive Cancer Center, Buffalo, NY
- TP 706 **Elucidating Novel Mechanisms of Action and Effects on Biological Pathways of Next Generation Anti-Cancer/Bacteria Complexes Using UHR-MS/MS;** Kung-Ching Cookson Chiu¹; Yuko P. Y. Lam¹; Christopher A. Wootton¹; Hannah Bridgewater¹; Feng Chen¹; Mark P. Barrow¹; John Moat¹; Peter J. Sadler¹; Peter B. O'Connor¹; ¹University of Warwick, Coventry, United Kingdom
- TP 707 **Insights into NEDD8 Inhibition on Proteostasis with Multiplexed Proteome Dynamics Profiling and super-Resolution Orbitrap Mass Spectrometry;** Nico Zinn¹; Konstantin Aizikov²; Dmitry Grinfeld²; Arne Kreuzmann²; Daniel Mourad²; Oliver Lange²; Maria Fälth-Savitski¹; Markus Queisser³; Alexander Makarov²; Marcus Bantscheff¹; ¹Cellzome, a GSK company, Heidelberg, Germany; ²Thermo Fisher Scientific, Bremen, Germany; ³GSK, Stevenage, United Kingdom
- TP 708 **Carrier Proteome Effect in Mass Spectrometry Based Approaches to Single Cell Proteomics;** Christopher M. Rose¹; Atticus McCoy¹; Donald S. Kirkpatrick¹; ¹Genentech, Inc., South San Francisco, CA
- TP 709 **Intact Glycopeptide Analysis of Triple Negative Breast Cancer Cell Lines Using IsoTaG;** Fernando Garcia-Marques¹; Catherine C. Going¹; Abel Bermudez¹; Marc D Driessen²; Alisha Birk¹; Carolyn R Bertozzi²; Christina Woo³; Sharon J. Pitteri¹; ¹Stanford University School of Medicine, Canary Center at Stanford for Cancer Early Detection, Palo Alto, CA; ²Department of Chemistry and Howard Hughes Medical Institute, Stanford University, Stanford, CA; ³Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA



- TP 710 **Isobaric Reporter Ion Cascades for High Capacity Multiplexing**; Brian Erickson¹; Ryan Kunz¹; Steven P Gygi²; [Craig Braun](#)¹; ¹*IQ Proteomics LLC, Cambridge, MA*; ²*Harvard Medical School, Boston, MA*
- TP 711 **Detection of Peptide Level Changes in Cerebro Spinal Fluid Proteomes of Neurodegenerative Disease by Data-Independent Acquisition**; [Deanna Plubell](#)¹; Eric Huang¹; Michael S. Bereman²; Thomas Montine³; Michael J MacCoss¹; ¹*University of Washington, Genome Sciences, Seattle, WA*; ²*North Carolina State University, Raleigh, NC*; ³*Stanford University, Stanford, CA*
- TP 712 **Investigation and Characterization of the Jumping Translocation Breakpoint (JTB) Protein Using Mass Spectrometry Based Proteomics**; [Madhuri Jayathirtha](#)¹; Devika Channaveerappa¹; Kangning Li¹; Costel C Darie¹; ¹*Clarkson University, Potsdam, NY*
- TP 713 **Effects to the Human Proteome Due to Legacy Chemical Exposure in the Great Lakes**; [Emmalyn J Dupree](#)¹; Bernard Crimmins¹; Thomas Montine³; James Pagano²; Brooke Thompson³; Krista Christensen³; Michelle Raymond³; Jon Meiman³; Costel C Darie¹; ¹*Clarkson University, Potsdam, NY*; ²*SUNY Oswego, Oswego, NY*; ³*Wisconsin Department of Health Services, Madison, WI*
- TP 714 **High-Throughput Quantitative Profiling of Small GTPases in Brain Tissues of Alzheimer's Disease Patients**; Ming Huang¹; Yinsheng Wang²; ¹*University of California, Riverside, CA*; ²*University of California, Riverside, Riverside, CA*
- TP 715 **Discovery of Novel Guanine-Quadruplex-Unwinding Proteins**; [Zi Gao](#)¹; Lin Li¹; Preston Williams¹; Yinsheng Wang¹; ¹*University of California, Riverside, Riverside, CA*
- TP 716 **Quantitative Profiling of Small GTPases in Secretome of Cultured Human Cancer Cells Using Scheduled MRM Coupled with Stable Isotope-Labeled Peptides**; [Tianyu Qi](#)¹; Ming Huang¹; Yinsheng Wang¹; ¹*UC Riverside, Riverside, CA*
- TP 717 **Proteome Quality Control Addressing Qualitative and Quantitative Needs for Trapped Ion Mobility Spectrometry and Parallel Accumulation Serial Fragmentation**; [Michael Krawitzky](#)¹; Chris Adams¹; Conor Mullens²; Shourjo Ghose²; Matthew Willetts²; Gary Kruppa²; ¹*Bruker Daltonics Inc., San Jose, CA*; ²*Bruker Daltonics Inc., Billerica, MA*
- PROTEOMICS: TOP DOWN ANALYSIS II**
718-737
- TP 718 **Proteoform Family Identification and Quantification Using Proteoform Suite**; [Leah V Schaffer](#)¹; Michael R Shortreed¹; Anthony J Cesnik¹; Jarred W Rensvold²; Adam Jochem²; Trisha Tucholski¹; Mark Scalfi¹; Brian L Frey¹; Ying Ge¹; David J Pagliarini^{1,2}; Lloyd M Smith¹; ¹*University of Wisconsin - Madison, Madison, WI*; ²*Morgridge Institute for Research, Madison, WI*
- TP 719 **An Iodine-Based N-Terminal Mass Defect Labelling Strategy for Improved de novo Top-Down Protein Sequencing**; [Lavrentis Dimitrios Galanopoulos](#)¹; Lennete Kjaer¹; Adam Karpinski²; Sam Hughes¹; David J Clarke¹; ¹*University of Edinburgh, Edinburgh, United Kingdom*; ²*University of Warsaw, Warsaw, Poland*
- TP 720 **FLASHDeconv: Ultra-Fast High-Quality Deconvolution Enables Online Processing of Top-Down MS Data**; [Kyowon Jeong](#)¹; Jihyung Kim¹; Manasi Gaikwad²; Siti Nurul Hidayah²; Hartmut Schlüter²; Oliver Kohlbacher^{1,3,4,5,6}; ¹*Applied Bioinformatics, Department for Computer Science, University of Tübingen, Tübingen, Germany*; ²*Mass Spectrometric Proteomics, Institute of Clinical Chemistry and Laboratory Medicine, Campus Forschung, Universitätsklinikum Hamburg-Eppendorf, Hamburg, Germany*; ³*Center for Bioinformatics, University of*
- Tübingen, Tübingen, Germany*; ⁴*Center for Quantitative Biology, University of Tübingen, Tübingen, Germany*; ⁵*Biomolecular Interactions, Max Planck Institute for Developmental Biology, Tübingen, Germany*; ⁶*Translational Bioinformatics, University Hospital Tübingen, Tübingen, Germany*
- TP 721 **Isotope Pattern Matching Software for Mass Analysis of Intact Proteins**; [Greg T. Blakney](#)¹; Lissa C Anderson¹; Allen G. Marshall¹; Christopher L. Hendrickson^{1,2}; ¹*National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL*; ²*Florida State University, Tallahassee, FL*
- TP 722 **A Fast and High-Throughput Sample Preparation Platform Coupled with Top-Down Mass Spectrometry for Therapeutic Antibody Analysis**; [Hae-Min Park](#)¹; Jared Drader²; Valerie J. Winton¹; Sheri Manalili-Wheeler²; Neil L. Kelleher¹; Philip D. Compton²; ¹*Northwestern University, Evanston, IL*; ²*Integrated Protein Technologies, Inc., Evanston, IL*
- TP 723 **Comprehensive Characterization of Kinases by Top-Down Mass Spectrometry**; [Zhijie Wu](#)¹; Yutong Jin¹; Bifan Chen¹; Ying Ge¹; ¹*University of Wisconsin, Madison, Madison, WI*
- TP 724 **Early Diagnostics of Clinical Samples by Top-Down Proteomics Using Capillary Electrophoresis-Electrospray Ionization-Mass Spectrometry (CESI-MS)**; [Amir Prior](#)¹; David Morgenstern¹; Alexandra Gabashvili¹; Dalia Elinger¹; Hila Wolf-Levy¹; Moshe E. Gatt²; Yishai Levin¹; ¹*Weizmann Institute of Science, Rehovot, Israel*; ²*Hadassah-Hebrew University Medical School, Jerusalem, Israel*
- TP 725 **High-Throughput Top-Down FAIMS Data Analysis with ProSight PD Nodes in the Thermo Scientific Proteome Discoverer Software**; Susan E. Abbatiello¹; Michael W. Belford²; Philip D. Compton³; Kenneth R. Durbin⁴; Ryan Fellers⁴; Vincent Gerbasi³; Joseph Greer⁴; [Mick Greer](#)⁵; David Horn²; Romain Huguet²; Neil L. Kelleher³; Richard LeDuc⁴; Scott M. Peterman²; Paul M Thomas³; ¹*Northwestern University, Boston, MA*; ²*Thermo Fisher Scientific, San Jose, CA*; ³*Northwestern University, Evanston, IL*; ⁴*Proteinaceous, Inc., Evanston, IL*; ⁵*Thermo Fisher Scientific, Austin, TX*
- TP 726 **Proteomic Characterization of Truncated Proteoforms in MDSC Extracellular Vesicles**; [Dapeng Chen](#)¹; Fabio P Gomes¹; Suzanne Ostrand-Rosenberg²; Catherine Fenselau¹; ¹*Department of Chemistry and Biochemistry, University of Maryland, College Park, MD*; ²*Department of Biological Sciences, University of Maryland Baltimore County, Baltimore, MD*
- TP 727 **Top Down Quantitation of Oxidative Proteomics**; [Surendar Tadi](#)¹; Joshua S Sharp²; ¹*University of Mississippi, Oxford, MS*; ²*University of Mississippi, University, MS*
- TP 728 **Native State Chemical Tagging Approaches for the Free Radical-Initiated Sequencing of Intact Protein Complexes**; [Carolina Rojas Ramirez](#)¹; Daniel A. Polasky¹; Brandon T. Ruotolo¹; ¹*University of Michigan, Ann Arbor, MI*
- TP 729 **Direct Thermal Proteome Profiling Using Quantitative Top-Down Proteomics**; [Kellye A Cupp-Sutton](#)¹; Zhe Wang¹; Si Wu¹; ¹*University of Oklahoma, Norman*
- TP 730 **MASH Explorer, a Universal, Comprehensive, and User-Friendly Software Environment for Top-down Proteomics**; [Sean J McIlwain](#)¹; Zhijie Wu²; Kent Wenger³; Molly Wetzel³; Trisha Tucholski²; Xiaowen Liu^{4,5}; Ruixiang Sun⁶; Irene M Ong^{1,7}; Ying Ge^{2,3,8,9}; ¹*Department of Biostatistics and Medical Informatics, University of Wisconsin, Madison, WI*; ²*Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706*; ³*Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI*; ⁴*Department of BioHealth Informatics, Indiana University-Purdue*



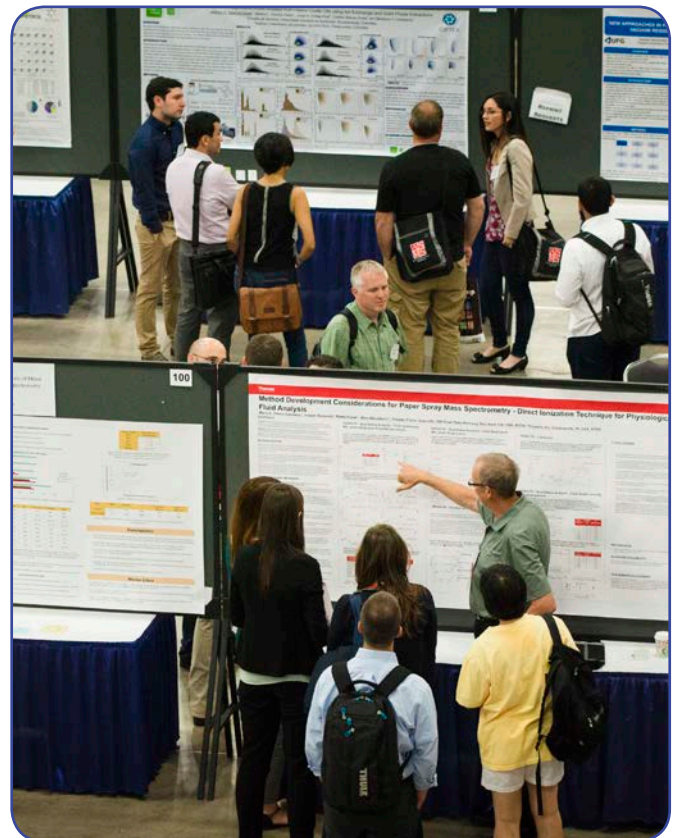
- University Indianapolis, Indianapolis, Indiana; ⁵Center for Computational Biology and Bioinformatics, Indiana University School of Medicine, Indianapolis, Indiana; ⁶Institute of Computing Technology, CAS, Beijing, China; ⁷Department of Obstetrics and Gynecology, University of Wisconsin-Madison, Madison, WI; ⁸Molecular and Cellular Pharmacology Program, University of Wisconsin, Madison, WI; ⁹Human Proteomics Program, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI
- TP 731 **Comparison of ECD versus ETD for Low-Charge State Proteins in Orbitrap and Q-ToF Instruments**; Yury V. Vasil'ev^{1,2}; Jared B. Shaw³; Valery G. Voinov^{1,4}; Joseph C. Meeuwssen⁵; Nathan I. Lopez^{1,2}; Joseph S. Beckman^{2,6}; ¹Linus Pauling Institute, Oregon State University, Corvallis, OR; ²e-Msion, Inc., Corvallis, OR; ³Pacific Northwest National Laboratory, Richland, WA; ⁴e-Msion Inc., Corvallis, OR; ⁵Oregon State University, Corvallis, OR; ⁶Linus Pauling Institute, Oregon State University, Corvallis, OR
- TP 732 **Targeting a Subset of the Membrane Proteome for Top-Down Mass Spectrometry; the Proteolipids that Extract into Chloroform**; Whitaker Cohn¹; Lucy Gao¹; Julian Whitelegge¹; ¹University of California LA, Los Angeles, CA
- TP 733 **Deep Intact Proteome Quantification Using Protein-Level Tandem Mass Tag (TMT) Labeling and Online 2D Liquid Chromatography**; Dahang Yu¹; Zhe Wang¹; Kellye A Cupp-Sutton¹; Kenneth Smith²; Xiaowen Liu³; Si Wu¹; ¹University of Oklahoma, Norman, OK; ²Oklahoma Medical Research Foundation, Oklahoma City, OK; ³Indiana University-Purdue University Indianapolis, Indianapolis, IN
- TP 734 **Investigating the Stability of Linear Polyacrylamide Coating for Capillary Zone Electrophoresis-Tandem Mass Spectrometry-Based Top-Down Proteomics**; Tian Xu; Michigan State University, East Lansing, MI
- TP 735 **Top-Down Proteomics in Support of the Industrial Milk Production Process**; Catherine Rawlins^{1,2}; Stéphane Claverol³; Audrey Romelard³; Caroline Tokarski^{1,2}; ¹Institute of Chemistry and Biology of Membrane and NanoObjects, UMR CNRS 5248, Bordeaux, France; ²Proteome Platform, Center of Functional Genomics of Bordeaux, University of Bordeaux, Bordeaux, France; ³Ingredia Dairy Experts, Arras, France
- TP 736 **Investigating the Protein Recovery of Membrane-Based Sample Preparation Methods for Top-Down Proteomics**; Qianjie Wang; Michigan State University, East Lansing, MI
- TP 737 **Top-Down Analysis of Snake Venom Proteoforms through de novo Sequencing**; Kira Vyatkina¹; Daniel Petras²; ¹SPb Academic University, St Petersburg, Russian Federation; ²University of California, San Diego, CA
- SMALL MOLECULES: QUALITATIVE ANALYSIS**
738-756
- TP 738 **Interpretation of Mass Spectrometric Data for Structure Elucidation of a New Endogenous Organosulfur Metabolite**; Qibo Zhang¹; Lisa A. Ford¹; Anne M. Evans¹; Douglas R. Toal¹; ¹Metabolon, Morrisville, NC
- TP 739 **Mass Spectroscopic Analysis of Phenol Derivatives by Gibbs Reaction**; Sabyasachy Mistry; Purdue University, West Lafayette
- TP 740 **An Efficient Approach to Oligomer Screening of Extractables Samples Using Liquid Chromatography Quadrupole Time-of-flight Mass Spectrometry (LC/Q-TOF)**; Kuang-Wei Yang¹; Jin Ren¹; Benben Song¹; ¹Pall Corporation, Westborough, MA
- TP 741 **Pharmaceutical Degradation Product Profiling on an Orbitrap ID-X Tribrid Mass Spectrometry Platform**; G. Charles Cheng¹; Kate J. Comstock²; Xiaojie C. Ding²; Seema Sharma²; ¹Blueprint Medicines, Cambridge, MA; ²Thermo Fisher Scientific, San Jose, CA
- TP 742 **Investigation and Profiling of Organic Solvent Based Lithium Ion Battery Electrolytes and the Decomposition Products**; Nan Hu; Agilent Technologies, Beijing, China
- TP 743 **An Alternative Screening Protocol for Determining Amines in Industrial Materials Using Combined Flow Injection (FI) Electrospray-TOFMS and Electrospray-TOFMS/MS Methods**; Dale A. Willcox¹; Jenan M. Elias²; Kelli Magarelli¹; Marshall Henry¹; ¹Intertek Allentown, Allentown, PA; ²Intertek, Allentown, PA
- TP 744 **Identification of Degradation Products of Epirubicin Based on multiple heart-cut2D LC-Q TOF**; Yaping Zhang¹; Hui Ouyang²; Congfang Lai³; ¹Agilent Technologies, Shanghai, China; ²Jiangxi University of Traditional Chinese Medicine, Nanchang, China; ³Agilent Technologies(China) Co. Ltd., Beijing, China
- TP 745 **Elucidating Disperse Dye Photodegradation Pathways Using Tandem Mass Spectrometry and Density Functional Theory**; Ciera E Cipriani¹; Erol Yildirim²; Cody P Zane¹; Stephanie E Atkinson¹; Nelson R Vinuesa¹; Melissa A Pasquinelli¹; ¹Wilson College of Textiles, North Carolina State University, Raleigh, NC; ²Institute of High Performance Computing, Agency for Science, Technology and Research, Singapore
- TP 746 **Simplified Approach for Structural Elucidation and Quantitation for Pharmaceutical API and Related Impurities Using Q-TOF**; Purushottam Janardan Sutar¹; Shaileendra Rane¹; Shailesh Damale¹; Rashi Kochhar¹; Deepti Bhandarkar¹; Anant Lohar¹; Ashutosh Shelar¹; Bhaumik Trivedi¹; Navin Devadiga¹; Ajit Datar¹; Pratap Rasam¹; Jitendra Kelkar¹; ¹Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India
- TP 747 **So Which Is It? In-Column Thermal Isomerization of Volatile Acid Emitted from Urethane Conformal Coating and Determining Identification Confidence**; Curtis D. Mowry¹; Lance L. Miller¹; Jessica Roman¹; Adam S. Pimentel¹; Raymond Fuentes¹; Jason R. Brown¹; ¹Sandia National Laboratories, Albuquerque, NM
- TP 748 **Development of LC-MS/MS Method to Detect and Evaluate Clinically Relevant Antibiotics in Human Stool Samples from Patients with Cholera**; Laura Bailey¹; Ashton Marrazzo¹; Manasi Kamat¹; Eric J. Nelson¹; Kari B. Green¹; ¹University of Florida, Gainesville, FL
- TP 749 **Improved Structural Characterisation of Molecules with a Chimeric Collision Cell with both Electron-Based and Collision-Induced Dissociation Capability**; Yves Le blanc¹; Takashi Baba²; Pavel Ryumin²; Bill Loyd²; Eva Duchoslav²; ¹SCIEX, Concord, ON, ON; ²SCIEX, Concord, ON
- TP 750 **Detection of Reactive Dye from soil via QuEChERS extraction and Quadrupole Time-Of-Flight Mass Spectrometry**; Xinyi Sui¹; Chengcheng Feng¹; Yufei Chen²; Mary Ankeny³; Nelson Vinuesa¹; ¹North Carolina State University, Raleigh, NC; ²Jordi Labs, Mansfield, MA; ³Cotton Incorporated., Cary, NC
- TP 751 **Application of Mass Spectrometry for Studying the Degradation of Amino Acids and Volatile Organic Compounds by Chlorine Dioxide**; Ngee Sing Chong¹; Abdul Hoque^{1,2}; Heather Deal¹; Beng Guat Ooi¹; ¹Middle Tennessee State University, Murfreesboro, TN; ²University of Cincinnati, Cincinnati, OH
- TP 752 **Identification of Impurities in the Organic Solvents Used in the Semiconductor Field by Using GC-HRTOFMS with EI/FI**; Koji Okuda¹; John Dane¹; Robert Cody¹; ¹JEOL USA, Inc., Peabody, MA
- TP 753 **Selective Gas-Phase Mass Tagging via Ion/Molecule Reactions Combined with Single Analyzer Neutral Loss Scans to Probe Pharmaceutical Mixtures**; Dalton T. Snyder¹; Lucas J. Szalwinski¹; Alice Pilo²; Nina K. Jarrah²; R. Graham Cooks¹; ¹Purdue University, West Lafayette, IN; ²Merck & Co., Inc., Rahway, NJ



- TP 754 **Evaluation of Alternate MS/MS Fragmentation Tools, Including UVPD and EID, for the Structural Eluciation of Trace Level Metabolites;** [Jeffrey Gilbert](#)¹; Jesse L Balcer¹; David G McCaskill¹; Nick N Wang¹; Chengli C Zu¹; Yelena A Adelfinskaya¹; J.C. Yves Le blanc²; ¹Corteva Agriscience, Indianapolis, IN; ²SCIEX, Concord, ON
- TP 755 **A New Electrochemical Route for Carbon-Carbon Bond Formation: Electrochemistry-Assisted Intermolecular [3+2] Annulation of N-cyclopropyl-3, 5-dimethylaniline and Styrene;** [Qi Wang](#)¹; Qile Wang²; Nan Zheng²; Richard N Zare³; Yuexiang Zhang⁴; Hao Chen^{1,4}; ¹New Jersey Institute of Technology, Newark, NJ; ²University of Arkansas, Fayetteville, AR; ³Stanford University, Stanford, CA; ⁴Ohio University, Athens, OH
- TP 756 **Building Local Proprietary Libraries with Automated MSn Spectral Tree Curation and New Library Searching Tools;** [Xiaojie C. Ding](#)¹; Kate J. Comstock²; Seema Sharma²; Mark Sanders²; Michal Raab³; ¹Thermo Scientific, San Jose, Ca, CA; ²Thermo Fisher Scientific, San Jose, CA; ³HighChem, Bratislava, Slovakia
- SYSTEMS BIOLOGY**
757-780
- TP 757 **Molar Quantification of Metabolic Pathways Elucidates the Mechanism of Metabolic Shift In *Caenorhabditis elegans*;** [Bharath Kumar Raghuraman](#)¹; Sider Penkov¹; Teymuras V. Kurzchalia¹; Andrej Shevchenko¹; ¹Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany
- TP 758 **Using Highly-Multiplexed Panels of Quantitative MRM Assays to Establish Normal Tissue Protein Concentrations in Mice;** [Sarah Michaud](#)¹; Helena Pětrošová¹; Angela Jackson¹; Andrea L. Palmer¹; Nicholas J. T. Sinclair¹; Ann Flenniken^{2,3}; Lauryl Nutter^{2,4}; Colin McKerlie^{2,4}; Milan Ganguly^{2,4}; Ingo Feldmann⁵; Olga Shevchuk⁵; Yassene Mohammed^{1,6}; David Schibli¹; Albert Sickmann⁵; Christoph H. Borchers^{1,7,8,9}; ¹University of Victoria-Genome BC Proteomics Centre, Victoria, BC; ²The Centre for Phenogenomics, Toronto, ON; ³Lunenfeld-Tanenbaum Research Institute, Sinai Health System, Toronto, ON; ⁴The Hospital for Sick Children, Toronto, ON; ⁵Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Dortmund, Germany; ⁶Center for Proteomics and Metabolomics, Leiden University Medical Center, Leiden, Netherlands; ⁷Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC; ⁸Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; ⁹Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC
- TP 759 **Interferon Stimulated Gene 15 Controls Phagosome Maturation;** [Frederic Lamoliatte](#)¹; Tiaan Heunis¹; Anetta Svitorka Hartlova¹; Matthias Trost¹; ¹ICAMB, Newcastle University, Newcastle Upon Tyne, United Kingdom
- TP 760 **Multi-Omics Profiling and Customized gRNA Library CRISPR-CAS9 Genomic Screening Identify Cancer Vulnerabilities in Brain Tumors;** [Hong Wang](#)¹; Mingming Niu²; Timothy I. Shaw²; yuxin Li²; Ji-Hoon cho²; Anthony High¹; Vishwajeeth Pagala²; Xusheng Wang²; Junmin Peng¹; ¹St. Jude Children's Research Hospital, Memphis, TN; ²St. Jude children's Research hospi, Memphis, TN
- TP 761 **Longitudinal Metaproteomic Characterization Simultaneously Reveals the Presence and Functions of Bacteria and Eukaryotes in the Gut Microbiomes of Preterm Infants;** [Samantha L. Peters](#)^{1,2}; Patrick T. West³; Feiqiao Brian Yu⁴; Brian A. Firek⁵; Michael J. Morowitz⁵; Jillian F. Banfield⁶; Robert L. Hettich^{2,7}; ¹Oak Ridge National Laboratory, Oak Ridge, Tennessee; ²University of Tennessee, Knoxville, TN; ³University of California Berkeley, Berkeley, California; ⁴Chan Zuckerberg Biohub, San Francisco, CA; ⁵University of Pittsburgh School of Medicine, Pittsburgh, PA; ⁶University of California, Berkley, Berkeley, CA; ⁷Oak Ridge National Laboratory, Oak Ridge, TN
- TP 762 **Advancing Insights in Molecular Regulation of *Leishmania donovani* by Integration of Multi-Omics Data.;** [Bart Cuypers](#)^{1,2}; Malgorzata A. Domagalska²; Pieter Meysman¹; Wout Bittremieux^{1,3}; Hideo Imamura²; Dirk Valkenburg⁴; Geert Baggerman^{1,5}; Inge Mertens^{1,5}; Jean-Claude Dujardin^{1,2}; Kris Laukens¹; ¹University Of Antwerp, Antwerp, Belgium; ²Institute Of Tropical Medicine, Antwerp, Belgium; ³University of Washington, Seattle, WA; ⁴University of Hasselt, Diepenbeek, Belgium; ⁵Vito, Mol, Belgium
- TP 763 **A Novel HLA-Peptide Profiling Workflow Called MAPTAC (Mono-Allelic-Purification-with-Tagged-Allele-Constructs) Leverages Mass Spectrometry to Improve Neoantigen Prediction;** [Daniel Rothenberg](#)¹; Jennifer Abelin¹; Dominik Bartheleme¹; Rob C Oslund¹; Amanda L Creech¹; Tyler Colson¹; Scott P Goulding¹; Lia R Serrano¹; Chris McGann¹; Ying S Ting¹; Yusuf Nasrullah¹; Janani Sridar¹; Dewi Harjanto¹; Matt Malloy¹; Christina Kuksin¹; Joel Greshock¹; Terri A Addona¹; Michael S Rooney¹; ¹Neon Therapeutics, Cambridge, MA
- TP 764 **MS-Based Metaproteomics Reveals Details of Microbiome Adaptation to Increasing Plant Biomass Substrate Loading to Maintain Undiminished Lignocellulose Solubilization;** [Payal Chirania](#)^{1,2}; Suresh Poudel²; Richard J. Giannone^{1,2}; Xiaoyu Liang³; Evert K. Holwerda³; Lee R. Lynd³; Robert L. Hettich^{1,2}; ¹University of Tennessee, Knoxville, Knoxville, TN; ²Oak Ridge National Laboratory, Oak Ridge, TN; ³Dartmouth College, Hanover, NH
- TP 765 **Identifying Novel TBK1 Substrates Using an Optimized TMT-Based Phosphoproteomics Method;** [Laura E Herring](#)¹; Emily M Wilkerson¹; Lianxin Hu¹; Dennis Goldfarb¹; Lee M Graves¹; Qing Zhang¹; ¹UNC-Chapel Hill, Chapel Hill, NC
- TP 766 **Metagenomic-based Metaproteomic Functional Characterization of the Sargasso Sea in a Three Year Time Series Dataset;** [Mak Saito](#)¹; Brian Searle²; Dawn Moran³; Jaci Saunders³; Noelle Held³; Chris Dupont⁴; Rod Johnson⁵; Matthew McIlvin³; ¹Woods Hole Oceanographic Inst., Woods Hole Ma 02543, MA; ²Institute for Systems Biology, Seattle, Washington; ³Woods Hole Oceanographic Institution, Woods Hole; ⁴J. Craig Venter Institute, La Jolla, CA; ⁵Bermuda Institute of Ocean Sciences, St. Georges, Bermuda
- TP 767 **Single Colony Metaproteomes of a Marine Bacterium: Exploring Heterogeneity in the Natural Environment;** [Noelle Held](#)^{1,2}; Matthew McIlvin¹; Eric Webb³; Mak Saito¹; ¹Woods Hole Oceanographic Institution, Woods Hole; ²Massachusetts Institute of Technology, Cambridge, MA; ³University of Southern California, Los Angeles, CA
- TP 768 **Cellular Dynamics of Protein-Protein Interactions Mediated by Serine Phosphorylation;** [Kyle Mohler](#)¹; Karl Barber¹; Jack Moen¹; Svetlana Rogulina¹; Jesse Rinehart¹; ¹Yale University, West Haven, CT
- TP 769 **Quantitative Protein Expression and Phosphorylation Level Profiling Using 11-plex TMT Reagents: Application to 110 Yeast Kinase and Phosphatase Deletion Strains;** [Jiaming Li](#)¹; Joao A. Paulo¹; David Nusinow¹; Edward Huttlin¹; Steven Gygi¹; ¹Harvard Medical School, Boston, MA
- TP 770 **Targeted Proteomics-Driven Computational Modeling of the Mouse Macrophage Toll-like Receptor Signaling Pathway;** [Nathan P Manes](#)¹; Jessica M Calzola¹; Pauline R Kaplan¹; Iain DC Fraser¹; Ronald N Germain¹; Martin Meier-Schellersheim¹; Aleksandra Nita-lazar¹; ¹National Institutes of Health, Bethesda, MD



- TP 771 **Universal Proteomic Approach of Capturing Novel and Dynamic Trafficking Organelle Assemblies;** Nan Wang¹; Thomas Lee¹; Mary Katherine Connacher¹; Tianjing Hu¹; Scott Stuart¹; Natalie Ahn¹; ¹Department of Biochemistry, University of Colorado, Boulder, CO
- TP 772 **Investigating Proteome Changes Caused by ABCA7 Missense Variants that Confer Alzheimer's Disease Risk in African Americans;** Tyra M. Avery¹; Kaitlyn E. Stepler¹; Prem Prakash²; Jamaine S. Davis²; Renā A.S. Robinson^{1, 3, 4, 5, 6}; ¹Vanderbilt University Department of Chemistry, Nashville, TN; ²Meharry Medical College Department of Biochemistry and Cancer Biology, Nashville, TN; ³Vanderbilt University Medical Center Department of Neurology, Nashville, TN; ⁴Vanderbilt Memory and Alzheimer's Center Vanderbilt University Medical Center, Nashville, TN; ⁵Vanderbilt Institute of Chemical Biology, Nashville, TN; ⁶Vanderbilt Brain Institute, Nashville, TN
- TP 773 **A Peptidogenomics Approach Reveals the Identification of the *Canidae hepcidin*;** Martin K Mead¹; Melissa Claus^{2, 3}; Ed Litton^{4, 5}; Lisa Smart^{2, 3}; Anthea Rasis^{2, 3}; Gabriele Rossi^{2, 3}; Robert D Trengove^{1, 6}; Joel P. A. Gummer^{1, 6}; ¹Separation Science and Metabolomics Laboratory, Research and Innovation, Murdoch University, Perth, Australia; ²College of Veterinary Medicine, Murdoch University, Perth, Australia; ³School of Veterinary Science, Murdoch University, Perth, Australia; ⁴Intensive Care Unit, Fiona Stanley Hospital, Perth, Australia; ⁵School of Medicine, University of Western Australia, Perth, Australia; ⁶Metabolomics Australia, Western Australia Node, Murdoch University, Perth, Australia
- TP 774 **Proteome-Wide Optimization of Orthogonal Translation Systems;** Jack M Moen¹; Kyle Mohler¹; Svetlana Rogulina¹; Jesse Rinehart¹; ¹Yale University, West Haven, CT
- TP 775 **Proteotyping 30 Mouse Knockouts Using Targeted Quantitative Plasma Proteomics with Heavy-Labeled Internal Standards and the Software Tool KOPF Gene;** Yassene Mohammed^{1, 2}; Simon Roome¹; Sarah A. Michaud¹; Helena Pětrošová¹; Ann Flenniken^{3, 4}; Lauryl Nutter^{3, 5}; Colin McKerlie^{3, 5}; Milan Ganguly^{3, 5}; Christoph H. Borchers^{1, 6, 7, 8}; ¹University of Victoria-Genome BC Proteomics Centre, Victoria, BC; ²Center for Proteomics and Metabolomics, Leiden University Medical Center, Leiden, Netherlands; ³The Centre for Phenogenomics, Toronto, ON; ⁴Lunenfeld-Tanenbaum Research Institute, Sinai Health System, Toronto, ON; ⁵The Hospital for Sick Children, Toronto, ON; ⁶Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC; ⁷Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; ⁸Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC
- TP 776 **Top-down Proteomics for Deciphering Hypertrophic Cardiomyopathy in a Patient-Specific Engineered Cardiac Tissue Disease Model;** Stanford D. Mitchell^{1, 2}; Willem J. de Lange³; Jianhua Zhang⁴; Gina Kim⁴; Trisha Tucholski⁵; Timothy J. Kamp^{1, 4}; J. Carter Ralphe³; Ying Ge^{1, 2, 5}; ¹Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI; ²Molecular and Cellular Pharmacology Graduate Training Program, Madison, Wisconsin; ³Department of Pediatrics, School of Medicine and Public Health, University of Wisconsin-Madison, MADISON, WI; ⁴Department of Medicine, School of Medicine and Public Health, University of Wisconsin - Madison, Madison, Wisconsin; ⁵Department of Chemistry, University of Wisconsin-Madison, Madison, WI
- TP 777 **Quantitative Lipidomics and Proteomics Analysis of HDL Particles from Patient Samples Separated by Preparative Two Dimensional Gel Electrophoresis;** Zsuzsanna Kuklennyik¹; Katrin Niisuke²; Michael Gardner¹; Antony Lehtikoski¹; Christopher Toth¹; John R Barr¹; Tomas Vaisar^{3, 4}; Bela Asztalos²; ¹Centers for Disease Control and Prevention, Atlanta, Georgia; ²Tufts University, Boston, MA; ³University of Washington, DEOHS, Seattle, WA; ⁴University of Washington, UWMDI, Seattle, WA
- TP 778 **A Proteogenomic Systems Analysis Reveals Alterations in RNA Binding Proteins and RNA Splicing in Alzheimer's Disease Brain;** Erik C.B. Johnson¹; Eric B. Dammer¹; Duc M. Duong¹; Luming Yin¹; Madhav Thambisetty²; Juan C. Troncoso³; James J. Lah¹; Allan I. Levey¹; Nicholas T. Seyfried¹; ¹Emory University, Atlanta, GA; ²National Institute on Aging, National Institutes of Health, Baltimore, MD; ³Johns Hopkins University School of Medicine, Baltimore, MD
- TP 779 **Systematic AP/MS and Genetic Interaction Mapping of the Ras Pathway Reveals New Effectors and Vulnerabilities;** Peter K Jackson¹; Marcus R Kelly¹; Kaja Kostyrko²; Kyuho Han¹; Michael Bassik¹; Alejandro Sweet-Cordero²; ¹Stanford University School of Medicine, Stanford, CA; ²UCSF, San Francisco, CA
- TP 780 **Integrated Proteome and Phosphoproteome Analysis Suggest a Role of JNK3 in Myelination and Synaptic Function;** Jan-Philip Schülke¹; Mercedes Priego Luque²; Norma Hernandez²; Daniel Bader¹; Barbara Kracher¹; Sarah Elschenbroich¹; Uli Ohmayer¹; Oxana Lavrova³; Jim Rosinski⁴; Christoph Schaab¹; Gerardo A Morfini²; Ignacio Munoz-Sanjuan³; ¹Evotec (München) GmbH, Martinsried, Germany; ²University of Illinois at Chicago, Department of Anatomy and Cell Biology, Chicago, IL; ³CHDI Foundation, Los Angeles, CA; ⁴CHDI Foundation, Princeton, NJ





WEDNESDAY POSTERS

Set up all Wednesday posters
7:00 - 8:00 am

Odd-numbered posters present
10:30 - 11:30 am PLUS 12:30 - 2:30 pm

Even-numbered posters present
10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

Remove all Wednesday posters
7:00 - 8:00 pm

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AMBIENT IONIZATION: APPLICATIONS I 001-031

- WP 001 **Open Probe Fast GC-MS and its Recent Real Time Forensic Medical and Food Safety Analysis Applications;** Benjamin Neumark¹; Uri Keshet¹; Alexander B. Fialkov¹; Tal Alon¹; Aviv Amirav¹; ¹Tel-Aviv University, Tel-Aviv, Israel
- WP 002 **Open Ambient Ionisation Source Coupled to a Mass Detector for Rapid Detection of Undeclared Active Ingredient(s) in Online Health Supplements;** Chris Henry; Waters Corporation, Cheshire, United Kingdom
- WP 003 **Protein Screening of Native Brain Sections Using LESA-TIMS-MS;** Yaxia L. Cintron-Diaz¹; Mario E. Gomez Hernandez¹; Jennifer Dziedzic¹; Tomas R. Guilarte¹; Francisco A. Fernandez-Lima¹; ¹Florida International University, Miami, FL

- WP 004 **Absolute Quantitation of Tryptophan Metabolites in Brain Tissue Using Paper Spray Ionization-High Resolution Mass Spectrometry;** Richard C Dilworth¹; Vanessa Y. Rubio¹; Gary P Wang¹; Timothy J. Garrett¹; ¹University of Florida, Gainesville, FL
- WP 005 **Rapid Drug Detection by Ultrasonic Nebulizer Coupled with Atmospheric-Pressure Chemical Ionization for Food-Product Analyses;** Linxia Song¹; Yi You²; Theresa Evans-Nguyen³; ¹University of Florida, Tampa, FL; ²Federal Institute for Materials Research and Testing (BAM), Berlin, Germany; ³University of South Florida, Tampa, FL
- WP 006 **A Novel Approach to Simultaneous Quantification of Tropane Alkaloids in Plant Tissue (Datura spp.) Using DART-HRMS and PLS Linear Regression;** Samira Beyramysoltan¹; Rabi A. Musah¹; ¹Department of Chemistry, State University of New York at Albany, Albany, NY
- WP 007 **A Coated Blade Spray - Mass Spectrometry (CBS-MS) Method for Simultaneous Screening of 68 Drugs and Metabolites in Urine;** Shirin Hooshfar¹; Simone Tchu¹; German A. Gómez-Ríos^{2,3}; Daniel A. Rickert³; Janusz Pawliszyn³; Kara Lynch¹; ¹University of California, San Francisco (UCSF), San Francisco, CA; ²Restek Corporation, Bellefonte, PA; ³University of Waterloo, Waterloo, ON
- WP 008 **Real-Time Analysis of the Metabolic Profile of Microglia Using Liquid Microjunction Surface Sampling Coupled with High-Resolution Mass Spectrometry;** Taylor M. Domenick¹; Vinata Vedam-Mai¹; Timothy J. Garrett¹; Richard A. Yost¹; ¹University of Florida, Gainesville, FL
- WP 009 **DART-MS: Enabling Safer Reaction Monitoring and Analysis Conditions with In Hood Vaporization;** Brittany Laramee¹; Frederick Li¹; Paul Liang¹; Brian Musselman¹; ¹IonSense, Inc, Saugus, MA
- WP 010 **High Throughput 96-Pin Solid Phase Microextraction Array for Direct Analysis in Real Time;** Paul Liang¹; Frederick Li¹; Brittany Laramee¹; Brian Musselman¹; ¹IonSense, Inc, Saugus, MA
- WP 011 **Can Reducing Sample Volume and Desorption Time Lead during Ambient Ionization lead to Improved Drug Detection from Biological Fluids;** Brian D. Musselman¹; Paul Liang²; ¹IonSense, Inc., Saugus, MA; ²IonSense, Inc., Saugus, MA
- WP 012 **The Eight(y) Million Pound Question: Using DESI Ambient MS Imaging for the Forensic Analysis of Cheque Fraud;** Huqin Zhong¹; Zhengwei Jia¹; Wei Rao¹; ¹Waters Technologies (Shanghai) Co, Ltd, Shanghai, China
- WP 013 **Rapid Screening of New Synthetic Drugs in Plasma Samples Using Paper Spray Mass Spectrometry with Integrated Solid-Phase Extraction Cartridge;** Greta J. Ren¹; Brandon J. Bills¹; Nicholas E. Manicke¹; ¹IUPUI Department of Chemistry & Chemical Biology, Indianapolis, IN
- WP 014 **Sub-Microliter Metabolomics via Triboelectric Nanogenerator-Induced Nanospray Mass Spectrometry;** Yafeng Li¹; Marcos Bouza Areces¹; Changsheng Wu²; Danning Huang¹; Gilad Doron³; Johnna S Temenoff^{3,4}; Arlene A. Stecenko⁵; Zhong Lin Wang^{2,6}; Facundo M Fernandez^{1,7}; ¹School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA; ²School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, Georgia; ³W.H. Coulter Department of Biomedical Engineering, Georgia Institute of Technology and Emory University, 315 Ferst Drive, Atlanta, GA 30332, Atlanta, Georgia; ⁴Petit Institute for Bioengineering and Bioscience, Georgia Institute of Technology, Atlanta, Georgia; ⁵Emory+Children's Center for Cystic Fibrosis and Airways Disease Research and Department of Pediatrics, Emory University School of Medicine and Children's Healthcare of Atlanta, Atlanta, Georgia; ⁶Beijing Institute of Nanoenergy and Nanosystems, Chinese Academy of



- Sciences, Beijing, China; ⁷Petit Institute of Bioengineering and Biosciences, Georgia Institute of Technology, Atlanta, Georgia
- WP 015 **Ambient Mass Spectrometry Immunoassays Using Small-Molecule Signal Amplifiers for Zeptomole Protein Detection;** Shuting Xu¹; Wen Ma¹; Yu Bai¹; Huwei Liu¹; ¹Peking University, Beijing, China
- WP 016 **Nitrogen and Ion Source Parameters: Considerations for Nitrogen Direct Analysis in Real Time;** Frederick Li¹; Paul Liang¹; Brittany Laramée¹; Brian Musselman¹; ¹IonSense, Inc., Saugus, MA
- WP 017 **Molecular Level Identification of Soil Organic Matter from Polar Region by solid phase LDI-FTICR-MS;** Seulgidan Lee¹; Sunghwan Kim¹; ¹Kyungpook National University, Daegu, South Korea
- WP 018 **Lower Detection Limits for Paper Spray Mass Spectrometry Using on Paper Extraction;** Brandon Bills¹; Nicholas E. Manicke¹; ¹IUPUI Department of Chemistry & Chemical Biology, Indianapolis, IN
- WP 019 **Rapid Identification of Wuyi Rock Tea Regions using the Direct Analysis in Real Time (DART) MS System with LiveID;** Yuhong Qin¹; Wei Rao¹; Huiqin Zhong¹; Fang Shu¹; Zhengwei Jia¹; Defeng Huang¹; Clara Chen¹; Kate Yu¹; ¹Waters Technologies (Shanghai) Co., Ltd, Shanghai, China
- WP 020 **Acoustic Mist Ionisation (AMI) a Rapid Approach for the Development of Mass Spectrometry Libraries;** Michael McCullagh¹; Sara Stead¹; Gareth Rhys Jones¹; Michelle Wood¹; Severine Goscinny²; Nayan Mistry¹; Kenneth Rosnack³; ¹Waters Corporation, Wilmslow, United Kingdom; ²Sciensano, Brussels, Belgium; ³Waters Corporation, Milford, MA
- WP 021 **A Validated Method for Quantification of Mescaline in Recreationally-abused EchinopsisCacti by Direct Analysis in Real Time Mass Spectrometry;** Cameron Longo¹; Rabi A. Musah¹; ¹University at Albany - SUNY, Albany, NY
- WP 022 **Detection of Organometallic Compounds on a Waters QDa Mass Spectrometer Equipped with a Helium-Plasma-Ionization (HePI) Source;** Athula B. Attygalle¹; Julius Pavlov¹; David Douce²; Steve Bajic³; ¹Stevens Institute of Technology, Hoboken, NJ; ²Waters corporation, Wilmslow, United Kingdom; ³Waters Corporation, Wilmslow, United Kingdom
- WP 023 **Rapid Quantitative Analysis of Six Anti-arrhythmic Drugs in Human Serum Using Direct Analysis in Real Time Mass Spectrometry;** Yuzhou Gui¹; Xiaokun Duan²; Kerry Song²; Jiale Xu²; Charles C. Liu²; Hong Yan³; Youli Lu¹; Gangyi Liu¹; ¹Central Laboratory, Shanghai Xuhui Central Hospital/Zhongshan - Xuhui Hospital, Fudan University /Shanghai Clinical Center, Chinese Academy of Sciences, Shanghai, China; ²ASPEC Technologies Limited, Beijing, China; ³Shanghai Institute of Medical Genetics, Shanghai Children's Hospital, Shanghai Jiao Tong University School of Medicine, Shanghai, China
- WP 024 **Direct insertion probe and atmospheric pressure ionization coupled to high-resolution mass spectrometry for the description of lignocellulosic biomass;** Clément Castilla¹; Christopher P. Rüger¹; Hélène Lavanant¹; Carlos Afonso¹; ¹Normandie Univ, INSA Rouen, UNIROUEN, CNRS, COBRA, Rouen, France, Rouen, France
- WP 025 **A Prototype Direct Sampling Inlet for the Rapid Analysis of Target Analytes in the Chemical Industry;** Rachel Sanig¹; David Douce¹; Jeff Goshawk¹; Caitlyn Da Costa¹; Gordon Jones¹; Eleanor Riches¹; ¹Waters Corporation, Wilmslow, United Kingdom
- WP 026 **Ambient Ionisation Mass Spectrometry: A novel diagnostic tool for debugging electronic circuits;** Barry Smith¹; Cedric Boisdon¹; Simon Maher¹; ¹University of Liverpool, Liverpool, United Kingdom
- WP 027 **Wood Discrimination Analyses of Pterocarpus tinctorius and Endangered P. santalinus Using DART-FTICR-MS Coupled with Multivariate Statistics;** Maomao Zhang^{1,2}; Yafang Yin^{1,2}; Wen Zhou³; Jiang Zhou³; Xiaokun Duan⁴; Charles C. Liu⁴; ¹Department of Wood Anatomy and Utilization, Research Institute of Wood Industry, Chinese Academy of Forestry, Beijing, China; ²Wood Collections (WOODPEdia), Chinese Academy of Forestry, Beijing, China; ³Peking University, Beijing, China; ⁴ASPEC Technologies, Beijing, China
- WP 028 **Direct Analysis in Real Time Mass Spectrometry and Multivariate Data Analysis for Profiling of Chinese Propolis;** Yilei Huang¹; Zhongping Huang¹; Charles C. Liu²; Kezhi Jiang³; Lili Wang⁴; Xiaokun Duan²; ¹Zhejiang University of Technology, Hangzhou, China; ²ASPEC Technologies, Beijing, China; ³Hangzhou Normal University, Hangzhou, China
- WP 029 **Intact Metabolomics by PESI/MS/MS and its Application to Metabolic Profiling of Acetaminophen-Induced Acute Hepatic Injury Model Mice;** Tomomi Ohara¹; Kenta Kondo¹; Tasuku Murata²; Tetsuya Ishikawa³; Akira Ishii¹; Hitoshi Tsuchihashi¹; Koretsugu Ogata²; Yumi Hayashi^{3,4}; Kei Zaitzu^{1,4}; ¹Department of Legal Medicine and Bioethics, Nagoya University Graduate School of Medicine, Nagoya, Japan; ²Shimadzu Corporation, Kyoto, Japan; ³Pathophysiological Laboratory Sciences, Department of Radiological and Medical Laboratory Sciences, Nagoya University Graduate School of Medicine, Nagoya, Japan; ⁴In Vivo Real-Time Omics Laboratory, Institute for Advanced Research, Nagoya University, Nagoya, Japan
- WP 030 **Rapid Analysis of Drugs in Plasma Using Probe Electro-spray Ionization Mass Spectrometry;** Hidekazu Saiki¹; Tasuku Murata¹; Koretsugu Ogata¹; Takahiro Inoue²; Kenji Nakayama³; Koji Shimizu²; Osamu Ogawa²; ¹Shimadzu corp., Kyoto, Japan; ²Kyoto University, Kyoto, Japan; ³Shimadzu Techno-Research, Inc., Kyoto, Japan
- WP 031 **Direct Analysis of Cell Wall Lipids from Mycobacterium via LESA-MS;** Rian L Griffiths¹; Luke Alderwick²; ¹University of Nottingham, Nottingham, United Kingdom; ²University of Birmingham, Birmingham, United Kingdom

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- WP 032 **MALDI-In-Source Decay FT-ICR MS for Top-Down and Middle-Down Characterization of Monoclonal antibodies;** Christoph J. Gstöttner¹; Yuri E.M. van der Burg¹; David P. A Kilgour²; Yury Tsybin³; Manfred Wuhrer¹; Simone Nicolardi¹; ¹Center for Proteomics and Metabolomics, LUMC, Leiden, Netherlands; ²Department of Chemistry, Nottingham Trent University, Nottingham, United Kingdom; ³Spectroswiss, Lausanne, Switzerland
- WP 033 **A Comparative Study of N-Glycosylation Assays for the Characterization of Fc and Fab N-Glycans on Monoclonal Antibodies;** John F. Kelly¹; Tammy-Lynn Tremblay¹; Denis Brochu¹; Robotham Anna¹; ¹Human Health Therapeutics, National Research Council of Canada, Ottawa, ON
- WP 034 **MS-based Characterization of a Novel Antibody Against Marburg Virus Nucleoprotein;** Yanchun Lin¹; Britney Johnson²; Angela Zou²; Kathleen C.F. Sheehan²; Gaya Amarasinghe²; Daisy Leung²; Michael L. Gross¹; ¹Department of Chemistry, Washington University in St Louis, St Louis, MO; ²Department of Pathology and Immunology, Washington University School of Medicine, St Louis, MO
- WP 035 **Rapid Conjugation, Proteolysis and Purification of Antibodies Using High Capacity CaptureTM Membranes;** Christian Hoppmann¹; Mandy Li¹; Michael Vierra¹; Boris Levitan¹; Gia Jokhadze¹; Andrew Farmer¹; ¹Takara Bio USA, Mountain View, CA



- WP 036 **Quantitative MFLC-MS/MS Analysis of the Antibody Drug Conjugate SigmaMAb Extracted from Rat Plasma Using Thermo Scientific MSIA Microcolumns;** Chad Christianson¹; Jennifer Zimmer¹; Kwasi Antwi²; Chris Ross²; Shane R Needham¹; ¹Alturas Analytics, Moscow, ID; ²Thermo Fisher Scientific, West Palm Beach, FL
- WP 037 **Top-down Proteogenomics Analysis of Serum Autoantibody Repertoire for the Discovery of Biomarker of Systemic Lupus Erythematosus;** Zhe Wang¹; Xiaowen Liu²; Kenneth Smith³; Si Wu¹; ¹University of Oklahoma, Norman, OK; ²Indiana University-Purdue University Indianapolis, Indianapolis, IN; ³Oklahoma Medical Research Foundation, Oklahoma City, OK
- WP 038 **High Sensitivity Native Analysis of Monoclonal antibodies by Electrokinetically Pumped Sheath-Flow Capillary Zone Electrophoresis-Mass Spectrometry on a Q-TOF Mass Spectrometer;** Xiaojing Shen¹; Zhichang Yang¹; David Wong²; Qiangwei Xia³; Liangliang Sun¹; ¹Michigan State University, East Lansing, MI; ²Agilent Technologies, Santa Clara, CA; ³CMP Scientific Corp, New York, NY
- WP 039 **Characterization of Monoclonal Antibody Biosimilar through C-terminal and Disulfide Bond Peptides Sequencing Analysis on Q-TOF Mass Spectrometer;** Udi Jumhawan¹; Zhaoyi Zhan¹; ¹Shimadzu Asia Pacific, Singapore, Singapore
- WP 040 **Application of a Label-Free and Domain-Specific Free Thiol Method in Monoclonal Antibody Characterization;** Yi Pu¹; Yunqiu Chen¹; Tai Nguyen¹; Chong-Feng Xu¹; Li Zang¹; Zoran Sosic¹; Tyler Carlage¹; ¹Biogen, Cambridge, MA
- WP 041 **Enabling Single-cell Clone Selection for Knob-in-Hole Bispecific Antibodies via Automated Affinity Capture Coupled to High-throughput RapidFire Mass Spectrometry;** William Sawyer¹; Neha Srikumar²; Joseph Carver²; Phillip Y. Chu²; Amy Shen²; Ankai Xu²; Ambrose Williams²; Cong Wu²; Yichin Liu²; John C. Tran²; ¹Genentech, South San Francisco, CA; ²Genentech, Inc., South San Francisco, CA
- WP 042 **Towards Better Characterizing Drug-Antibody Ratios in Antibody-Drug Conjugates with Ion Mobility Separations in Structures for Lossless Ion Manipulations;** Gabe Nagy¹; Isaac K. Attah¹; Yue-Mei Zhang²; James Lanter²; Jared B. Shaw¹; Sandilya V. B. Garimella¹; Harsha P. Gunawardena²; Richard D. Smith¹; Yehia M. Ibrahim¹; ¹Pacific Northwest National Laboratory, Richland, WA; ²Janssen Research and Development, Spring House, PA
- WP 043 **Regulated LCMS bioanalysis of Monoclonal Antibodies in Human Serum for Inflammatory Immune Disease Management Using Novel Fab-Selective nSMOL Chemistry;** Noriko Iwamoto¹; Atsushi Yonezawa^{2,3}; Kazuo Matsubara³; Takashi Shimada^{1,4}; ¹Shimadzu Scientific Instruments, Bothell, WA; ²Kyoto University, Kyoto, Japan; ³Kyoto University Hospital, Kyoto, Japan; ⁴Shimadzu Corporation, Kyoto, Japan
- WP 044 **A Proteomic Approach to Single Chain Camelid Antibody Discovery;** Anand Patel¹; Natalie Castellana¹; Thiago Lima¹; Stefano Bonissone¹; ¹Digital Proteomics, LLC., San Diego, CA
- WP 045 **Affinity Based LC-MS Method for Improved Determination of HCP-ELISA Reagent Coverage;** Christina Seisenberger¹; Stefanie Wohlrab¹; ¹Roche Diagnostics GmbH, Penzberg, Germany
- WP 046 **A Large Scale Comparison of MS-based Antibody De Novo Protein Sequencing and Targeted DNA Sequencing;** Zac McDonald¹; Signy Chow^{2,3}; Kathleen Gorospe¹; Xin Xu¹; Paul Taylor¹; Qixin Liu¹; Trevor J Pugh²; Suzanne Trudel²; Bin Ma⁴; ¹Rapid Novor Inc., Kitchener, ON; ²University Health Network/Princess Margaret Hospital, Toronto, ON; ³Sunnybrook Health Sciences Centre, Toronto, ON; ⁴University of Waterloo, Waterloo, ON
- WP 047 **Exploring the Effects of Media on Glycosylation of Biotherapeutics with Reduced Mass and Multi-Attribute Method (MAM) Analysis;** Yuko Ogata¹; Nancy S Nightlinger¹; Richard S Rogers¹; ¹Just Biotherapeutics, Seattle, WA
- WP 048 **Monitoring of DAR/ADC attributes for Trastuzumab Emtansine;** Sibylle Heidelberger¹; Ferran Sanchez²; ¹AB Sciex UK Ltd, Warrington, United Kingdom; ²SCIEX, Madrid, Spain
- WP 049 **Rapid and Automated LCMS Characterization of Antibody and Protein Drug Conjugates;** Mark E. Hall¹; Robert Schuster¹; Kevin McCarl¹; ¹Novatia LLC, Newtown, PA
- WP 050 **Interactions of Hepatitis B Virus Capsids with Importin β and Anti-viral Drugs Monitored by Charge Detection Mass Spectrometry;** Christine Kim¹; Nicholas A. Lykтей¹; Adam Zlotnick¹; Martin F. Jarrold¹; ¹Indiana University, Bloomington, IN
- WP 051 **In-Depth Characterization of *in vivo* Biotransformations for Trastuzumab Emtansine by Orbitrap MS;** Jintang He¹; Shang-Fan Yu¹; Sharon Yee¹; Surinder Kaur¹; Keyang Xu¹; ¹Genentech Inc., South San Francisco, CA
- WP 052 **Characterization of N-Glycan Species of VEGF Decoy Receptor Fusion Protein by Novel HILIC-LC Separation with High Sensitive Mass Spectrometric Characterization;** Mihir Mahendra Thakar¹; Faraz Rasid²; Dipankar Malakar²; Bobby Virasingh¹; Manoj Pillai²; ¹Phenomenex India Pvt Ltd, Hyderabad, India; ²SCIEX INDIA, GURUGRAM, India
- WP 053 **Affinity Purification of IdeZ Digest for Glycosylation Profile of Immunoglobulins Using a Linear Benchtop MALDI-TOFMS;** Yuzo Yamazaki¹; Shuichi Nakaya¹; ¹Shimadzu Corporation, Kyoto, Japan
- WP 054 **Investigation of Ocular Tissue Disposition of Antibody-Drug Conjugates Using Novel LC-MS-Based Strategies;** Xiaoyu Zhu¹; Ming Zhang²; Jie Pu¹; Shihan Huo¹; Chao Xue¹; Jun Qu^{1,2}; ¹University at Buffalo, Buffalo, NY; ²New York State Center of Excellence in Bioinformatics & Life Sciences, Buffalo, New York
- WP 055 **Strategies for Sample Handling and Characterization of Antibody-Drug Conjugates by Quadrupole Mass Spectrometry;** Malin Källsten^{1,2}; Matthijs Pijnappel²; Rafael Hartmann^{1,2}; Fredrik Lehmann³; Lucia Kovac²; Sara Bergström Lind¹; Jonas Bergquist¹; ¹Uppsala University, Uppsala, Sweden; ²Recipharm OT Chemistry AB, Uppsala, Sweden; ³Oncopeptides AB, Stockholm, Sweden
- WP 056 **Optimization of a LC/MS Method for Disulfide Characterization and Free Cysteine Quantification in Protein Therapeutics;** Song Nie¹; Xin Chen¹; Jun Lun¹; ¹Catalent Pharma Solutions, Madison, WI
- WP 057 **A New Preparation Method Enabling Targeted Quantification of Biotherapeutics, Biomarker/Target Levels in FFPE Tissues with High Protein Recovery and Reproducibility;** Chao Xue¹; Jie Pu¹; Shihan Huo¹; Xiaoyu Zhu¹; Ming Zhang²; Jun Qu^{1,2}; ¹University at Buffalo, Buffalo, NY; ²New York State Center of Excellence in Bioinformatics & Life Sciences, Buffalo, New York
- WP 058 **Cleavage of Intact Monoclonal Antibodies by Cathepsin L and D Studied by Native Mass Spectrometry;** Wilfred Tang¹; Marshall Bern¹; Andrew C Nichols¹; Jing Zhu²; Tomislav Caval²; Albert J.R. Heck²; ¹Protein Metrics Inc., Cupertino, CA; ²Utrecht University, Utrecht, Netherlands
- WP 059 **High Resolution MS-based Structural Characterization Plays a Key Role in ADC Process Development;** Zhiqi Hao¹; Diana Y. Liu¹; Qiuting Hong^{2,3}; Michael Kim¹; William Haskins^{1,4}; Tomasz Baginski¹; Yan Chen¹; ¹Genentech,



- South San Francisco, CA; ²Eurofins Lancaster Laboratories, Inc., Lancaster, PA; ³Allakos Inc., Redwood City, CA; ⁴Gryphon Bio Inc, South San Francisco, CA
- WP 060 **Development of a Fully Automated Peptide Mapping Procedure;** Chen Qian¹; Rob Brian Jimenez¹; Ben Niu¹; Methal Albarghouthi¹; ¹MedImmune, Gaithersburg, MD
- WP 061 **Assessment of Anti-drug Antibodies in Cynomolgus Monkey Dosed with an Antibody Drug Conjugate Using Immunocapture-LC/MS;** Luying Chen^{1,2}; Linlin Dong¹; Nicole Bebrin¹; Hiroshi Sugimoto¹; Martin Paton¹; Dong Wei¹; Mark Qian¹; ¹Takeda Pharmaceuticals International, Inc., Cambridge, MA; ²Linus Pauling Institute, College of Pharmacy, Oregon State University, Corvallis, OR
- WP 062 **Antibody Subunit LC-MS Analysis from Pre-Clinical Studies for Biotransformation & Catabolism Determination;** John Kellie; GSK, King Of Prussia, PA
- WP 063 **Using Low-Resolution MS for Protein Therapeutic Process Monitoring during Development after One-Time Characterization with High-Resolution MS;** Chien-Hsun Chen¹; Eike Zimmermann¹; Kenji Furuya¹; Scott Corley¹; ¹Boehringer Ingelheim, Fremont, CA
- WP 064 **A novel Immunocapture Middle-Up LC-MS Method to Evaluate the *in vivo* Stability of Fc Conjugated Antibody Drug Conjugates (ADCs);** Srikanth Kotapati¹; David Passmore¹; Qiang Cong¹; Yam B Poudel¹; Mei-Chen Sung¹; Mary Huber¹; Patrick Holder¹; Sayumi Yamazoe¹; Sanjeev Gangwar¹; Chetana Rao¹; Vangipuram S. Rangan¹; Chin Pan¹; Pina M. Cardarelli¹; Shrikant Deshpande¹; Pavel Strop¹; Gavin Dollinger¹; Arvind Rajpal¹; ¹Bristol-Myers Squibb, Redwood City, CA
- BIOMARKERS: DISCOVERY II**
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- WP 065 **A Flexible Analytical Platform for the Discovery of Biomarkers of Disease;** Laura McGregor¹; Pete Grosshans¹; Anthony Buchanan¹; Bob Green¹; Nick Bukowski¹; ¹SepSolve Analytical, Peterborough, United Kingdom
- WP 066 **The Discovery of Potential Cancer Biomarkers in Human Plasma Using GC- and GCxGC-TOFMS;** David E Alonso¹; Habtom Ressom²; Cristina Di Poto²; Joseph E Binkley³; ¹Leco Corporation, St. Joseph, MI; ²Georgetown University Medical Center, Washington, DC; ³LECO Corporation, St Joseph, MI
- WP 067 **AlbuVoid™ Enrichment & Antibody Depletion - Solving the Challenges of Serum Proteomics;** Matt Kuruc¹; Swapan Roy¹; Haiyan Zheng^{2,3}; Amenah Soherwardy^{2,3}; ¹Biotech Support Group LLC, Monmouth Junction, NJ; ²Rutgers University, New Brunswick, NJ; ³Rutgers Proteomics Center, Piscataway, NJ
- WP 068 **Applications of SurfaceGenie: A Web-Based Tool for Mining Experimental Data for Informative Surface Proteins;** Matthew Waas¹; Shana T. Snarrenberg¹; Jack Littrell¹; Rebekah L. Gundry¹; ¹Medical College of Wisconsin, Milwaukee, WI
- WP 069 **Plasma Proteins as New Biomarkers of Irradiation in Humans;** Ales Tichy¹; Gabriela Kultova^{1,2}; Helena Rehulkova^{1,2}; Pavel Rehulka¹; Alena Myslivcova-Fucikova^{1,2}; ¹University of Defence, Hradec Kralove, Czech Republic; ²University of Hradec Králové, Czech Republic, Hradec Králové, Czech Republic
- WP 070 **Global Plasma Proteome Quantification Using Internal Standard Triggered Targeted Analyses;** Sebastien Gallien^{1,2}; Jing Wang¹; Aaron S. Gajadhar³; Bhavin Patel⁴; Markus Kellmann⁵; Tabiwang N. Arrey⁶; Alexander Harder⁶; Romain Hugué³; Graeme McAlister³; Derek Bailey³; Shannon Eliuk³; Yue Xuan⁶; Andreas Huhmer³; Emily I. Chen¹; ¹Thermo Fisher Scientific, Precision Medicine Science Center, Cambridge, MA; ²Thermo Fisher Scientific, Paris, France; ³Thermo Fisher Scientific, San Jose, CA; ⁴Thermo Fisher Scientific, Rockford, IL; ⁵Thermo Fisher Scientific, Bremen, Germany
- WP 071 **Modification of Lipid Expression in human Clear Cell Renal Cell Carcinoma;** Lucia Martin-Saiz¹; Olatz Fresnedo²; Jone Garate¹; Roberto Fernandez¹; Peio Errarte³; Maider Beitia³; Gorka Larrinaga³; Jon Danel Solano-Iturri⁴; Beatriz Abad⁵; Jose Andrés Fernández¹; Begoña Ochoa²; ¹Dep. of Physical Chemistry, Fac. of Science and Technology, University of the Basque Country (UPV/EHU), Leioa, Spain; ²Department of Physiology, Fac. of Medicine and Nursing, University of the Basque Country (UPV/EHU), Leioa, Spain; ³Department of Nursing, Fac. of Medicine and Nursing, University of the Basque Country (UPV/EHU), Leioa, Spain; ⁴Department of Pathology, Cruces University Hospital, Barakaldo, Spain; ⁵Liquid Chromatography and lipidomics platform, SGIKER, University of the Basque Country (UPV/EHU), Leioa, Spain
- WP 072 **Amniotic Fluid Proteome of Neonates with Congenital Diaphragmatic Hernia;** Sumit Bhatnada¹; Karin Tran-Lundmark²; Carmen Mesas-Burgos²; Peter Conner²; Bjorn Frenckner²; Suneel Apte¹; ¹Cleveland Clinic, Cleveland, OH; ²Karolinska Institutet, Stockholm, Sweden
- WP 073 **Characterizing Glycans and Glycan Isomers Associated with Breast Cancer Tissue Phenotypes;** Sakshi Gautam¹; Wenjing Peng¹; Xue Dong¹; Jingfu Zhao¹; Yifan Huang¹; Aiyi Yu¹; jieqiang Zhong¹; Yehia Mechref¹; ¹Texas Tech University, Lubbock, TX
- WP 074 **Proteomic Profiling and Immunoassay-based Validation of Biomarkers in Human Plasma from Alzheimer's Patients;** Mei Chen¹; Abby S. Gelb¹; Weiming Xia^{1,2}; ¹Geriatric Research Education and Clinical Center (GRECC), ENR Memorial Veterans Hospital, Bedford, MA; ²Boston University School of Medicine, Boston, MA
- WP 075 **LC-MS/MS Proteomic: Identification of Candidate Biomarkers of Breast Cancer Subtypes;** Jingfu Zhao¹; Wenjing Peng¹; Aiyi Yu¹; Yifan Huang¹; Xue Dong¹; Yehia Mechref¹; ¹Texas Tech University, Lubbock, TX
- WP 076 **Proteomic Profiling of Ovarian Cancer Extracellular Vesicles for Biomarker Discovery;** Dylan Z Dieters-Castator^{1,2}; Jiahui Liu¹; Gilles Lajoie²; Lynne-Marie Postovit^{1,2}; ¹University of Alberta, Edmonton, AB; ²Western University, London, ON
- WP 077 **Multiplexed, Quantitative Proteomic Comparison of a Novel Nrf2 Pathway – Targeting Therapeutic Compound in Two Separate, but Complementary, Matrices;** Damon Young¹; Amanda L. Edwards¹; Sharon O'Neill¹; Ashley Nelson¹; Ankur Thomas¹; Brian Wipke¹; Michael Rooney¹; Omar Mabrouk¹; Danielle Graham¹; ¹Biogen, Cambridge, MA
- WP 078 **Identifying Novel Upstream Kinases of the Microtubule-Associated Protein Tau Using Fluorescence Complementation Mass Spectrometry (FCMS) in an Alzheimer's-like cell model;** Der-Shyang Kao¹; Yanyan Du²; W. Andy Tao²; ¹Purdue University, West Lafayette, Indiana; ²Purdue University, West Lafayette, Indiana
- WP 079 **Secretotranscriptomic Identification and Validation of New Prognostic Liquid Biopsy Biomarkers;** J. Astor Ankney¹; John A. Wrobel¹; Ling Xie¹; Xian Chen^{1,2}; ¹Department of Biochemistry and Biophysics, University of North Carolina, Chapel Hill, NC; ²Lineberger Comprehensive Cancer Center, University of North Carolina at Chapel Hill, Chapel Hill, NC
- WP 080 **Region-Specific N-Glycome Mapping of the Human Brain in Alzheimer's Patients by nanoLC chip-Q-TOF MS Analysis;** Jennyfer Tena¹; Mariana Barboza¹; Maurice Wong¹; Carlito B Lebrilla¹; ¹University of California, Davis, Davis, CA
- WP 081 **The Urinary Metabolome and Lipidome of Prostate Cancer;** Iqbal Mahmud¹; Timothy J Garrett¹; ¹University of Florida Department of Pathology, Immunology, and Laboratory Medicine, Gainesville, FL



- WP 082 **Proteomic Discovery of Potential Biomarkers in Zika Virus Infected Monkeys**; Bao Q. Tran¹; Gabrielle Rizzo²; Michael Ward³; Lisa Cazares³; Trevor Glaros⁴; ¹20th CBRNE Command, APG, MD; ²Excet, Inc., Springfield, VA; ³United States Army Medical Research Institute of Infectious Diseases, Fort Detrick, MD; ⁴ECBC, Aberdeen Proving Ground, Maryland
- WP 083 **Serum Proteomic Profiling for Biomarker Discovery in Ischemic Stroke**; Miji Shin¹; Jiyeong Lee²; Arum Park²; Sora Mun¹; You-rim Lee¹; Ae Eun Seok²; Hyo-jin Kim¹; Yoo-jin Lee¹; Hee-gyoo Kang^{1,2}; ¹Department of Senior Healthcare, BK21 Plus Program, Graduate School, Eulji University, Daejeon, South Korea; ²Department of Biomedical Laboratory Science, College of Health Sciences, Eulji University, Seongnam-si, South Korea
- WP 084 **Phosphatidylcholines as a Biomarker Potential Candidate of Multiple Sclerosis**; Fernando Brunale Leite¹; Danielle Zildeana Furtado¹; Cleber Nunes Barreto¹; Erica Souza Silva¹; Nilson Antonio Assuncao¹; ¹Unifesp, São Paulo, Brazil
- WP 085 **Proteome and Phosphoproteome Biomarker Discovery Strategies for Biopsy-Free Bladder Cancer Diagnosis Based on Urinary Extracellular Vesicles**; Xiaofeng Wu¹; Sebastian Paez¹; Hristos Kaimakliotis²; Anton B. Iliuk³; Weiguo Andy Tao¹; ¹Purdue University, West Lafayette, IN; ²Indiana University School of Medicine, Indianapolis, Indiana; ³Tymora Analytical Operations, West Lafayette, IN
- WP 086 **Aging Markers and Ageotypes Revealed by Deep Longitudinal Profiling**; Sara Ahadi¹; Wenyu Zhou¹; Reza Sailani¹; Kevin Contrepois¹; Michael Snyder¹; ¹Stanford University School of Medicine, Stanford, CA, 94305
- WP 087 **Deciphering Racial Disparities in Breast Cancer by Novel Extracellular Matrix Proteomic Approaches on Formalin-Fixed, Paraffin-Embedded Clinical Specimens**; Peggii M. Angel¹; Baylye Boxall¹; Jennifer R. Bethard¹; Lauren E. Ball¹; Jeffrey R. Marks²; Richard R. Drake¹; ¹Medical University of South Carolina, Charleston, SC; ²Duke University School of Medicine, Durham, NC
- WP 088 **Stability-Based Protein Fractionation of Plasma Reveals Insights into Familial Amyloid Polyneuropathy Treatment with Tafamidis**; Jolene K. Diedrich¹; Chung-Yon Lin¹; Jeffery W. Kelly¹; John R. Yates, III¹; ¹The Scripps Research Institute, La Jolla, CA
- WP 089 **Serum Proteomic Profiling for Biomarker Discovery in Rheumatoid Arthritis**; Sora Mun¹; Jiyeong Lee²; Arum Park²; Ae Eun Seok²; Hyo-jin Kim¹; Yoo-jin Lee¹; Hee-gyoo Kang^{1,2}; You-rim Lee¹; ¹Department of Senior Healthcare, BK21 Plus Program, Graduate School, Eulji University, Daejeon, South Korea; ²Department of Biomedical Laboratory Science, College of Health Sciences, Eulji University, Seongnam-si, South Korea
- WP 090 **Development of a Bioanalytical Method for the Measurement of Symmetric-Dimethylarginine (SDMA) in Formalin-Fixed Paraffin-Embedded (FFPE) and Frozen Samples by LC/MS/MS**; Max Lein¹; David Pirman¹; Gina Lein²; Katherine Sellers¹; Everton Mandley¹; Taryn Slegler¹; Katya Marjon¹; Guowen Liu¹; Yue Chen¹; ¹Agios Pharmaceuticals, Cambridge, MA; ²Sigilon Therapeutics, Cambridge, MA
- WP 091 **UTIDx: 60 Second Assay for Detecting Urinary Tract Infections**; Dominique G. Bihan¹; Spencer D. Wildman¹; Daniel B. Gregson²; Thomas Rydzak¹; Ryan A. Groves¹; Carly Y. Chan¹; Deirdre L. Church²; Ian A. Lewis¹; ¹University of Calgary, Calgary, AB; ²Calgary Laboratory Services, Alberta Health Services, Calgary, AB
- WP 092 **A Tunable Approach for Median-Polish of Ratio (TAMPOR) across Batches of Proteomics Datasets Deals a Blow to Stubborn Technical Variance**; Eric B. Dammer^{1,2,3}; Tyler W.A. Bradshaw⁴; Lenora A. Higginbotham^{3,5}; Lingyan Ping^{3,5,6}; Duc M. Duong^{2,3,5}; James J. Lah^{3,5}; Allan I. Levey^{3,5}; Scott H. Soderling⁴; Nicholas T. Seyfried^{2,3,5}; ¹Emory University, Atlanta, GA; ²Emory Integrated Proteomics Core, Emory University, Atlanta, Georgia; ³Emory School of Medicine, Atlanta, GA; ⁴Duke University School of Medicine, Durham, NC; ⁵Emory University - Center of Neurodegenerative Diseases, Atlanta, GA; ⁶Emory University-Biochemistry, Atlanta, GA
- WP 093 **Metabolomic Approach for the Discovery of Internal Standard Substances of Bloodstain**; Hee-gyoo Kang¹; You-rim Lee¹; Jiyeong Lee¹; Ae Eun Seok¹; Arum Park¹; Sora Mun¹; Hyojin Kim¹; Yoo Jin Lee¹; ¹Department of Senior Healthcare, BK21 Plus Program, Graduate School, Eulji University, Daejeon, South Korea; ²Department of Biomedical Laboratory Science, College of Health Sciences, Eulji University, Seongnam-si, South Korea
- WP 094 **Lipid Signature to Distinguish between Patient with type II Diabetes and Type II Diabetes with Cardiovascular Disease**; yashwant kumar; *Translational health science and technology institute, Faridabad, India*
- WP 095 **Proteomic Analysis of NMuMG Cells Undergoing Epithelial Mesenchymal Transition**; Santanu Palchoudhuri¹; Faraz Rashid²; Dipankar Malakar²; Manoj G Pillai²; ¹Amity University, Kolkata, India; ²SCIEX, Gurgaon, India
- BIOMARKERS: QUANTITATIVE ANALYSIS III**
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- WP 096 **A Sensitive and RobustUPLC-MS/MS Method for Quantitation of Estrogens and Progestogens in Human Serum**; Junmei Zhang¹; Chenxiao Tang¹; Patrick J. Oberly¹; Margaret B. Minnigh¹; Sharon L. Achilles^{1,2}; Samuel M. Poloyac¹; ¹University of Pittsburgh, Pittsburgh, PA; ²Magee-Womens Research Institute, Pittsburgh, PA
- WP 097 **Identification of Candidate Biomarkers for Head and Neck Cancer Using LC-SRM and Longitudinal Samples from the DOD Serum Repository**; Ju Yeon Lee¹; Tujin Shi¹; Vladislav Petyuk¹; Athena Schepmoes¹; Thomas Fillmore¹; Wayne Cardoni²; George Coppit²; Joseph Goodman²; Shiv Srivastava³; Craig Shriver²; Tao Liu¹; Karin Rodland¹; ¹Pacific Northwest National Laboratory, Richland, WA; ²Walter Reed National Military Medical Center, Bethesda, MD; ³Center for Prostate Disease Research, Bethesda, MD
- WP 098 **Assessment of Food Impact on Serum Bile Acid Changes in a clinical methodology study by LC-MS/MS Analysis**; Lina Luo¹; John Pettersen²; Michael Aleo¹; Christopher Holliman¹; Ragu Ramanathan¹; ¹Pfizer WRD, Groton, CT; ²University of Connecticut, Storrs, CT
- WP 099 **TNF- α Regulated Metabolic Reprogramming in Breast Cancer Using High-Resolution Proteomics**; Ha Yun Lee¹; Eugene C. Yi^{1,2}; Kritarth Singh³; Rajesh Singh³; Hanbyeol Kim⁴; ¹Seoul national university, Seoul, South Korea; ²Department of Molecular Medicine and Biopharmaceutical Sciences, Graduate School of Convergence Science and Technology, Seoul National University, Seoul, South Korea; ³Department of Bio-Chemistry, The M.S. University of Baroda, Vadodara, India; ⁴Department of Integrated OMICS for Biomedical Science, Graduate School, Yonsei University, Seoul, South Korea
- WP 100 **Identification Clostridium chauvoei by MALDI-TOF MS from Paraffin Embedded Sections of Lower Extremity Infections, in Three Diabetes Patients after Amputations**; Barbara Dominiak¹; Maria Anita Mendes^{2,3,4,5}; ¹Temple University, Philadelphia, PA; ²Dampster Mass Spectrometry Lab, Sao Paulo-SP, Brazil; ³William Oxberry, Brooklyn, New York, SUNY Downstate Medical Center; ⁴Patrick Chen, Brooklyn, SUNY Downstate Medical Center, New York; ⁵Ernieque ER Sanches, Dampster Mass Spectrometry Lab., Brazil



- WP 101 **Pre-Analytical Variation and Sample Quality Control of Human Blood for Metabolomics**; Xinyu Liu; *Dalian Institute OF Chemical Physics, Chinese Academy of Sciences, Dalian, China*
- WP 102 **Surface Modification of Gold Nanoparticles and their Applications as Mass Tags for Protein Marker Detection in Laser Ionization Mass Spectrometry**; Siu Chung Toby Tam¹; Yu-Hong Cheng¹; Kwan-Ming Ng¹; ¹*The University of Hong Kong, Hong Kong, Hong Kong*
- WP 103 **Investigating Phytophthora methylation using Trapped Ion Mobility Spectrometry Mass Spectrometry**; Han Chen¹; Qing Zhang²; Heiner Koch³; Lucy Woods⁴; Hongyu Ma¹; ¹*Nanjing Agricultural University, Nanjing, China*; ²*Bruker (Beijing) Scientific Technology Co., Ltd, Beijing, China*; ³*Bruker Daltonik GmbH, Bremen, Germany*; ⁴*Bruker Daltonics, 28359 Bremen, Germany*
- WP 104 **Improvement of Phospho-monoester Lipids LC-MS Detection by Selective Capture using Molecularly Designed Materials**; Giuliana Grasso¹; Carlo Crescenzi¹; Börje Sellergren²; ¹*University of Salerno, Fisciano, Italy*; ²*Biofilm Research Center for Biointerfaces, Malmö University, Malmö, Sweden, SE, Sweden*
- WP 105 **Proteomic Analysis of Cerebrospinal Fluid in Alzheimer's disease**; Justin McKetney¹; Daniel Panyard¹; Sterling C Johnson¹; Cynthia Carlsson¹; Corinne D Engelman¹; Joshua J Coon¹; ¹*University of Wisconsin-Madison, Madison, WI*
- WP 106 **Utilizing Blood Cards for Quantitative Assessment of Glutathione as an Important Biomarker Test for Autism Spectrum Disorder and Neurodegenerative Diseases**; Ashley Trouten¹; H. m. Skip Kingston¹; ¹*Duquesne University, Pittsburgh, PA*
- WP 107 **Development of a Quantification Method for Intact Phosphorylated Alpha-Synuclein in Mouse Brain**; Jens Fogh¹; François Fenaille²; Line Roerbaek Olsen¹; Anne-Marie Jacobsen¹; François Becher²; ¹*H. Lundbeck A/S, Valby, Denmark*; ²*CEA Saclay, Service de Pharmacologie et Immunoanalyse (SPI) - Laboratoire d'Etude du Métabolisme des Médicaments, Gif-Sur-Yvette, France*
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- WP 114 **Simultaneous Quantification of Nine Polyunsaturated Fatty Acids (PUFAs) in Rat Plasma by Reverse Phase LC-MS/MS**; Roger Pham¹; Michelle Chen²; Josh Dekeyser³; Christopher A. James²; Omar S. Barnaby²; ¹*Amgen, Inc., Thousand Oaks, CA*; ²*Amgen, Inc., Thousand Oaks, CA*; ³*Amgen Inc., Boston, MA*
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- WP 124 **Development of an Automated LC-MS Based Assay Using a SISCAPA Workflow to Enable Quantitation of Peptide Biomarkers of Neurodegeneration;** Julie Lee¹; Paul L Auger¹; Kristin Wildsmith¹; ¹Genentech Inc., South San Francisco, CA
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- WP 126 **Developing an Automated Plasma Sample Preparation Method for LC/MS Analysis of Metabolites;** Koen Raedschelders¹; Weston Spivia¹; Jennifer Van Eyk¹; ¹Cedars-Sinai Medical Center, Los Angeles, CA
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- WP 138 ***In situ* Production of Hydroxyl Radicals by Ozone from Laser Photolysis of Solvated Oxygen at Physiological pH for Protein Footprinting;** Simin D. Maleknia¹; Callan Wilcox²; Scott Kable²; ¹University of Technology Sydney, Sydney, Australia; ²School of Chemistry, University of New South Wales, Sydney, NSW, Australia
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- WP 141 **Uncovering the Molecular Architecture of Human Fibrin Clots by Crosslinking Mass Spectrometry;** Oleg Klykov^{1,2}; Carmen van der zwaan³; Alexander B. Meijer³; Albert J.R. Heck^{1,2}; Richard A. Scheltema^{1,2}; ¹Utrecht University, Utrecht, Netherlands; ²Netherlands Proteomics Center, Utrecht, Netherlands; ³Sanquin Research, Amsterdam, Netherlands
- WP 142 **Mechanistic Studies of Radical Trifluoromethylation and Its Application for Membrane Protein Labeling and Epitope Mapping;** Ming Cheng¹; Chunyang Guo¹; George Mathai²; Gary Gerstenecker¹; Don Rempel¹; Michael L. Gross¹; ¹Washington University, St. Louis, MO; ²Sacred Heart College, Cochin, India
- WP 143 **In-Cell Fast Photochemical Oxidation of HCT116 Spheroids;** Raquel Short¹; Jesica Lukowski²; Amanda B. Hummon³; Lisa M Jones¹; ¹University of Maryland Baltimore, Baltimore, MD; ²University of Notre Dame, Notre Dame, IN; ³The Ohio State University, Columbus, OH
- WP 144 **Evaluation of FAIMS Technology for Mass Spec Analysis of Chemical Cross-Linked Peptides;** Rosa Viner¹; Leigh A Foster²; Ryan D. Bomgarden²; Michael W. Belford¹; Satendra Prasad¹; Romain Huguet¹; Eloy R. Wouters¹; ¹Thermo Fisher Scientific, San Jose, CA; ²ThermoFisher Scientific, Rockford, IL
- WP 145 **Photo Affinity Fragment (PhABit) Screening: A High Throughput Assay Platform and Identification of PhABit Binding Sites;** Chad J Quinn¹; Ken Fantom²; Craig Wagner¹; Emma Grant²; Jacob Bush²; Chun-wa Chung²; Mike Hann²; Roland S Annan¹; Francesca Zappacosta¹; ¹GSK, Collegeville, PA; ²GSK, Stevenage, United Kingdom
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- ²University of California at San Francisco, San Francisco, CA; ³University of Washington, Seattle, WA
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- WP 167 **Does Your Dog Have Anxiety After a Rough Day at the Lake: Analysis of CBD Extracts for Dog Treats**; Matthew Curtis¹; Mike Adams²; Karen Kaikaris²; Sarah Aijaz³; Sue D'Antonio¹; Anthony Macherone^{1,4}; ¹Agilent Technologies, Inc., Santa Clara, CA; ²CWC Labs, Cedar Creek, TX; ³MilliporeSigma, Bellefonte, PA; ⁴Johns Hopkins University School of Medicine, Baltimore, MD
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- Hedge¹; Nathan Mitchell¹; Scott Stanley^{1,2}; Rui Yu¹;
¹United States Equestrian Federation Equine Drug Testing
and Research Laboratory, Lexington, KY; ²University of
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- WP 173 **Screening CBD Oil Pet Supplements for Mycotoxins
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School of Medicine, Baltimore, MD
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- WP 177 **Liquid Chromatography and Tandem Mass
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Jingcun Wu⁴; Josh Ye⁵; Feng Qin⁵; ¹PerkinElmer, Canada,
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⁵PerkinElmer Inc., Woodbridge, ON
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- WP 179 **GC/MS and HPLC/MS Characterization of the Terpenes,
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Ibrahim¹; Richard D. Smith¹; ¹Pacific Northwest National
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- WP 181 **Quantitative Glycomics with Improved Multiplexing
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²; ¹Department of Chemistry, University of Wisconsin,
Madison, WI; ²School of Pharmacy, University of Wisconsin-
Madison, Madison, WI
- WP 182 **Introduction of a Novel Labelling Strategy to Facilitate
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Widdowson¹; Zoltan Szabo²; Sheheer Khan²; Jonathan
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United Kingdom; ²Thermo Fisher Scientific, Oyster Point,
California; ³National Institute for Bioprocessing Research
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Hemel Hempstead, United Kingdom
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¹Academia Sinica, Taipei, Taiwan; ²Institute of Atomic and
Molecular Sciences, Academia Sinica, Taipei City, Taiwan
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Rebekah L. Gundry¹; ¹Medical College of Wisconsin,
Milwaukee, WI
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¹University of Michigan, Ann Arbor, MI
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²Penn State University - Scranton, Dunmore, PA; ³University
of New Hampshire, Durham, NH
- WP 187 **The Quantification of Chondroitin Sulfate in
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Jackson^{1,3}; ¹C. Eugene Bennett Department of Chemistry,
West Virginia University, Morgantown, WV; ²INRA
UR1268 BIA, Nantes, France; ³Department of Forensic
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Morgantown, WV
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²University of Georgia, Athens, GA; ³Utrecht Univeristy,
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- WP 193 **Investigating Isoform Structures Found In Enoxaparin
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- WP 194 **A Novel Isobaric Tag Enabled Multiplexed Quantitative
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- WP 195 **The Unexpected Dissociation Mechanism of Sodiated
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Ni¹; ¹Institute of Atomic and Molecular Sciences, Academia
Sinica, Taipei, Taiwan; ²Department of Chemistry, National
Taiwan University, Taipei, Taiwan



- WP 196 **Investigation on Isomeric Gangliosides using LC/MS/MS towards Mouse Brain Regional Mapping;** Jua Lee¹; Jaekyung Yun¹; Heeyoun Hwang¹; Hee-sup Shin²; Hyun Joo An¹; ¹Chungnam National University, Daejeon, South Korea; ²Institute for basic science, Daejeon, South Korea
- WP 197 **Isomeric Separation of Permethylated Glycans by Extra-Long Reversed-Phase Liquid Chromatography (RPLC)-MS;** Xue Dong¹; Yifan Huang¹; Jingfu Zhao¹; Aiyang Yu¹; Yehia Mechref¹; ¹Texas Tech University, Lubbock, TX
- WP 198 **Discrimination of Metal Adducted Sialylated Carbohydrate Isomers by Ion Mobility Spectrometry, Electron Transfer, and Vibrational Activation;** Anna J. Diepenbrock¹; Eric D. Dodds¹; ¹University of Nebraska - Lincoln, Lincoln, NE
- WP 199 **Degradation Pathway of β -Cyclodextrin by Electrospray Ionization Mass Spectrometry and Liquid Chromatography with Evaporative Light Scattering Detection;** Hengwen Zhong¹; Peter Wang¹; Tao Jiang¹; ¹Mallinckrodt, Hazelwood, MO
- WP 200 **Characterization of Sodium and Lithium Cationized Mono and Disaccharides Using High Resolution IMS and Tandem IMS Techniques;** Paul Scott Soma¹; Matthew T Campbell¹; Andrew Baker²; Martin Palmer³; Dale Cooper-Shepherd³; Gary Glish¹; ¹University of North Carolina, Chapel Hill, NC; ²Waters Corporation, Pleasanton, CA; ³Waters, Wilmslow, United Kingdom
- WP 201 **Determining the Structure of the Glycan Bearing the Bisecting GlcNAc on Human Placenta Membrane Using Mass Spectrometry;** Qiushi Chen¹; Yuanliang Zhang¹; Zhilong Lin¹; Yan Ren¹; Siqi Liu¹; ¹BGI-Shenzhen, Beishan Industrial Zone 11th Building, Yantian District, Shenzhen City, China
- WP 202 **A Facile and Unbiased Method for Comprehensive Glycome Characterization;** Juan Wei¹; Yang Tang²; Pengyu Hong³; Catherine E. Costello^{1,2}; Cheng Lin¹; ¹Department of Biochemistry, Boston University School of Medicine, Boston, MA; ²Department of Chemistry, Boston University, Boston, MA; ³Department of Computer Science, Brandeis University, Waltham, MA
- WP 203 **Isoforms of Carbohydrates Identified by 2D UV-MS of Non-Covalent Complexes with Aromatics;** Oleg V. Boyarkine; EPFL, Lausanne, Switzerland
- WP 204 **Separation and Identification of Glycan Anomers Using Ultrahigh-Resolution Ion Mobility Spectrometry Combined with Cryogenic IR Spectroscopy;** Stephan Warnke¹; Ahmed Ben Faleh¹; Thomas R. Rizzo¹; ¹Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland
- WP 205 **Dual Enzymatic Digestion Enabling Simultaneous Release of Glycans from Glycoproteins and Glycolipids;** Seth D Williamson¹; Andrew Cho¹; Jair Montford¹; Yehia Mechref¹; ¹Texas Tech University, Lubbock, TX
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- WP 207 **An Ultra-Sensitive Paper-Based Diagnostic Platform of Detecting Colorectal Cancer via Mass Spectrometry;** Suji Lee¹; Abraham K. Badu-Tawiah¹; ¹The Ohio State University, Columbus, OH
- WP 208 **Rapid, Robust and High-Throughput Proteome Analysis by High-Flow LC-MS/MS;** Yangyang Bian¹; Runsheng Zheng¹; Yun-Chien Chang¹; Jana Zecha¹; Stephanie Heinzlmeir¹; Daniel P. Zolg¹; Oleksandr Boichenko²; Mike Baynham³; Bernhard Kuster^{1,4,5}; ¹Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; ²Thermo Fisher Scientific, Germering, Germany; ³Thermo Fisher Scientific, Runcorn, United Kingdom;
- ⁴Center for Integrated Protein Science Munich, Freising, Germany; ⁵Bavarian Center for Biomolecular Mass Spectrometry, Freising, Germany
- WP 209 **A High Throughput and High Resolution LC-MS/MS Method to Measure IGF1 in Serum for Clinical Research;** Xiaolei Xie; ThermoFisher Scientific, San Jose, CA
- WP 210 **Faecal Metabolomics by Conventional UHPLC-HRMS as well as Novel LA-REIMS Reveals Relevant Metabolic Perturbations in Type 2 Diabetes;** Lieven Van Meulebroek¹; Simon Cameron²; Bruno Lapauw³; Zoltan Takats²; Lynn Vanhaecke¹; ¹Ghent University, Merelbeke, Belgium; ²Imperial College, London, United Kingdom; ³Ghent University Hospital, Ghent, Belgium
- WP 211 **Clinical Evaluation of Coated Blade Spray Mass Spectrometry for the Concomitant Determination of Four Immunosuppressive Drugs in Whole Human Blood;** Daniel Ricker¹; German Augusto Gomez-Rios^{1,2}; Emir Nazdrajić¹; Marcos Tascon^{1,3}; Vathany Kulasingam^{4,5}; Janusz Pawliszyn¹; ¹University of Waterloo, Waterloo, ON; ²Restek Corporation, Bellefonte, PA; ³Instituto de Investigación e Ingeniería Ambiental (3iA), Universidad Nacional de San Martín (UNSAM), San Martín, Argentina; ⁴Department of Laboratory Medicine and Pathobiology, University of Toronto, Toronto, Ontario; ⁵Department of Clinical Biochemistry, University Health Network, Toronto, Ontario
- WP 212 **An Approach to Screening Clinical Samples for Novel Fentanyl using High Resolution Tandem Mass Spectrometry;** Kenneth D. Swanson¹; Rebecca L. Shaner¹; William A. Bragg¹; Logan C. Krajewski²; Elizabeth I. Hamelin¹; Melissa D. Carter¹; Rudolph C. Johnson¹; ¹Emergency Response Branch, Division of Laboratory Sciences, National Center for Environmental Health, Centers for Disease Control and Prevention, Atlanta, GA; ²Battelle Memorial Institute at the Centers for Disease Control and Prevention, Atlanta, GA
- WP 213 **Different Approaches for Vitamin D Determination in Newborns by LC-MS/MS;** Rafal Rola^{1,2}; Konrad Kowalski²; Tomasz Bienkowski²; Jacek Witwicki³; ¹Nicolaus Copernicus University, Torun, Poland; ²Masdiag Sp. z o.o., Warsaw, Poland; ³Bielanski Hospital, Warsaw, Poland
- WP 214 **A Simple Analysis of Catecholamines in Cell Cultures by LC/MS/MS Using an Ion-Pairing Reagent Added to Final Extracts;** Yi Zhao¹; Peiling Hou²; Shu Qing Chan³; Weiyong Sim¹; Lisa Helen Ong¹; Jie Xing²; ¹Department of Clinical Research, Singapore General Hospital, Outram Road, Singapore; ²Application Development & Support Centre, Shimadzu (Asia Pacific) Pte Ltd, Singapore; ³School of Chemical and Life Sciences, Singapore Polytechnic, Singapore
- WP 215 **Application of the HPLC-MS/MS Method in Studying Individual Metabolic Differences of Cyclosporin A in Bone Marrow Transplant Patients;** Wang Lei^{1,2}; Liu hong xing^{2,3,4}; Liu rui¹; Yang zi yi¹; ¹HebeiYanda Lu Daopei Hospital, Langfang, China; ²Beijing Lu Daopei Hospital, Beijing, China; ³HebeiYanda Lu Daopei Hospita, Langfang, China; ⁴Beijing Lu Daopei Institute of Hematology, Beijing, China
- WP 216 **Intra-Surgical Diagnosis of IDH Mutation in Human Glioma using a Miniature Mass Spectrometer;** Fan Pu¹; Clint M Alfaro¹; Hannah M Brown¹; Zheng Ouyang^{1,2}; Graham R. Cooks¹; ¹Department of Chemistry, Purdue University, West Lafayette, IN 47907; ²Singhua University, Beijing, China
- WP 217 **High-Throughput Analysis of Neuroleptic Drugs in Plasmas using LDTD-MS/MS Technology;** Jacques Corbeil^{1,2}; Serge Auger³; Pier-Luc Plante^{1,2}; Jean Lacoursière³; Pierre Picard³; ¹Université Laval, Quebec, Quebec; ²Infectiology Research Centre, CHU de Québec, Laval University, Québec, QC; ³Phytronix Technologies, Quebec, QC



- WP 218 **Reliable Quantification of 52 Amino Acids in Human Plasma by LC-MS/MS;** Stephanie Samra¹; Valérie Thibert²; Claude Netter²; ¹Thermo Fisher Scientific, San Jose, CA; ²Thermo Fisher Scientific, Courtaboeuf, France
- WP 219 **High-Sensitivity Analysis of a Steroid Panel Samples using Micro-Flow LC-MS/MS for Clinical Research;** Narumi Shirai¹; Takanari Hattori²; Mikael Levi²; Shoji F. Nakayama³; Shigeru Suzuki¹; ¹Chubu University, Kasugai, Japan; ²Shimadzu Corporation, Kyoto, Japan; ³National Institute for Environmental Studies, Tsukuba, Japan
- WP 220 **Using Superficially Porous Phenyl Phase Selectivity for Benzodiazepine Separations;** William Long¹; Carl Griffin²; Anne E Mack²; Emily Parry²; Charles Lofton²; ¹Agilent Technologies, Wilmington, DE; ²Agilent Technologies, Inc., Wilmington, DE
- WP 221 **A Systematic Study of Hydrolytic Degradation of Acylcarnitines During Sample Preparation and Analysis in Newborn Screening Using Tandem Mass Spectrometry;** Timothy Lim¹; Donald H Chace¹; Konstantinos Petritis¹; ¹Centers for Disease Control and Prevention, Chamblee, GA
- WP 222 **Translation of a Top-Down Proteomics IgG Workflow to the Mayo Clinic to Characterize Monoclonal Gammopathies;** Ryan T Fellers¹; Richard D Leduc¹; Bryan P Early¹; Rafael D. Melani¹; Joseph B Greer¹; Surendra Dasari²; Patrick M Vanderboom²; Angela Dispenzieri²; David L Murray²; Paul M Thomas¹; Neil L Kelleher¹; ¹Northwestern University, Evanston, IL; ²Mayo Clinic, Rochester, MN
- WP 223 **Isotopic Peak Index: A Novel Nomenclature to Help Simultaneously Detect and Identify 13 IGF-1 Variants during Routine Clinical Analysis;** Ievgen Motorykin¹; Michael P Caulfield¹; Michael J McPhaul¹; Zengru Wu¹; ¹Quest Diagnostics, San Juan Capistrano, CA
- WP 224 **Case-Control Study: Expanded Proteomics and Lipidomic Profiling for Early Prediction of Major Adverse Cardiac Events;** Qin Fu¹; Irina Tchernyshyov¹; Ronald Holewinski¹; Vidya Venkatraman¹; David Sarracino²; Casey Johnson¹; Kelly Njine Mouapi¹; Susan Cheng³; Chrisandra Shufelt³; Brennan Spiegel⁴; Noel Bairey Merz³; Scott Peterman²; Jennifer Van Eyk^{1,3}; ¹Advanced Clinical Biosystems Research Institute, The Smidt Heart Institute, Cedars-Sinai Medical Center, Los Angeles, CA 90048, Los Angeles, CA; ²Thermo Fisher Scientific, Cambridge, MA; ³Barbra Streisand Women's Heart Center, The Smidt Heart Institute, Cedars-Sinai Medical Center, Los Angeles, CA; ⁴Clinical and Translational Science Institute, Cedars-Sinai Medical Center, Los Angeles, CA
- WP 225 **Biomarker Detection Utilizing a Desktop IMS-MS Device with Electrospray Ionization High Resolution Drift Time Ion Mobility-Linear Ion Trap Mass Spectrometer;** Julia L. Kaszycki¹; Gregory F. Brabeck¹; Aurelio La Rotta¹; Ching Wu¹; ¹Excellims Corporation, Acton, MA
- WP 226 **The MasSpec Pen for the Rapid Detection of Primary Breast Cancer and Breast Cancer Metastasis;** Kyana Y Garza¹; Jialing Zhang¹; John Lin¹; Stacey Carter²; James Suliburk²; Chandandeep Nagi²; Livia S Eberlin¹; ¹University of Texas at Austin, Department of Chemistry, Austin, TX; ²Baylor College of Medicine, Houston, TX
- WP 227 **Ambient Mass Spectrometry Mapping of Lipid Fingerprints in Healthy and Cancerous Human Colorectal Tissues;** Yasmin Shanneik¹; Emrys A. Jones²; Bipasha Chakrabarty³; Kaye J. Williams⁴; Omer Aziz³; Steven Pringle²; Adam W. McMahon¹; ¹Wolfson molecular imaging centre, The University of Manchester, Manchester, United Kingdom; ²Waters Corporation, Manchester, United Kingdom; ³The Christie NHS Foundation Trust, Manchester, United Kingdom; ⁴The University of Manchester, Division of Pharmacy & Optometry, Manchester, United Kingdom
- WP 228 **Quantitative N-Glycan Profiling of Clinical Tissue Samples by On-Line Fluorescence-MS Using a Rapid Labeling Tag;** Sarah Totten¹; Andres Guerrero²; John Yan³; Aled Jones³; James D. Brooks⁴; Abel Bermudez¹; Sharon J. Pitteri¹; ¹Stanford University School of Medicine, Canary Center at Stanford for Cancer Early Detection, Palo Alto, CA; ²ProZyme, A part of Agilent, Hayward, CA; ³ProZyme, Hayward, CA; ⁴Department of Urology, Stanford University School of Medicine, Stanford, California
- WP 229 **Development of LC-MS/MS Method for Detection Endogenous Steroids;** Konrad Piotr Kowalski¹; Joanna Was²; Magdalena Niedolistek²; Masdiag Sp. z o.o., Warszawa, Poland; ²Department of Medical Biology, Institute of Cardiology, Warsaw, Poland
- WP 230 **Structures for Lossless Ion Manipulations (SLIM)-Mass Spectrometry (MS) for High Resolution Ion Mobility Analysis of Immunosuppressive Drugs;** Kelly Wormwood¹; Laura Maxon¹; Daniel DeBord¹; ¹MOBILion Systems Inc., Exton, PA
- WP 231 **Method Development and Validation of LC-MS/MS Based Assay for Detection of Carfentanil and Norcarfentanil in Human Urine;** Difei Sun¹; Danijela Korforte¹; Jan Palaty²; ¹Lifelabs Medical Laboratories, Toronto, ON; ²Lifelabs Medical Laboratories, Burnaby, BC
- WP 232 **HarmCheck: Direct Mass Spectrometry Harm Reduction Drug Checking for use in the Opioid Overdose Crisis;** Scott A. Borden^{1,2}; Jan Palaty³; Erik T. Krogh^{1,2}; Christopher G. Gill^{1,2,4,5}; ¹Appl. Env. Res. Labs. (AERL), Vancouver Island University, Chemistry Department, Nanaimo, BC; ²University of Victoria, Chemistry Department, Victoria, BC; ³Lifelabs Medical Laboratories, Burnaby, BC; ⁴Simon Fraser University, Chemistry Department, Burnaby, BC; ⁵University of Washington, DEOHS, Seattle, WA
- WP 233 **Quantitative Proteomic Assessment of Differences and Stability of Human Serum and Plasma Proteins;** Sumio Ohtsuki¹; Madoka Nanbu¹; Shin Nishiumi²; Takashi Kobayashi²; Shingo Ito¹; Takeshi Masuda¹; Masaru Yoshida²; ¹Kumamoto University, Kumamoto, Japan; ²Kobe University, Kobe, Japan
- WP 234 **Probe ElectroSpray Ionization Mass Spectrometry for Cholangiocarcinoma Tumor and Healthy Tissues Rapid Identification;** Silvia Giordano¹; Hidekazu Saiki²; Hiroki Nakajima²; Matteo Donadon³; Matteo Cimino³; Cristiana Soldani³; Barbara Franceschini³; Guido Torzilli³; Enrico Davoli¹; ¹Istituto di Ricerche Farmacologiche Mario Negri IRCCS, Milan, Italy; ²Shimadzu Corporation, Kyoto, Japan; ³Humanitas Clinical and Research Center IRCCS, Rozzano, Italy

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- WP 236 **Drug Discovery Applications of ADE-OPP-MS (Acoustic-Droplet-Ejection coupled Open-Port-Probe Mass Spectrometry) Platform;** Hui Zhang¹; Wenyi Hua¹; Chang Liu²; Jianua Liu¹; David Cox²; Anthony Carlo¹; Matt Troutman¹; Tom Covey²; ¹Pfizer Inc., Groton, CT; ²SCIEX, Concord, ON
- WP 237 **Acoustic Droplet Ejection (ADE) and Open Port Probe (OPP) Sampling Interface for High Throughput Analysis of ADME Assays;** Tom Hollenbeck¹; John Isbell¹; Patrick White¹; Lucas Westling¹; Ashley Chong¹; Stefan Thibodeaux²; ¹GNF (Novartis), San Diego, CA; ²Novartis, Cambridge, MA



- WP 238 **High-Throughput Analysis of Synthetic Samples from High-Density Microplates with ESI-MS Enabled by the Acoustic-Droplet-Ejection to the Open-Port Probe sampling interface;** Wenyi Hua¹; Chang Liu²; Kenneth Dirico¹; Joseph Tucker¹; Thomas R. Covey²; Hui Zhang¹; ¹Pfizer Inc., Groton, CT; ²SCIEX, Concord, ON
- WP 239 **Effect of Increased Plate Density on Sensitivity in High-Throughput LDTD-MS;** Pierre Picard¹; Pier-Luc Plante²; Sarah Demers¹; Serge Auger¹; Jean Lacoursière¹; ¹Phytonix Technologies, Inc., Quebec, QC; ²Université Laval, Quebec, Quebec
- WP 240 **Enzyme Activity Assay of an Engineered Human Homocyst(e)inase in Mammalian Serum using LC-MS/MS;** Dale Schoener¹; Silvia Ferrati²; Forrest Helfrich¹; Jennifer Zarzoso¹; Susan Alters²; Mike Buonarati¹; ¹Intertek Pharmaceutical Services, San Diego, CA; ²Aeglea Biotherapeutics, Austin, TX
- WP 241 **Improved Kinome Coverage and Automated Data Analysis Pipeline for Large-Scale Kinase Inhibitor Screens;** Maria Reinecke^{1,2}; Florian Seefried¹; Svenja Petzold^{1,2}; Tobias Schmidt¹; Patroklos Samaras¹; Mathias Wilhelm¹; Stephanie Heinzlmeir¹; Benjamin Ruprecht¹; Guillaume Medard¹; Bernhard Kuster¹; ¹Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; ²German Cancer Consortium (DKTK), DKFZ partner site, Munich, Germany
- WP 242 **MS-Based Drug-Screening Platform for *in vitro* Biomedical Efficiency and *in vivo* Target Engagement of Covalent Inhibitors against KRAS G12C Mutant;** Shujia Dai¹; Junqing Shen¹; Gejing Deng¹; Hong Cheng¹; Bailin Zhang¹; ¹Biochemistry & Bioanalytics, Translational Sciences, Sanofi US, Cambridge, MA
- WP 243 **Characterization of a Novel BCL6 PROTAC to Provide Molecular Insights by Chemical Biology Approaches;** Fiona Pachl¹; William McCoull²; Tony Cheung³; Kate Byth³; Aarti Kawatkar¹; Timothy Rasmusson¹; Paola Castaldi¹; ¹Discovery Sciences, IMED Biotech Unit, AstraZeneca, Waltham, MA; ²Chemistry, IMED Biotech Unit, AstraZeneca, Cambridge, United Kingdom; ³Bioscience, Oncology, IMED Biotech Unit, AstraZeneca, Waltham, MA
- WP 244 **Quantifying Heterogeneity in Drug-Uptake, Metabolism and Response in Single-Cells by an Integrated Raman-Spectroscopy and Mass spectrometry Approach;** Ahmed Ali¹; Yasmine Abouleila¹; Yoshihiro Shimizu¹; Eiso Hiyama²; Arno Germond¹; Toshio Yanagida¹; ¹RIKEN, Osaka, Japan; ²Hiroshima University, Hiroshima, Japan
- WP 245 **High Resolution MS for 3D Culture Hepatic *in vitro* Models Metabolite Identification;** Sujoy Lahiri¹; Kate Comstock²; ¹Thermo Fisher Scientific, Frederick, MD; ²Thermo Fisher Scientific, San Jose, CA
- WP 246 **Dual-Stream LC Coupled with 'Plug and Play' Automation for Routine Bioanalysis in Drug Discovery;** Emile G Plise¹; Jonathan Cheong¹; Katherine Gaffney¹; Jamie Jorski¹; Loren Olson²; Neal Liddle²; Anthony Romanelli²; Joseph Janiszewski³; Wayne Lootsma³; John Janiszewski⁴; ¹Genentech, Inc., South San Francisco, CA; ²SCIEX, Concord, ON; ³Sound Analytics, Niantic, CT; ⁴J2-Bioanalytical, Westerly, RI
- WP 247 **Development and Optimization of an Integrated Trap-and-Elute Microflow LC-MS/MS Platform;** Brendon Kapinos¹; Mary Piotrowski¹; Hui Zhang¹; John Janiszewski²; Wayne Lootsma³; Steve Ainley³; ¹Pfizer, Groton, CT; ²J2-Bioanalytical, Westerly, RI; ³Sound Analytics, Niantic, CT
- WP 248 **Stereoisomer Separation of Drugs and Biomarkers Using Supercritical Fluid Chromatography to Support PK/PD Studies;** Fangbiao Li¹; Bang-lin Wan²; Guangping Bi²; Rena Zhang²; Daniel Spellman²; ¹Merck & Co., Inc., West Point, PA; ²Merck & Co., Inc., West Point, PA
- WP 249 **LC-MS for Bioanalysis of a Wide Range of Biotherapeutic Modalities;** Hao Jiang¹; Alex Kozhich¹; Linlin Luo¹; Wendy Miller¹; Craig Titsch¹; Johanna Mora¹; Gerry Kolaitis¹; ¹Bristol-Myers Squibb, Princeton, NJ
- WP 250 **Ion Mobility-Enabled Metabolite Identification of Tienilic Acid and Tienilic Acid Isomer;** Lauren Mullin¹; Giorgis Isaac¹; Ian D Wilson²; Gordon Murray³; Nathan Andersen¹; Robert S Plumb¹; ¹Waters Corporation, Milford, MA; ²Imperial College London, London, SW7 2AZ; ³Waters Corp., Beverly, MA
- WP 251 **Structures for Lossless Ion Manipulations (SLIM)-Mass Spectrometry (MS) for High Resolution and High Throughput Glycan Biomarker Analysis;** Kelly Wormwood¹; Liulin Deng¹; Daniel DeBord¹; Laura Maxon¹; Hirsh Nanda²; Jarrat Jordan²; Sunil Nagpal²; Harsha Gunawardena²; ¹MOBILion Systems Inc., Exton, PA; ²Janssen Research and Development, Spring House, PA
- WP 252 **Pharmacokinetic Analysis of an Alzheimer's Disease Therapeutic in Rat Serum via 908devices ZipChip CZE-MS;** Zachary Kelley¹; Mark Lovell^{1,2}; Bert C. Lynn¹; ¹Department of Chemistry, University of Kentucky, Lexington, KY; ²Sanders-Brown Center on Aging, University of Kentucky, Lexington, KY
- WP 253 **Streamlining the Metabolite Identification Workflow in Drug Discovery: Evaluation of Different Fragmentation Techniques and Software for Data Analysis;** Catalina Suarez¹; Qi Wu¹; Yongying Jiang¹; ¹MD Anderson Cancer Center, Houston, TX
- WP 254 **Evaluation of Microflow LC-MS/MS in a Quantitative Discovery Bioanalysis Setting;** Jun Zhang¹; Wilson Shou¹; Jonathan Ho²; Tairo Ogura²; Yohei Arao²; Shu Li¹; Harold Weller¹; ¹Bristol-Myers Squibb, Hopewell, NJ; ²Shimadzu Scientific Instruments, Inc., Columbia, MD
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- WP 256 **Application of REIMS to Describe Genetic, Environmental, and Processing Factors Affecting;** Harmonie M Bettenhausen; ¹Colorado State University, Fort Collins, CO
- WP 257 **Classification and Visualization of Beer Quality Using GC-MS and GC-FID;** Yusuke Takemori¹; Yui Higashi¹; Takero Sakai²; Ryo Takechi³; Motoki Sasaki⁴; Narihiro Suzuki⁴; ¹Shimadzu Corporation, Kyoto, Japan; ²Shimadzu Corporation, Nakagyo-ku, Japan; ³Shimadzu Scientific Instruments, Inc., Columbia, Maryland; ⁴Ise Kadoya Brewery, Ise, Japan
- WP 258 **MALDI-MS Analysis of Phospholipids from Colombian Cacao Beans;** Deisy Giraldo Davila¹; Marianny Y. Combariza¹; Cristian Blanco-Tirado¹; ¹Universidad Industrial de Santander, Bucaramanga, Colombia
- WP 259 **Non-Targeted Metabolomic Study on Variation of Phenolics in Different Cranberry Cultivars Using UPLC-IM-HRMS;** Yifei Wang^{1,2}; Nicholi Vorsa³; Peter de B. Harrington²; Pei Chen¹; ¹U.S. Department of Agriculture, Agricultural Research Service, Beltsville Human Nutrition Research Center, Food Composition and Methods Development Laboratory, Beltsville, MD; ²Center for Intelligent Chemical Instrumentation, Department of Chemistry & Biochemistry, Ohio University, Athens, OH; ³Philip E. Marucci Center for Blueberry and Cranberry Research and Extension, Rutgers University, Chatsworth, NJ
- WP 260 **Comparing Chemical Constituency using Data-Driven Botanical Extraction Solvent Assessment by UHPLC-PDA-CAD-HRMS;** Christopher J. Pulliam¹; Vincent P.



- Sica¹; Timothy R. Baker¹; ¹*The Procter and Gamble Co., Cincinnati, OH*
- WP 261 **Application of Metabolomics Methods on LC/GC-QTOF Data to Discriminate Extra Virgin Olive Oils from Different Protected Designations of Origin**; Lucía Olmo-García¹; Karin Wendt²; Nikolas Kessler²; Aadil Bajoub³; Artem Filipenko⁴; Alberto Fernández-Gutiérrez¹; Carsten Baessmann²; Alegría Carrasco-Pancorbo¹; ¹*Department of Analytical Chemistry, Faculty of Science, University of Granada, Granada, Spain*; ²*Bruker Daltonik GmbH, Bremen, Germany*; ³*Department of Basic Sciences, National School of Agriculture, Meknès, Morocco*; ⁴*Bruker Daltonics Inc., Billerica, MA*
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- WP 264 **The Effects of Boiling Time on the Wort Proteome during Beer Production**; Katherine Cordova¹; Ray Bacala¹; Marta Izydorczyk¹; Dave Hatcher¹; ¹*Canadian Grain Commission, Winnipeg, MB*
- WP 265 **Lipid Profiling of Beef Muscle Tissues by LC-MS/MS and GC Analysis and Possible Health Benefits of Odd Chain Fatty Acids**; Beate Fuchs¹; Dirk Dannenberger¹; ¹*Leibniz-Institut für Nutztierbiologie (FBN), Dummerstorf, Germany*
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- WP 268 **Metabolite Fingerprinting and Mapping the Phytonutrients through LCMS and HPTLC Analysis of Rice Varietals, Endogenous to North-East Region of India**; Krishna N Dutta¹; Akanksha Singh²; Paramita Choudhury¹; Rajlakhmi Devi¹; Narayan C Talukdar¹; Suman K Samanta¹; Dipankar Malakar²; Manoj G Pillai²; ¹*Life Sciences Division, Institute of Advanced Study in Science and Technology, Guwahati, India*; ²*SCIEX, Gurgaon, India*
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- WP 273 **Evaluation of Trimethylamine in the De-Dimerization of 2-Hydroxy-4-(methylthio)butanoic Acid (HMB) Utilizing GC-MS and TMS- and tBMS-Derivatization**; Thomas P. Mawhinney¹; Yiyi Li¹; Deborah L Chance¹; James K Waters¹; ¹*University of Missouri, Columbia, MO*
- WP 274 **In-Depth Profiling of Beetroot Bioactive Compounds by DAD-ESI-LC/MS/MS**; Nebiyu Abshiru¹; Boris Nemzer¹; ¹*VDF FutureCeuticals, Inc, Momence, IL*
- WP 275 **Dereplication of Betalain Derivatives in Different Color of Djulis (Chenopodium formosanum) using UHPLC-DAD-ESI-Orbitrap**; Gui-ru Xie¹; Hong-Jhang Chen¹; ¹*National Taiwan University, Taipei, Taiwan*
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- WP 276 **Veterinary Drug Detection in Pork and Milk Using a Small, Innovative Triple Quad with an ESI Ion Source**; Jarod Grossman¹; Theresa Sosienski¹; ¹*Agilent Technologies, Santa Clara, CA*
- WP 277 **Determination of Acrylamide in Coffee by LC-MS/MS**; Jd De-Alwis¹; Euan Ross¹; Joanne Williams¹; Kenneth Rosnack²; ¹*Waters, Wilmslow, United Kingdom*; ²*Waters Corporation, Milford, MA*
- WP 278 **Optimized System for Pulsed Injections and Backflushing in GC/MS Analysis of Pesticides with Acetonitrile Solvent**; Anastasia Andrianova¹; Bruce Quimby¹; ¹*Agilent Technologies, Wilmington, DE*
- WP 279 **High-Throughput Online Miro-SPE with LCMS/MS Analysis of Multiple Pesticides Residues in Fruits and Vegetables**; jianzhong li¹; Ye Kong¹; Zhe Cao¹; ¹*No.3, Wang Jing Bei Lu, Beijing, China*
- WP 280 **Fast Analysis of Multi-Class Pesticides Panel in Wine and Olive Oil Extracts using a Single Run LC-Triple Quadrupole Mass Spectrometry**; Illaria Palini¹; Silvia Bani¹; Debora D'Addona²; Charles T. Yang³; Dipankar Ghosh³; ¹*ISVEA, Poggibonsi, Italy*; ²*Thermo Fisher Scientific, Milano, Italy*; ³*Thermo Fisher Scientific, San Jose, CA*
- WP 281 **Determination of Glycoalkaloids in Potato by Molecular Imprinted Polymer@Magnetic Nanoparticles Combined with Liquid Chromatography Mass Spectrometry**; Cheng-Hsing Yeh¹; Chung-Yu Chen¹; Peipei Qi²; Maw-Rong Lee¹; ¹*National Chung-Hsing University, Taichung, Taiwan*; ²*Zhejiang Academy of Agricultural Sciences, Hangzhou, China*
- WP 282 **Screening and Quantitation of Drugs Illegally Added to Health Foods by UHPLC-hybrid Quadrupole-Orbitrap Mass Spectrometry**; Long Sun¹; Tao Bo¹; ¹*Thermo Fisher Scientific, Beijing, China*
- WP 283 **A Rapid and Original Method for the Determination of Heterocyclic Aromatic Amines in Cooked Meat using QuEChERS Extraction and UHPLC-APCI-MS/MS**; Sylvie Chevolleau^{1,2}; Alyssa Bouville^{1,2}; Laurent Debrauwer^{1,2}; ¹*Axiom Platform, UMR 1331 Toxalim, MetaToul-MetaboHUB, National Infrastructure of Metabolomics and Fluxomics, Toulouse, France*; ²*Toxalim, Université de Toulouse, INRA, INP-ENVT, INP-EI-Purpan, Université de Toulouse 3 Paul Sabatier, Toulouse, France*
- WP 284 **Multi-class Veterinary Drug Screening and Quantitation with a Comprehensive Workflow**; Ed George¹; Viet Dang²; ¹*ThermoFisher Scientific, San Jose, CA*; ²*Iowa State University, Ames, IA*
- WP 285 **Methodology for Detection and Structural Characterization of Phosphodiesterase-5 (PDE-5) Inhibitor Adulterants in an Herbal Coffee Product**; Marian Twohig¹; Andy Aubin¹; Sarah Dowd²; Gordon Fujimoto²; Simon Hird³; Kenneth Rosnack¹; ¹*Waters Corporation, Milford, MA*; ²*Waters Corporation, Beverly, MA*; ³*Waters Corporation, Wilmslow, United Kingdom*
- WP 286 **A Quantitative Method to Detect Penicillin in Limited Amounts of Bovine Tissues Using Liquid Chromatography and Tandem Mass Spectrometry (LC/MS/MS)**; Linge Li¹; Karyn D. Howard¹; Christine Kilonzo¹;



- WP 287 Raoul Gonzales¹; Michael Myers¹; ¹FDA/Center for Veterinary Medicine, Office of Research, Laurel, MD 20708
Optimization of Detection and Separation Conditions in LC-MS/MS Method for Determination of Phenothiazine Dyes in Fish Muscle; Luiza Kijewska¹; Kamila Mitrowska¹; Luigi Giannetti²; Bruno Neri²; ¹Department of Pharmacology and Toxicology, National Veterinary Research Institute (PIWet), Pulawy, Poland; ²Istituto Zooprofilattico Sperimentale Regioni Lazio e Toscana Via Appia Nuova, Rome, Italy
- WP 288 **Determination of Glyphosate in Animal Feed Matrices by QuPPE Extraction and LC-MS/MS Detection**; Joanne L Baillie¹; Fang Shi¹; ¹Canadian Food Inspection Agency, Calgary, AB
- WP 289 **Sensitive Determination of Polar Anionic Pesticides in Wheat Flour by Stable Isotope Dilution Ion Chromatography-Tandem Mass Spectrometry**; Yingchen Li¹; Qilei Guo¹; Tao Bo¹; ¹Thermo Fisher Scientific, Beijing, China
- WP 290 **Fragmentation Pathways of Synthetic Drugs Added in Health Food Based on Higher Energy Collisional Dissociation in High-Resolution Quadrupole-Orbitrap Mass Spectrometry**; Long Sun¹; Qilei Guo¹; Tao Bo¹; ¹Thermo Fisher Scientific, Beijing, China
- WP 291 **QuEChERS Coupled to Gas Chromatography-Mass Spectrometry for Determination of Leachables of Packaging Material in Beverages**; Ya-Ying Chen¹; Chung-Yu Chen¹; Poppy Wulandari Sitanggang¹; Peipei Qi²; Maw-Rong Lee³; ¹National Chung-Hsing University, Taichung, Taiwan; ²Zhejiang Academy of Agricultural Sciences, Hangzhou, China
- WP 292 **Combination of GC/MS/MS and LC/MS/MS to Analyze Multiclass Pesticides in Orange Using One QuEChERS Sample Preparation Method**; zhiming zhang¹; Ge Meng¹; Dan-hui Dorothy Yang²; Jianzhong Li³; Jinlan Sun³; Cuijing Wu³; ¹Agilent Technologies (Shanghai) Co., Ltd., Shanghai, China; ²Agilent Technologies, Santa Clara, CA; ³Agilent Technologies(China) Co. Ltd., Beijing, China
- WP 293 **Analysis of Bifenazate and Derived Metabolite, Bifenazate-Diaen, in Six Livestock Products using Liquid Chromatography-Tandem Mass Spectrometry**; Da-Hee Park¹; Kyung-Hee Yoo¹; Seong-Kwan Kim¹; Ho-Chul Shin¹; ¹Konkuk university, Seoul, South Korea
- WP 294 **Rapid and Easy Analysis of Tetrodotoxin by Direct Probe Ionization/Tandem Mass Spectrometry (DPiMS)**; Tasuku Murata¹; Koretsugu Ogata¹; Yuji Nagashima²; ¹Shimadzu Corporation, Kyoto, Japan; ²Food Industry, Department of Food Industry, Niigata Agro-Food University, Niigata, Japan
- WP 295 **Development of a Confirmatory Method for Determination of Xenobiotics in Honey by HPLC-MS/MS**; Pavel Metalnikov¹; Ilya Batov¹; Renat Selimov¹; Denis Nekrasov¹; Tatyana Sukhova¹; Alexandre Komarov¹; ¹VGNKI, Moscow, Russian Federation
- WP 296 **Screening and Low-Level Quantitation of Chloramphenicol (CAP) in Commercial Honey Samples Using Miniaturized LC/MS System**; Vikrant Goel¹; Saikat Banerjee²; Samir Vyas³; ¹Agilent Technologies, Gurgaon, India; ²Agilent Technologies India Pvt Ltd, Hyderabad, India; ³Agilent Technologies India Pvt Ltd, Mumbai, India
- WP 297 **The Analysis of Chloramphenicol in Milk Using Ultra High Pressure Liquid Chromatography/Compact Mass Spectrometry**; Changtong Hao¹; Daniel Eikel¹; Simon Prosser¹; ¹Advion Inc., Ithaca, NY
- WP 298 **QuEChERS Extracted Pesticide Quantitation by LCMS QTOF using High Resolution Accurate Mass Acquisition Acquired at High Data Acquisition Speed**; Alan Barnes¹; Steve Williams²; Christopher Titman¹; Neil Loftus¹; ¹Shimadzu Corporation, Manchester, United Kingdom; ²Concept Life Sciences, Cambridge, United Kingdom
- WP 299 **High-Throughput Analysis of Indole, Skatole and Androstene in Pork Fat Using a LDTD-MS/MS System**; Jean Lacoursière¹; Serge Auger¹; Sarah Demers¹; Pierre Picard¹; ¹Phytronix Technologies, Quebec, QC
- WP 300 **Thyrostatic Drug Analysis in Animal Tissues using LC-SRM and High-Field Asymmetric Waveform Ion Mobility Spectrometry (FAIMS)**; Randall W Purves^{1,2}; Kim Souster¹; Caleb M.E. Fisher¹; Michelle West¹; Roger Munro¹; Haixia Zhang²; Michael W. Belford³; Albert Vandenberg²; Bryn O Shurmer¹; ¹Canadian Food Inspection Agency, Saskatoon, SK; ²University of Saskatchewan, Saskatoon, SK; ³Thermo Fisher Scientific, San Jose, CA
- WP 301 **Off-Line Hydrogen Cleaning of GC/MS Ion Source Increases Sample Throughput for Pesticides in Foods**; Jochen Stoeppeler¹; Joerg Riener²; Klaus Wilmers¹; Thorsten Bernsmann¹; Courtney Milner³; ¹Chemisches und Veterinäruntersuchungsamt Münsterland-Emscher-Lippe (CVUA-MEL), Muenster, Germany; ²Agilent Technologies, Waldbronn, Germany; ³Agilent, Santa Clara, CA
- WP 302 **Is Washing and/or Cooking of Vegetables Enough to Minimize the Risk of Population Exposure to Pesticide Residues?**; Joshua Ye¹; Jingcun Wu²; Erasmus Cudjoe²; Feng Qin²; ¹PerkinElmer Inc., Woodbridge, ON; ²PerkinElmer, Inc., Woodbridge, ON
- WP 303 **Rapid Measurement of Agrochemicals by PaperSpray Mass Spectrometry**; Steven Lawrence Reeber¹; Neloni R. Wijeratne¹; Mary L. Blackburn¹; ¹Thermo Fisher Scientific, San Jose, CA
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- WP 304 **Reduction of Disulfide Bonds Using a High-Powered Femtosecond Laser**; Simon K. Gammelgaard^{1,2}; Steffen B. Petersen²; Kim F. Haselmann¹; Peter Kresten Nielsen¹; ¹Novo Nordisk A/S, Måløv, Denmark; ²Aalborg University, Aalborg, Denmark
- WP 305 **Impact of Charge Sites on Fragmentation of Peptides and Proteins: Carbamylation and Guanidination**; Amanda Helms¹; Jennifer S Brodbelt¹; ¹University of Texas at Austin, Austin, TX
- WP 306 **GC-MS with Photoionization of Cold Molecules in Supersonic Molecular Beams – Approaching the Softest Ionization Method**; Alexander B. Fialkov¹; Elias Ikonen²; Tiina Laaksonen²; Aviv Amirav¹; ¹Tel-Aviv University, Tel-Aviv, Israel; ²Neste Oyj, Porvoo, Finland
- GC/MS: INSTRUMENTATION AND APPLICATIONS II**
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- WP 307 **New Evaluation Methods for Expanding an Electron Ionization Mass Spectral Library**; Weihua Ji¹; Sanford P. Markey¹; Gary Mallard¹; Dmitrii V. Tchekhovskoi¹; Yuri A. Mirokhin¹; Oleg V. Toropov¹; Alexey Mayorov¹; William E. Wallace¹; Stephen E. Stein¹; ¹NIST, Gaithersburg, MD
- WP 308 **Improved Separation and Identification of Essential Oil Constituents in Commercial Products using GCxGC-HR-ToF-MS**; Vimbai Mhuka¹; Simiso Dube²; Mathew M Nindi²; ¹UNISA, Florida Park, Roodepoort, South Africa; ²UNISA, Florida Park, Roodepoort, South Africa
- WP 309 **Rapid "Shotgun" APCI-Ion Mobility Mass Spectrometry for the Analysis of Phytosterols in Honey Bee Dietary Pollen**; Jeffrey T Morre¹; Priyadarshini Chakrabarti¹; Diana Oppenheimer¹; Ramesh R Sagili¹; Claudia S. Maier¹; ¹Oregon State University, Corvallis, OR
- WP 310 **Is a Never-Clean Ion Source Possible? Is it Possible to Prove It?**; Lorne Fell¹; Todd Richards¹; Joseph E Binkley¹; ¹LECO Corporation, St Joseph, MI
- WP 311 **Comprehensive Evaluation of NIST Library Search Software**; Arun Moorthy¹; Anthony J Kearsley¹; William E. Wallace¹; Stephen E. Stein¹; ¹NIST, Gaithersburg, MD



- WP 312 **Combining Deconvolution, Library Search, and Principal Component Analysis to Detect and Identify Important Flavour and Fragrance Compounds with High-Resolution GC/MS;** Jason Cole¹; John Voss¹; Xin Zheng²; Scott Quarmby¹; ¹Thermo Fisher Scientific, Ausitn, TX; ²Thermo Fisher Scientific, Austin, TX
- WP 313 **Improving GC/MS Library Search on a Single Quadrupole Using Complementary and Orthogonal Metrics Within the Run;** Don Kuehl¹; Stacey Simonoff¹; Yongdong Wang¹; ¹Cerno Bioscience, Norwalk, CT
- WP 314 **Progress in the Development of a Plasma Based CI-Source for GC-MS;** Kai Kroll¹; Hendrik Kersten¹; Thorsten Benter¹; ¹University of Wuppertal, Wuppertal, Germany
- WP 315 **What is Identification?: Comprehensive Characterization of Exposome Samples via GCxGC-High Resolution TOFMS;** Todd Richards¹; Joseph E Binkley¹; David Alonso¹; Lorne Fell¹; ¹LECO Corporation, St Joseph, MI
- WP 316 **Stir Bar Sorptive Extraction-in-port Derivatization-Gas Chromatography-Mass Spectrometry for Determination of Perfluorocarboxylic Acids in Environmental Water;** Chun-Hung Wang¹; Chung-Yu Chen¹; Maw-Rong Lee¹; ¹National Chung-Hsing University, Taichung, Taiwan
- WP 317 **Comprehensive Analysis of Short-Chained Chlorinated Paraffins and other POPs in Environmental Samples by GCxGC-HR-TOFMS with a Novel Ion Source;** Scott Pugh¹; George Tikhonov¹; Viatcheslav Artaev¹; ¹LECO Corporation, St Joseph, MI
- WP 318 **Determination of Methamphetamines in Human Saliva by GC-MS and Two Step Injection On-Column derivatization;** Xiaolei Shi; Shimadzu (China) Co., Ltd., Shanghai Office, Shanghai, China
- WP 319 **Comparing the Results of Trace Chemical Analyses of ~200 Compounds Using GC-HRMS vs. APGC-QQQ Systems;** Daryl Smith¹; Wendy Zhao¹; Xiangjun Liao¹; Sue Quade¹; Amy Sadler¹; Valerie Casey¹; Thea Rawn¹; ¹Health Canada, Government of Canada, Ottawa, ON
- WP 320 **Emerging Contaminants in Valparaiso, Chile Rain Water: Changes in Composition and Concentration Levels over Fifteen Years (2003-2017);** Olga Polyakova¹; Viatcheslav Artaev²; Victor Vidal³; Francisco Cereceda³; Katalina Gonzalez Arincibia³; Albert Lebedev¹; ¹Moscow State University, Moscow, Russian Federation; ²LECO Corporation, St Joseph, MI; ³Universidad Técnica Federico Santa María, Valparaiso, Chile
- WP 321 **DMEITM Source with a Reaction Cell - A New Advances in Ion Generation for GC-MS/MS;** Harikrishnan Sukumar¹; Heather Gamble¹; Dante Sanchez¹; Victor Titov¹; Anna Kornilova¹; Reza Javahery¹; ¹PerkinElmer Inc., Woodbridge, ON
- WP 322 **Vacuum Assisted Sorbent Extraction (VASE) and a Dual-Column Thermal Desorption Approach for GC-MS Analysis of Trace-Level Polycyclic Aromatic Hydrocarbons;** Sage J. B. Dunham¹; Victoria L. Noad¹; Daniel B. Cardin¹; ¹Entech Instruments Inc, Simi Valley, CA
- WP 323 **Vacuum Assisted Sorbent Extraction for the Detection of Butyric Acid and other Short-Chain Fatty Acids by Headspace-GCMS-Headspace without Derivatization;** Tyler B. Van Ry¹; Sage J.B. Dunham²; Victoria L. Noad²; Daniel B. Cardin²; James Eric Cox¹; ¹Department of Biochemistry, University of Utah, Salt Lake City, UT; ²Entech Instruments, Simi Valley, CA
- WP 324 **Detection and Quantification of Fragrance Allergens in Complex Matrices Using GC-Orbitrap MS Technology;** Richard Law¹; Xin Zheng²; Cristian I Cojocariu¹; Jason Cole²; ¹Thermo Fisher Scientific, Runcorn, United Kingdom; ²Thermo Fisher Scientific, Ausitn, TX
- WP 325 **Development of an Integrated Qualitative Analysis Coupled with EI and Soft Ionization Data for GC-HRTOFMS System;** Masaaki Ubukata¹; Kenji Nagatomo¹; Ayumi Kubo¹; Takaya Satoh¹; John Dane²; ¹JEOL, Ltd., Tokyo, Japan; ²JEOL USA, Inc., Peabody, MA
- WP 326 **Multicomponent Analysis of Metabolites in Chinese Caterpillar Fungus using Gas Chromatography-Triple Quadrupole Mass Spectrometry;** Xiaoming Bao¹; Peng Tan²; Jun Fan³; Taohong Huang³; ¹Shimadzu (China) Co., Ltd, Chengdu, China; ²Chengdu Institute for Food and Drug Control, Chengdu, China; ³Shimadzu (China) Co., Ltd, Shanghai, China
- WP 327 **Workflow Solutions for Direct Insertion, Real-Time Gas Chromatography -Mass Spectrometry;** Ken Lynam¹; Angela Henry¹; Luis Cuadra-Rodriguez²; Wei Song¹; ¹Agilent Technologies, Wilmington, DE; ²Agilent Technologies, Santa Clara, CA
- WP 328 **A Novel Soft Ionization Plasma Source for GC-MS/MS Applications;** Mehrnaz Sarrafzadeh¹; Charles Jolliffe¹; Dmitry Valyaev¹; Reza Javahery¹; ¹PerkinElmer Inc., Woodbridge, ON
- WP 329 **Dual Mode Ionization Source (DMEI Source);** Anna Kornilova¹; Dante Sanchez¹; Harikrishnan Sukumar¹; Reza Javahery¹; Harpreet Singh¹; ¹PerkinElmer, Inc., Woodbridge, ON
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- WP 330 **Comparison of the Ionization Efficiency of N-Linked Glycopeptides by Matrix Assisted Laser Desorption Ionization and Electrospray Ionization;** Richard J Bell¹; Eric D Dodds¹; ¹University of Nebraska - Lincoln, Lincoln, NE
- WP 331 **Evaluating the Utility of a HILIC Model for Predicting Glycan Retention across Differing Stationary Phases and Tagging Chemistries;** Naqlaa Sheiba¹; Mark Han²; Ron Orlando¹; ¹Complex Carbohydrate Research Center, University of Georgia, Athens, Georgia; ²Reference Standards Laboratory, The United States Pharmacopeial Convention, Rockville, Maryland 20852
- WP 332 **Analysis of Mucin Proteins by Charge Detection Mass Spectrometry;** Lauren F Barnes¹; Benjamin E Draper¹; Nicholas A Lykтей¹; Martin F Jarrold¹; ¹Indiana University, Bloomington, IN
- WP 333 **N-Linked Glycosylation Site Mapping in Prostate Cancer and Matched Normal Tissue: Defining Alterations in Glycan Microheterogeneity;** Sarah Michelle Totten¹; Abel Bermudez¹; Sharon J. Pitteri¹; James D. Brooks²; ¹Stanford University School of Medicine, Canary Center at Stanford for Cancer Early Detection, Palo Alto, CA; ²Stanford University School of Medicine, Stanford, CA, 94305
- WP 334 **Analysis of O-glycosylated Biopharmaceuticals using an O-glycan dependent Endoprotease and LC-MS;** Andreas Nägeli¹; Philip J. Widdowson²; Maria Nordgren¹; Tom Buchanan²; Rolf Lood¹; Fredrik Leo¹; Helen Nyhlen¹; Jonathan Sjögren¹; Rowan Moore²; Fredrik Olsson¹; ¹Genovis AB, Lund, Sweden; ²Thermo Fisher Scientific, Runcorn, United Kingdom
- WP 335 **Detection of Site-Specific N-Glycosylation on the AAV8 Capsid Protein using High-Resolution Mass Spectrometry;** Arya Aloor; Georgia State University, Atlanta, GA
- WP 336 **Modification of Cell Membrane Glycosylation with Inhibitors and Characterization with nanoLC-MS;** Qing W Zhou¹; Yixuan Xie²; Qiongyu Li¹; Maurice Wong³; Carlito B Lebrilla¹; ¹University of California, Davis, Davis, CA; ²University of California Davis, Davis, CA; ³University of California Davis, Davis, CA
- WP 337 **Ionic Charge Manipulation using Solution and gas-Phase Chemistry to Facilitate Analysis of Highly Heterogeneous Proteins by ESI-MS;** Yang Yang¹; Chendi Niu¹; Cedric E. Bobst¹; Igor A. Kaltashov¹; ¹Department of Chemistry, University of Massachusetts-Amherst, 240 Thatcher Way, Life Science Laboratories N369, Amherst, MA



- WP 338 **Ion Mobility Collisional-Cross Section Values Facilitate Identification and Quantification of N-Glycan Structure Isomers and Permit Automated Processing of HILIC-UPLC-FLD-TIMS-CID-MS/MS data;** Sven Bahrke¹; Robert Wilmanowski¹; Sheira Mujica²; Wolfgang Jabs²; Stuart Pengeley³; Detlev Suckau³; ¹*Glycotope GmbH, Berlin, Germany*; ²*Beuth-Hochschule, Berlin, Germany*; ³*Bruker Daltonik GmbH, Bremen, Germany*
- WP 339 **High Throughput Profiling of Glycans Released from Therapeutic Glycoproteins via micro-Permethylated at the CCRC;** Stephanie A Archer-Hartmann¹; Asif Shajahan¹; Nitin Tatyaso Supekar¹; Christian Heiss¹; Parstoo Azadi¹; ¹*University of Georgia, Athens, GA*
- WP 340 **Identification of N-Glycopeptides using Electron Transfer/High-energy Collision Dissociation (ETHcD);** Rui Zhang¹; Xue Dong²; Jianhui Zhu³; David M. Lubman³; Yehia Mechref²; Haixu Tang¹; ¹*Indiana University Bloomington, Bloomington, IN*; ²*Texas Tech University, Lubbock, TX*; ³*University of Michigan Medical Center, Ann Arbor, MI*
- WP 341 **Analysis of IgA1 O-Glycosylation in Familial IgA Nephropathy;** Ellenore P. Craine¹; Audra A. Hargett²; Hiroyuki Ueda^{2,3}; Yoshimi Ueda^{2,3}; Colin Reily²; Zina Moldoveanu²; Stacy D. Hall²; Dana V. Rizk²; Krzysztof Kiryluk⁴; Ali G. Gharavi⁴; Takashi Yokoo³; Bruce A. Julian²; Matthew Renfrow²; Jan Novak²; ¹*University of Alabama at Birmingham, Birmingham*; ²*University of Alabama at Birmingham, Birmingham, Alabama*; ³*The Jikei University School of Medicine, Tokyo, Japan*; ⁴*Columbia University College of Physicians and Surgeons, New York, 10032*
- WP 342 **Characterizing HIV-1 Envelope N-Glycan Shield: A Glycomics and Bioinformatics Method;** Audra Hargett¹; Qing Wei¹; Barbora Knoppova²; Stacy Hall¹; Milan Raska^{1,2}; Zina Moldoveanu¹; Todd Green¹; Jan Novak¹; Matthew B. Renfrow¹; ¹*University of Alabama at Birmingham, Birmingham, AL*; ²*Palacky University in Olomouc, Olomouc, Czech Republic*
- WP 343 **Site Specific N-Glycosylation of Afamin Expressed in a Baculoviral System;** Mislav Novokmet¹; Andreas Naschberger²; Stefan Lechner²; Bernhard Rupp²; Gordan Lauc^{1,3}; ¹*Genos, Glycoscience Laboratory, Borongajska cesta 83h, Croatia*; ²*Department of Genetic Epidemiology, Medical University Innsbruck, Schöpfstr. 41, Austria*; ³*University of Zagreb Faculty of Pharmacy and Biochemistry, A. Kovačića 1, Croatia*
- WP 344 **Enzyme Toolkit for Selective Enrichment and Analysis of Mucin-Domain Glycoproteins;** Stacy Malaker¹; Judy Shon¹; Kayvon Pedram¹; Nicholas M Riley¹; Carolyn R Bertozzi^{1,2}; ¹*Stanford University, Palo Alto, CA*; ²*Howard Hughes Medical Institute, Stanford, CA*
- WP 345 **Improving the Glycomics Fidelity of Cancer Cells *in vitro* by using a Physiological Cell Culture Medium;** Junyao Wang¹; Wenjing Peng¹; Yehia Mechref¹; ¹*Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, Texas*
- WP 346 **Glycopeptide Micro-Heterogeneity: A Case Study in Antibody Glycans;** Anand Patel¹; Stefano Bonissone¹; Natalie Castellana¹; ¹*Digital Proteomics, LLC., San Diego, CA*
- WP 347 **Identification of Core-Fucosylated Glycoprotein as Potential Biomarker of Alzheimer's Disease;** Ding Liu¹; Cheng Ma¹; Peng George Wang²; ¹*Georgia state university, Atlanta, GA*; ²*Georgia State University, Atlanta, GA*
- WP 348 **Determination of Human Immunoglobulin Glycoforms by timsTOF Pro Sequencing Analysis;** Kim Alving¹; Anjali Alving²; Aharon Cohen¹; Bing Wang¹; ¹*Sanofi, Waltham, MA*; ²*Bruker Scientific, Billerica, MA*
- WP 349 **Fast Analysis of Glycans using LC-MS and Proteinase K Digestion;** Suping Zheng¹; Jie Ding¹; ¹*PPD, Inc., Middleton, WI*
- WP 350 **Characterizing Intact N-linked Glycoproteins with 2-Dimensional HPLC-MS: A Machine Learning Pipeline for Mapping Glycoproteoforms in Multidimensional Space;** Jiana Duan¹; Weiwei Rong¹; Shengkun Dai¹; Steven Matthew Patrie¹; ¹*Northwestern University, Evanston, IL*
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- WP 351 **Metabolomics in Nonhuman Primate Models for Radiation Biodosimetry in Emergency Preparedness;** Evan Pannkuk¹; Evagelia C Laiakis¹; Kirandeep Gill¹; Shreyans K Jain¹; Khyati Y. Mehta¹; Denise Nishita²; Kim Bujold³; James Bakke²; Janet Cahagen²; Simon Authier³; Polly Chang²; Albert J Fornace¹; ¹*Georgetown University, Washington Dc, DC*; ²*SRI International, Menlo Park, CA*; ³*CiToxLAB North America, Laval, QC*
- WP 352 **A Clinical Assay for Botulinum Neurotoxins through Mass Spectrometric Detection;** Kaitlin M Hoyt¹; Suzanne R Kalb¹; John R. Barr¹; Carolina Luquez¹; Janet K. Dykes¹; ¹*Centers for Disease Control and Prevention, Chamblee, GA*
- WP 353 **Detection and Analysis of Simulated Chemical Warfare Agents via Portable Mass Spectrometry;** Camila Anguiano Virgen¹; James D. Fox²; Jaime L. Winfield²; Kenneth C. Wright²; Guido F. Verbeck¹; ¹*University of North Texas, Denton, TX*; ²*Infficon, East Syracuse, NY*
- WP 354 **Validation of an LC-MS/MS Method to Detect Ricin Activity;** Kathryn R. Pigg¹; Jakub Baudys¹; Dongxia Wang¹; Suzanne R. Kalb¹; John R. Barr¹; ¹*Centers for Disease Control and Prevention, Atlanta, Georgia*
- WP 355 **Sensitive Detection of Active Ricin by MALDI-TOF Mass Spectrometry through an Improved RNA Substrate;** Dongxia Wang¹; Jakub Baudys²; John R Barr²; Suzanne R Kalb²; ¹*Centers of Disease Control and Prevention (CDC), Atlanta, GA*; ²*Centers for Disease Control and Prevention, Atlanta, Georgia 30341*
- WP 356 **Detection and Identification of Model Peroxide Explosives Using Paper Spray Ionization Combined With Tandem Mass Spectrometry;** Madeleine Wood^{1,2}; Luke Metzler²; Theodore Corcovilos³; Michael Van Stipdonk²; ¹*Forensic Science and Law Program, Duquesne University, Pittsburgh, PA*; ²*Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA*; ³*Department of Physics, Duquesne University, Pittsburgh, PA*
- WP 357 **Method Development for the Identification of Trichothecenes: Mass Spectral Library Matching and Determination of Unknown Mycotoxins;** Maria C. Prieto Conaway¹; Mark Dreyer¹; Todd H. Corzett¹; Brian P. Mayer¹; Audrey P. Williams¹; ¹*Lawrence Livermore National Laboratory, Livermore, CA/94550*
- WP 358 **Detection and Quantitative Analysis of Ricin by Tryptic Digestion and PRM MS Method;** Jakub Baudys¹; Dongxia Wang¹; John R. Barr¹; Suzanne R. Kalb¹; ¹*Centers for Disease Control and Prevention, Atlanta, Georgia*
- WP 359 **Rapid Identification and Antibiotic Susceptibility Determination for Anthrax (Bacillus anthracis) using Lethal Factor Endopeptidase Activity Coupled with MALDI-MS;** Jon Rees¹; Yulanda Williamson¹; Anne E Boyer¹; Maribel Gallegos-Candela¹; Renato Lins²; John R Barr¹; ¹*CDC, Atlanta, GA*; ²*Batelle, Columbus, OH*
- WP 360 **High-Throughput Screening of Explosive Residues Using a Robust Thermal Extraction Ionization Source (TEIS);** Pierre Negri¹; Neil Davenport²; Ashley Sage²; Peter Luke³; Carl Fletcher³; ¹*SCIEX, Redwood City, CA*; ²*SCIEX, Warrington, United Kingdom*; ³*Mass Spec Analytical, Bristol, United Kingdom*



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- WP 361 **Lipid Profiling of Carotid Atherosclerotic Plaque with Mass Spectrometry Imaging;** Mirjam Visscher¹; Astrid M. Moerman¹; Peter C. Burgers¹; Heleen M.M. Van Beusekom¹; Antonius F.W. Van der Steen¹; Theo M. Luider¹; Kim Van der Heiden¹; Gijs Van Soest¹; ¹Erasmus MC, Rotterdam, Netherlands
- WP 362 **A Novel Strategy for Cancer Biomarker Discovery Powered by Lipids Profiling using Imaging MS together with UPLC-QTOF/QQQ Tandem MS;** Lei Wang¹; Xu Ma¹; Chunyan Lan^{1,2}; Hainan Li³; Linbo Cai³; Xiaofei Jia⁴; Huiqin Zhong⁴; ¹National Center for Human Genetic Resources, National Research Institute for Health and Family Planning, Beijing, China; ²Peking Union Medical College Graduate School, Beijing, China; ³Guang Dong San Jiu Brain Hospital, Guangzhou, China; ⁴Waters Technologies (Shanghai) Co., Ltd, Shanghai, China
- WP 363 **Integrating Ambient Ionization Mass Spectrometry with Machine Learning for Rapid Breast Cancer Diagnosis;** Hsin-Hsiang Chung¹; Ying-Chen Huang¹; Bo-Rong Chen²; Ming-Yang Wang²; Cheng-Chih Hsu¹; ¹Department of Chemistry, National Taiwan University, Taipei, Taiwan; ²Department of Surgery, National Taiwan University Hospital, Taipei, Taiwan
- WP 364 **Discrimination of Human Renal Oncocytoma from Normal Kidney and Renal Cell Cancer Subtypes Using Ambient Ionization Mass Spectrometry Imaging;** Jialing Zhang¹; Shirley Li¹; Wendong Yu²; Livia S Eberlin¹; ¹University of Texas at Austin, Austin, TX; ²Baylor College of Medicine, Houston, TX
- WP 365 **3D MALDI Imaging of Traumatic Brain Injury: Unveiling a Link to Parkinson's Disease;** Khalil Mallah¹; Jusul Quanico¹; Dennis Tredre²; Firas Kobeissy³; Isabelle Fournier¹; Michel Salzet¹; ¹PRISM Inserm U1192 - University of Lille, Villeneuve D'ascq Cedex, France; ²Bruker Daltonik GmbH, Bremen, Germany; ³Department of Biochemistry and Molecular Genetics, Faculty of Medicine, American University of Beirut, Beirut, Lebanon
- WP 366 **Predicting Lymph Node Metastasis in Endometrial Cancer by Multi-Modal Mass Spectrometry Imaging;** Parul Mittal¹; Mark R Condina²; Matthew T Briggs³; Alice Ly⁴; Janina Oetjen⁴; Gurjeet Kaur Chatar Singh⁵; Manuela Klingler-Hoffmann³; Peter Hoffmann³; ¹Adelaide Proteomics Centre, The University of Adelaide, Adelaide, Australia; ²Future Industries Institute, Adelaide, Australia; ³Future Industries Institute, Adelaide, Australia; ⁴Bruker Daltonik GmbH, Bremen, Germany; ⁵Institute for Research in Molecular Medicine, Universiti Sains Malaysia, Minden,, Malaysia
- WP 367 **Unraveling Pathogenesis of Renal Amyloidosis with MALDI Imaging Mass Spectrometry and Shotgun Proteomics on paraffin Embedded Renal Biopsy Tissue Section;** Yume Mukasa¹; Yuki Kuzuhara¹; Megumi Terada¹; Takashi Nirasawa²; Ryo Kajita²; Marion Rabant³; Jean-Paul Duong Van Huyen⁴; Hatsue Ishibashi-Ueda⁵; Nobuto Kakuda¹; Masaya Ikegawa¹; ¹Doshisha university, Kyotanabe City, Japan; ²Bruker Japan K. K., Yokohama, Japan; ³Necker-Enfants malades Hospital, Paris, France; ⁴Georges-Pambidou European Hospital, Anatomy-Pathology, Paris, France; ⁵National Cerebral and Cardiovascular Center Research Institute, Suita, Japan
- WP 368 **Lipid Fingerprint Enables Identification of Human Inflammatory Bowel Disease Using Imaging Mass Spectrometry;** Simona Salivo¹; Tom K. Abban¹; Lucia Martín-Saiz²; Albert Maimó-Barceló³; Juan Bestard-Escalas³; Daniel H. López³; Sam Khorrami^{3,4}; Marcelo García^{3,4}; Gwendolyn Barceló-Coblijn³; Matthew E. Openshaw¹; José A. Fernández²; ¹Shimadzu, Manchester, United Kingdom; ²Dep. of Physical Chemistry, Fac. of Science and Technology, University of the Basque Country (UPV/EHU), Barrio Sarriena, Spain; ³Institut d'Investigació Sanitària Illes Balears (IdISBa), Palma, Spain; ⁴Gastroenterology Unit, Hospital Universitari Son Espases, Palma, Spain
- WP 369 **Mass Spectrometric In-Depth Proteome Analysis of the Kidneys from Rat Model of Diabetic Nephropathy;** Yuki Kuzuhara¹; Yume Mukasa²; Takashi Nirasawa³; Ryo Kajita³; Hatsue Ishibashi-Ueda⁴; Nobuto Kakuda²; Masaya Ikegawa^{1,2}; ¹Graduate School, Major of Medical Life Systems, Doshisha University, Kyotanabe City, Japan; ²Department of Medical Life Systems, Doshisha University, Kyotanabe City, Japan; ³Bruker Japan K.K., Yokohama, Japan; ⁴National Cerebral and Cardiovascular Center Research Institute, Suita, Japan
- WP 370 **MALDI-MSI Investigation of Lipid Alterations in Developing Rat Cerebellum Following Hypoxic/Ischemic Insult;** Dominique Figueroa¹; Maureen A. Kane²; ¹University of Maryland Baltimore, Baltimore, MD; ²University of Maryland, Baltimore, Baltimore, MD
- WP 371 **Bisphenol S Exposure Induced the Proliferation of Human Breast Tumor by Disturbing Lipid Metabolism and Protein Profiling;** Chao Zhao¹; Zongwei Cai¹; ¹Hong Kong Baptist University, HK, China
- WP 372 **Laser Desorption Ionization from Silicon Nanopost Arrays for Mass Spectrometry Imaging of Neutral Lipids in Bacterially Infected Human Skin Tissue;** Jarod Fincher¹; Derek Jones²; Andrew Korte¹; Jacqueline Dyer¹; Paola Parlanti¹; Anastas Popratiloff¹; Christine Brantner¹; Nicholas Morris³; Russell Pirlo⁴; Victoria Shanmugam²; Akos Vertes¹; ¹The George Washington University, Washington, DC; ²The George Washington University, School of Medicine and Health Sciences, Washington, DC; ³UES, Inc., Dayton, OH; ⁴United States Naval Research Laboratory, Washington, DC
- WP 373 **Reproducibility of MALDI Imaging Based Tissue Classifications - Results of a Multi-Center Study;** Soeren-Oliver Deininger¹; Rita Casadonte²; Petra Wandernoth²; Kristina Schwamborn³; Christine Bollwein³; Christian Marsching⁴; Katharina Kriegsmann⁵; Carsten Hopf⁴; Wilko Weichert³; Jörg Kriegsmann²; Peter Schirmacher³; Mark Kriegsmann⁶; Alice Ly¹; ¹Bruker Daltonik GmbH, Bremen, Germany; ²Proteopath, Trier, Germany; ³Institute of Pathology, Technical University of Munich, Munich, Germany; ⁴Center for Biomedical Mass Spectrometry and Optical Spectroscopy (CeMOS), Mannheim University of Applied Sciences, Mannheim, Germany; ⁵Department of Hematology, Oncology and Rheumatology, University Hospital Heidelberg, Heidelberg, Germany; ⁶Institute of Pathology, University Hospital Heidelberg, Heidelberg, Germany
- WP 374 **Metabolomic/Lipidomic DESI Imaging of Different Cell Cultures;** Hadeer Mattar¹; Emrys A. Jones²; Emmanuelle Claude²; Clare mills¹; ¹Division of Infection, Immunity & Respiratory Medicine, Manchester Institute of Biotechnology, University of Manchester, Manchester, United Kingdom; ²Waters Corporation, Wilmslow, United Kingdom
- WP 375 **Spatial Information of Metabolites Using Mass Spectrometry Imaging on Breast Needle Biopsy Using DEFFI-MS;** Vincen Wu¹; Paolo Inglese²; Hui-Yu Ho²; Andreas Dannhorn³; Emine Kazanc²; Goncalo Correia²; James Mckenzie²; Stephanie Ling³; Evdokia Karali⁴; Nikolaos Koundouros⁴; Hiromi Kudo²; Peter Kreuzaler⁵; Sami Shousha²; Ian Gilmore⁶; Maria Yuneva⁵; Richard Goodwin³; Josephine Bunch⁶; George Poulgiannis⁴; Zoltan Takats²; ¹Imperial College London, London, United Kingdom; ²Imperial College, London, United Kingdom; ³AstraZeneca, iMED, United Kingdom; ⁴Institute of Cancer Research, London, United Kingdom; ⁵Francis Crick Institute, London, United Kingdom; ⁶National Physical Laboratory, London, United Kingdom



- WP 376 **Mapping Molecular Interactions in the *Clostridium difficile* Infected Gastrointestinal Tract Using Multimodal Imaging Mass Spectrometry**; Emma R. Guiberson^{1,2}; Aaron G Wexler³; William J. Perry^{1,2}; Eric P. Skaar³; Richard M. Caprioli^{1,2,4,5,6}; Jeffrey M. Spraggins^{1,2,4}; ¹Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; ²Department of Chemistry, Vanderbilt University, Nashville, TN; ³Department of Pathology, Microbiology and Immunology, Vanderbilt University School of Medicine, Nashville, TN; ⁴Department of Biochemistry, Vanderbilt University, Nashville, TN; ⁵Department of Medicine, Vanderbilt University, Nashville, TN; ⁶Department of Pharmacology, Vanderbilt University, Nashville, TN
- WP 377 **Multiple Chemical and Enzymatic Approaches for Comprehensive N-Glycome Determinations of Prostate Cancer Tissues by MALDI-FTICR Imaging Mass Spectrometry**; Connor A West¹; Fred David¹; Laura Spruill¹; Anand Mehta¹; Richard R Drake¹; ¹Medical University of South Carolina, Charleston, SC
- WP 378 **Desorption Electrospray Ionization Mass Spectrometry Imaging of Brain Tissue from a Mouse Model of Smith-Lemli-Opitz Syndrome**; Amy Li¹; Libin Xu¹; ¹University of Washington, Seattle, WA
- WP 379 **A Novel Strategy for the Pathological Study of Alzheimer's Disease Brain with MALDI Imaging Mass Spectrometry with Shotgun Proteomics**; Masaya Ikegawa¹; Nobuto Kakuda¹; Tomohiro Miyasaka¹; Takashi Nirasawa²; Ryo Kajita²; Shigeo Murayama³; Yasuo Ihara⁴; ¹Doshisha university, Kyotanabe City, Japan; ²Bruker Japan K.K., Yokohama, Japan; ³The Brain Bank for Aging Research, Tokyo Metropolitan Geriatric Hospital and Institute of Gerontology, Tokyo, Japan; ⁴Graduate School of Brain Science, Doshisha University, Kyotanabe City, Japan
- INFORMATICS: ALGORITHMS AND STATISTICAL ADVANCES II**
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- WP 380 **A Ground Truth MS1 Data Set for Quantitative Evaluation of Precursor-Aware Proteomics Mass Spectrometry Data Processing Algorithms**; Jessica Henning¹; Annika Tostengard¹; Robert Smith¹; ¹University of Montana, Missoula, MT
- WP 381 **EnvCNN: A Convolutional Neural Network Model for Evaluating Isotopomer Envelopes in Top-Down Mass Spectral Deconvolution**; Abdul Rehman Basharat¹; Xie Wang²; Si Wu²; Rachele Lubecky³; Liangliang Sun³; Xiaowen Liu^{1,4}; ¹Department of BioHealth Informatics, Indiana University-Purdue University Indianapolis, Indianapolis, Indiana; ²Department of Chemistry and Biochemistry, University of Oklahoma, Norman, Oklahoma; ³Department of Chemistry, Michigan State University, East Lansing, Michigan; ⁴Center for Computational Biology and Bioinformatics, Indiana University School of Medicine, Indianapolis, Indiana
- WP 382 **Targeted Database Search Strategies for Ricin Detection: Searching Only for Ricin Peptides**; Andy Lin¹; Deanna Plubell¹; Uri Keich²; William Stafford Noble¹; ¹University of Washington, Seattle, WA; ²University of Sydney, Sydney, Australia
- WP 383 **MIND: A Double-Linear Model to Accurately Determine Monoisotopic Precursor Mass in High-Resolution Top-Down Proteomics**; Frederik Lermyte¹; Piotr Dittwald²; Jürgen Claesen³; Geert Baggerman⁴; Frank Sobott⁵; Peter B. O'Connor¹; Kris Laukens⁴; Jef Hooyberghs⁶; Anna Gambin²; Dirk Valkenborg³; ¹University of Warwick, Coventry, United Kingdom; ²University of Warsaw, Warsaw, Poland; ³Hasselt University, Hasselt, Belgium; ⁴University Of Antwerp, Antwerp, Belgium; ⁵University of Leeds, Leeds, United Kingdom; ⁶Flemish Institute for Technological Research (VITO), Mol, Belgium
- WP 384 **pValid: Validation Beyond the Target-Decoy Approach for Peptide Identification in Shotgun Proteomics**; Wen-Jing Zhou¹; Hao Yang¹; Wen-Feng Zeng¹; Kun Zhang¹; Hao Chi¹; Si-Min He¹; ¹Institute of Computing Technology, CAS, Beijing, China
- WP 385 **Bayes' Formula and Fisher Information for Automated Analysis of Mass Spectra**; Alex Ulyanenko¹; Alexander Mikhalychev²; Svetlana Vlasenko²; ¹Atomius LLC, Seattle, WA; ²Atomius OOO, Minsk, Belarus
- WP 386 **MSstatsTMT: Statistical Detection of Differentially Abundant Proteins in Mass Spectrometry Experiments with Isobaric Labeling**; Ting Huang¹; Meena Choi¹; Manuel Tzouros²; Nikhil Janak Pandya²; Balazs Banfai²; Tom Dunkley²; Olga Vitek¹; ¹Northeastern University, Boston, MA 02115; ²Roche Pharmaceutical Research and Early Development (pRED), Roche Innovation Center Munich, Germany
- WP 387 **Identification of Alternative-Splicing Events Present in Proteins Using Mass Spectrometry and a Custom Sequence Database of Junction-Spanned Peptides**; Bang-Jie Han¹; Pang-Hung Hsu¹; Wen-Shyong Tzou¹; ¹National Taiwan Ocean University, Keelung, Taiwan
- WP 388 **Tree Based Machine Learning Methods Improve Error Rates in Quality Control of Mass Spectrometry-Based Proteomics**; Eralp Dogu¹; Shantam Gupta²; Roger Olivella³; Eduard Sabido³; Olga Vitek⁴; ¹Mugla University, Mugla, Turkey; ²Quantiphi Inc, Boston, Massachusetts; ³CRG, Barcelona, Spain; ⁴Northeastern University, Boston, MA
- WP 389 **Deep Learning Methods Applied to the Analysis of Metabolomics Data**; Shinji Kanazawa^{1,2,3}; Yohei Yamada¹; Hiroyuki Yasuda¹; Akihiro Kunisawa¹; Toru Shiohama¹; Shigeki Kajihara¹; Norio Mukai¹; Masaki Kakisako⁴; Go Fujisawa⁴; Yuzuru Yamakage⁴; Junko Iida^{1,2}; Eiichiro Fukusaki⁵; Fumio Matsuda³; ¹Shimadzu Corporation, Kyoto, Japan; ²Osaka University Shimadzu Analytical Innovation Research Laboratory, Osaka University, Osaka, Japan; ³Graduate School of Information Science and Technology, Osaka University, Osaka, Japan; ⁴Fujitsu Limited, Tokyo, Japan; ⁵Graduate School of Engineering, Osaka University, Osaka, Japan
- WP 390 **SPIX, a Newly Developed Free Software to Overcome Operator Subjectivity in MS and Characterize Unknown Chemical Reactions in Complex Mixtures**; Edith Nicol¹; Yao Xu^{2,3}; Zsuzsanna Varga¹; Stéphane Bouchonnet¹; Marc Lavielle^{2,3}; ¹Laboratory of Molecular Chemistry, École Polytechnique, Palaiseau, France; ²National Institute for Research in Computer Science and Automation (Inria), Saclay, France; ³Center for Applied Mathematics, École polytechnique, Palaiseau, France
- WP 391 **In vivo Proteome Dynamics from Tandem Mass Spectrometry**; Ahmad Borzou¹; Rovshan Sadygov¹; ¹University of Texas, Galveston, TX
- WP 392 **Diversity Indices Applied to Laser-Assisted Rapid Evaporative Ionisation MS (LA-REIMS) Microbial Profiles for Quality Control and Stratification for Classification Modelling**; Alvaro Perdone-Montero¹; Simon Cameron¹; Attila Kiss²; Richard Schaffer²; Julia Balog²; Keith Richardson³; Steven D Pringle³; Zoltan Takats¹; ¹Imperial College London, London, United Kingdom; ²Waters Research Center Kft., Budapest, Hungary; ³Waters Corporation, Wilmslow, United Kingdom
- WP 393 **The Titin Problem: Hitchhiking Siblings during Protein Inference**; Kyle Lucke¹; Max Thibeau¹; Levi Zell¹; Julianus Pfeuffer²; Xiao Liang³; Oliver Serang¹; ¹University of Montana, Missoula, MT; ²Eberhard Karls University of Tübingen, Tübingen, Germany; ³Freie Universität Berlin, Berlin, Germany



- WP 394 **Improving Resource Libraries for Data Independent Acquisition through iRT Residual Prediction using Deep Learning;** Timothy Man¹; Jan Muntel¹; Roland Bruderer¹; Lukas Reiter¹; ¹*Biognosys AG, Schlieren, Switzerland*
- WP 395 **Influence of Library Selection for Proteomics Experiments on Statistical Error Rate Estimation;** Seth Just¹; Caleb Emmons¹; Jacob C Lippincott¹; Susan Ludwigsen¹; Susan T Weintraub²; Brian C Searle^{1,3}; ¹*Proteome Software, Portland, OR*; ²*University of Texas Health Science Center at San Antonio, San Antonio, TX*; ³*Institute for Systems Biology, Seattle, WA*
- WP 396 **Updates on Philosopher: a complete toolkit for both conventional and open search-based shotgun proteomics data analysis;** Felipe Da Veiga Leprevost¹; Avinash K Shanmugam¹; Dattatreya Mellacheruvu¹; Hui-Yin Chang¹; Dmitry M Avtonomov¹; Andy T. Kong¹; Alexey I. Nesvizhskii¹; ¹*University of Michigan, Ann Arbor, MI*
- WP 397 **Automating Component Detection of Small Molecules in Complex Mixtures using HRAM Q-TOF data;** Simon Ashton¹; Kirsten Hobby¹; Alan Barnes¹; Neil Loftus¹; ¹*Shimadzu Corporation, Manchester, United Kingdom*
- WP 398 **Extending the Scope of ProsiT: Accurate Fragment Ion Intensity and Retention Time Prediction for (Un) Modified (Non-)Tryptic Peptides;** Tobias Schmidt¹; Michael Graber¹; Daniel P Zolg¹; Siegfried Gessulat¹; Patroklos Samaras¹; Johannes Zerweck²; Tobias Knaute²; Hans-Christian Ehrlich³; Stephan Aiche³; Bernard Delanghe⁴; Andreas Huhmer⁵; Karsten Schnatbaum²; Ulf Reimer²; Bernhard Kuster¹; Mathias Wilhelm¹; ¹*Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany*; ²*JPT Peptide Technologies GmbH, Berlin, Germany*; ³*SAP SE, Potsdam, Germany*; ⁴*Thermo Fisher Scientific, Bremen, Germany*; ⁵*Thermo Fisher Scientific, San Jose, CA*
- WP 399 **Reducing False Peptide-Spectrum Matches in Peptide Identification using Spectrum Clustering;** Lei Wang¹; Sujun Li¹; Haixu Tang¹; ¹*Indiana University Bloomington, Bloomington, IN*
- WP 400 **Computing Information Content of PTM Site Localization Assignments Using PTMProphet;** David D. Shteynberg¹; Eric W. Deutsch¹; David S. Campbell¹; Michael R. Hoopmann¹; Ulrike Kusebauch¹; Zhi Sun¹; Anthony Whetton²; Robert L. Moritz¹; ¹*Institute for Systems Biology, Seattle, Washington*; ²*University of Manchester, Manchester, United Kingdom*
- WP 401 **IsoSpec 2.0: a Hyperfast Fine Isotopic Envelope Calculator;** Michał Startek¹; Mateusz K. Łącki²; Dirk Valkenborg^{3,4,5}; ¹*University of Warsaw, Warsaw, Poland*; ²*University Medical Center Mainz, Mainz, Germany*; ³*Centre for Proteomics (University of Antwerp/VITO (Belgium)), Antwerp, Belgium*; ⁴*Flemish Institute for Technological Research (VITO), Mol, Belgium*; ⁵*Interuniversity Institute for Biostatistics and Statistical Bioinformatics, Hasselt, Belgium*
- WP 402 **A Novel Data-Adaptive Robust Method for Quantifying Tissue Specificity Scores;** Meng Wang¹; Lihua Jiang²; Hua Tang²; Michael Snyder²; ¹*Stanford University, Stanford*; ²*Stanford University, Palo Alto, CA*
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- WP 403 **Revealing Concurrent Change of Heterogeneity and Subpopulations of Cancer Cells Using Single Cell Metabolomics;** Renmeng Liu¹; Jiannong Li²; Ann Chen²; Zhibo Yang¹; ¹*Department of Chemistry and Biochemistry, University of Oklahoma, Norman, Oklahoma*; ²*Department of Biostatistics and Bioinformatics, H. Lee Moffitt Cancer Center and Research Institute, Tampa, Florida*
- WP 404 **Incorporating In-Source Fragments Improves Metabolite Identification Accuracy in Untargeted LC-MS and LC-MS/MS Datasets;** Jacob C Lippincott¹; Phillip M Seitzer¹; Brian C Searle^{1,2}; ¹*Proteome Software, Portland, OR*; ²*Institute for Systems Biology, Seattle, WA*
- WP 405 **Automated Protein Metabolite Structure Elucidation Using HPLC/ESI-Exact Mass-MSMS Data for Insulin and ANP;** Marshall M. Siegel¹; Gary E Walker¹; Ronnie Crepeau¹; Serhiy Hnatyshyn²; Asoka Ranasinghe²; ¹*MS Mass Spec Consultants, Fair Lawn, NJ*; ²*Bristol-Myers Squibb Co., Lawrenceville, NJ*
- WP 406 **Metabolic Profiling of Small Molecule Ion Mobility Assisted Data Independent Acquisition Data Using Skyline;** Brian S Pratt¹; Johannes PC Vissers²; Ian D Wilson³; Nyasha C Munjoma²; Marine PM Letertre³; Micheal J MacCoss¹; Brendan X MacLean¹; ¹*University of Washington, Seattle, WA*; ²*Waters Corporation, Wilmslow, United Kingdom*; ³*Section of Computational and Systems Medicine, Imperial College, London, United Kingdom*
- WP 407 **Exploratory Data Analysis and Interactive Visualization of FTICR-MS Data;** Allison M. Thompson^{1,2}; Lisa M. Bramer¹; Amanda M. White¹; Kelly G. Stratton¹; Daniel Claborn¹; Kirsten S. Hofmockel^{1,2}; Lee Ann McCue^{1,2}; ¹*Pacific Northwest National Laboratory, Richland, WA*; ²*Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA*
- WP 408 **SIRIUS 4 - Turning Tandem Mass Spectra into Metabolite Structure Information;** Kai Dührkop¹; Markus Fleischauer¹; Marcus Ludwig¹; Martin A. Hoffmann¹; Juho Rousu²; Sebastian Böcker¹; ¹*Friedrich-Schiller University, Jena, Germany*; ²*Aalto University, Espoo, Finland*
- WP 409 **A Novel Approach to Data-Driven Differential Network Analysis with Limited Sample Size In High-Throughput Metabolomics and Lipidomics Data;** Gayatri R Iyer¹; Janis Wigginton²; William Duren^{1,2}; Marci Brandenburg^{1,3}; George Michailidis^{2,4}; Alla Karnovsky¹; ¹*Department of Computational Medicine and Bioinformatics, University of Michigan Medical School, Ann Arbor, MI*; ²*Michigan Regional Comprehensive Metabolomics Resource Core, Ann Arbor, MI*; ³*Taubman Health Sciences Library, University of Michigan Medical School, Ann Arbor, MI*; ⁴*Department of Statistics, University of Florida, Gainesville, FL*
- WP 410 **Web Based Basic Mass Spectrometry Search Tool For Molecules To Search Public Data;** Mingxun Wang¹; Alan K. Jarmusch¹; Ricardo R. da Silva¹; Robert Quinn²; Alexey Melnik¹; Julia M Gauglitz¹; Justin van der Hooft¹; Andrés Rodríguez¹; Louis Felix Nothias¹; Jeremy Carver¹; Jeramie Watrous¹; Mohit Jain¹; Rob Knight¹; Nuno Bandeira¹; Pieter C. Dorrestein¹; ¹*UCSD, La Jolla, CA*; ²*Michigan State University, East Lansing*
- WP 411 **A Novel Tool for Evaluation of Data Preprocessing – an Essential Step in Untargeted Metabolomics;** Yasin El Abiead^{1,2,3}; Maximilian Milford¹; Gunda Koellensperger^{1,2,3}; ¹*University of Vienna, Department of Analytical Chemistry, Vienna, Austria*; ²*Vienna Metabolomics Center (VIME), Vienna, Austria*; ³*Chemistry Meets Microbiology, Vienna, Austria*
- WP 412 **Evaluation of Freely Available Software Tools for Untargeted Quantification of 13C Isotopic Enrichment in Cellular Metabolome from HR-LCMS Data;** Manohar Dange¹; Vivek Mishra¹; Murtaza Saifuddin Merchant¹; Damini Jaiswal¹; Bratati Mukherjee¹; Charulata B Prasannan¹; Pramod P Wangikar¹; ¹*Indian Institute of Technology Bombay, Mumbai, India*
- WP 413 **Feature-Based Molecular Networking of Untargeted Mass Spectrometry Data: Bridging MS-DIAL, MZmine2, MetaboScape, OpenMS, and XC-MS, with the GNPS Web-Platform;** Louis Felix Nothias¹; Daniel Petras¹; Mingxun Wang¹; Robin Schmid^{1,2}; Abinesh Sarvepalli¹; Zheng Zhang¹; Ricardo da Silva¹; Pieter Dorrestein¹; ¹*University of California, San Diego, La Jolla, CA*; ²*University of Muenster, Institute of Inorganic and Analytical Chemistry, Muenster, Germany*



- WP 414 **Deuterater: An Analyte-Agnostic Refactoring of Kinetic Analysis Software for Deuterium-Labeled Metabolomics**; Kyle J. Cutler¹; Russell Denton¹; John C Price¹; ¹Brigham Young University, Provo, UT
- WP 415 **Using Cloud Computing for Large Scale Data Processing in Clinical Metabolomics**; Oliver Fiehn¹; Ying Zhang^{1,2}; Brian C DeFelice¹; Sili Fan¹; Diego Pedrosa¹; Sajjan S Mehta¹; Gert Wohlgemuth¹; ¹UC Davis West Coast Metabolomics Center, Davis, CA; ²Chemistry Department UC Davis, Davis, CA
- WP 416 **Using Maximum Common Substructures to Interpret Hit Lists from Small-Molecule Tandem Hybrid Similarity Searches**; Brian T. Cooper^{1,2}; Arun S Moorthy²; Tytus D Mak²; Stephen E Stein²; ¹UNC Charlotte, Charlotte, NC; ²NIST, Gaithersburg, MD
- WP 417 **MetaboQuest: Tool for Metabolite Identification**; Mohammad R Nezami Ranjibar¹; Linge Yan¹; Yan Gao¹; Habtom W Resson¹; ¹OmicsCraft LLC, Washington, District of Columbia
- WP 418 **A High-Resolution Accurate-Mass GC Electron Ionization (EI) and Chemical Ionization (CI) mass Spectral Database of Chemical Standards**; Biswapriya Biswas Misra¹; Michael Olivier¹; ¹Wake Forest Baptist Medical Center, Winston-Salem, NC
- WP 419 **The Power of MS/MSALL Acquisition for High-Throughput Metabolomics Studies**; Mariateresa Maldini¹; Eva Duchoslav²; Cyrus Papan³; Khatereh Motamedchaboki⁴; ¹SCIEX, Milan, Italy; ²SCIEX, Concord, ON; ³SCIEX, Darmstadt, Germany; ⁴Sciex, Redwood City, CA
- WP 420 **Evaluations Factors for Intra- and Inter-Batches Variations in Targeted and Untargeted Metabolomics through SPC and QC-Dependent SC Strategies**; Li Zhang^{1,2}; Peter Sajjakulnukit¹; Maureen Kachman²; Costas Lyssiotis¹; ¹University of Michigan Medical School, Cancer Center, Ann Arbor, Michigan; ²University of Michigan Medical School, BRCF Metabolomics Core, Ann Arbor, Michigan
- WP 421 **MetGem Software for the Generation of Molecular Networks Based on the t-SNE Algorithm**; Nicolas Elie¹; Florent Olivon¹; Gwendal Grelier¹; Fanny Roussi¹; Marc Litaudon¹; David Touboul¹; ¹CNRS-ICSN, Gif-Sur-Yvette, France
- WP 422 **Characterizing Product Ions in a Reference Tandem Mass Spectral Library**; Xiaoyu Yang¹; Pedatsur Neta¹; Yuri Mirokhin¹; Dmitri Tchekhovskoi¹; Yuxue Liang¹; Alexey Mayorov¹; Stephen E. Stein¹; ¹NIST, Gaithersburg, MD
- WP 423 **Development of a Machine Learning Tool to Enhance Gas Chromatography-Mass Spectrometry-Based Metabolite Identification**; Feng Qiu^{1,2,3,4}; Zhentian Lei^{1,2,3,5}; Lloyd W. Sumner^{1,2,3,5}; ¹Department of Biochemistry, University of Missouri, Columbia, MO; ²Bond Life Sciences Center, University of Missouri, Columbia, MO; ³Interdisciplinary Plant Group, University of Missouri, Columbia, MO; ⁴International Flavors & Fragrances, Union Beach, NJ; ⁵Metabolomics Center, University of Missouri, Columbia, MO
- WP 424 **Secondary Chemical Processes of Acylcarnitines Revealed by LC-MS/MS**; Xinjian Yan¹; Sanford P. Markey¹; Yamil Simón-manso¹; Ramesh Marupaka¹; Qian Dong¹; Stephen E. Stein¹; ¹NIST, Gaithersburg, MD
- WP 425 **Contextualizing Metabolomics Data by Integrating Text Mining and Computational Chemistry**; Magnus Palmblad¹; Leiden University, Leiden, Netherlands
- WP 426 **Computational metabolomics to characterize metabolites in stable isotope-labeled organisms**; Hiroshi Tsugawa¹; Ryo Nakabayashi¹; Tetsuya Mori¹; Yutaka Yamada¹; Mikiko Takahashi¹; Amit Rai²; Ryosuke Sugiyama¹; Hiroyuki Yamamoto³; Taiki Nakaya²; Mami Yamazaki²; Rik Kooke⁴; Johanna A. Bac-Molenaar⁴; Nihal Oztolan-Erol⁴; Joost J.B. Keurentjes⁴; Masanori Arita¹; Kazuki Saito¹; ¹RIKEN, Yokohama, Japan; ²Chiba University, Chuo-ku, Japan; ³Human Metabolome Technologies, Tsuruoka, Japan; ⁴Wageningen University & Research, Netherlands
- WP 427 **Uniting Metabolomics Data Processing and Highly Confident Annotation across Six MS Instrumental Set Ups: MetaboScape 5.0**; Nikolas Kessler¹; Wiebke Timm¹; Sascha Winter¹; Ulrike Schweiger-Hufnagel¹; Sven W. Meyer¹; Aiko Barsch¹; Heiko Neuweget¹; ¹Bruker Daltonics, Bremen, Germany
- WP 428 **Retention Time Prediction of Dansyl Labeled Tripeptides Using Machine Learning Methods for Dansylation LC-MS Metabolomics**; Hao Li¹; Liang Li²; ¹University of Alberta, Edmonton; ²University of Alberta, Edmonton, AB
- WP 429 **Metabolite Classification into Major Chemical Classes using Supervised Machine Learning**; Elizabeth H. Mahood¹; Cornell University, Ithaca, NY
- WP 430 **A Scalable Approach to Curation of Public MS2 Spectra for Co-Analysis Using Untargeted Mass Spectrometry**; Alan K. Jarmusch^{1,2}; Mingxun Wang^{1,2}; Madeleine Ernst^{1,2}; Ricardo R. da Silva^{1,2}; Pieter C. Dorrestein^{1,2}; ¹Skaggs School of Pharmacy & Pharmaceutical Sciences, University of California – San Diego, La Jolla, CA; ²Collaborative Mass Spectrometry Innovation Center, University of California – San Diego, La Jolla, CA
- WP 431 **MZmine 3 - a Comprehensive Mass Spectrometry Data Processing Framework for Metabolomics**; Tomáš Pluskal¹; Robin Schmid²; Ansgar Korf²; Timothy R Fallon¹; Aleksandr Smirnov³; Matej Orešič⁴; Xiuxia Du³; Jing-ke Weng¹; ¹Whitehead Institute for Biomedical Research, Cambridge, MA; ²University of Muenster, Institute of Inorganic and Analytical Chemistry, Muenster, Germany; ³The University of North Carolina at Charlotte, Charlotte, NC; ⁴Örebro University, Örebro, Sweden

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- WP 432 **Improving Resolution of Frequency-Scanning ESI Ion Trap MS in Rough Vacuum using Periodic DC Focusing and Segment Quad Interface**; Jung-Lee Lin¹; Hsi-Chang Shih¹; Chung-Hsuan Chen¹; ¹The Genomics Research Center Academia Sinica, Taipei, Taiwan
- WP 433 **Software for Automated Laser Ablation and Capture from Tissue Sections**; Fabrizio Donnarumma¹; Touradj Solouki²; Kermit K Murray¹; ¹Louisiana State University, Baton Rouge, LA; ²Baylor University, Waco, TX
- WP 434 **Characterization of Quadrupole Mass Filters Regarding Elevated Entrance Ion Currents**; Markus Langner¹; Marco Thinius¹; Chris Heintz¹; Yessica Brachthaeuser²; Hendrik Kersten¹; Thorsten Benter¹; ¹Bergische Universität Wuppertal, Wuppertal, Germany; ²Carl Zeiss SMT, Oberkochen, Germany
- WP 435 **Time-of-Flight Compensated Ion Transmission: Theory, Simulation, and Application in Fourier Transform Ion Cyclotron Resonance Mass Spectrometry**; Qinghao Wu¹; Jared B. Shaw²; Ljiljana Pasa-Tolic²; ¹IonX Tech, LLC, Richland, WA; ²PNNL, Richland, WA
- WP 436 **Performance Evaluation of a Modified Quadrupole Orbitrap Mass Spectrometer**; Tabiwang N. Arrey¹; Rosa Jessie-Christensen Rakownikow¹; Julia Kraegenbring¹; Kerstin Strupat¹; Markus Kellmann¹; Catharina Crone¹; Thomas Moehring¹; Alexander Harder¹; ¹Thermo Fisher Scientific, Bremen, Germany
- WP 437 **Determining the Nature of MS Contamination with Various Sample Matrices**; Leigh Bedford¹; Yang Kang¹; Bradley B. Schneider¹; Thomas R. Covey¹; ¹SCIEX, Concord, ON



- WP 438 **Reliable and Deep Proteome Coverage by Gas-Phase Fractionation of Peptides with a FAIMS Pro Interface on a Modified Quadrupole Orbitrap**; [Julia Kraegenbring](#)¹; Tabiwang N. Arrey²; Michael W. Belford³; Satendra Prasad³; Kerstin Strupat²; Markus Kellmann²; Thomas Moehring²; Alexander Harder²; ¹*Thermo Fisher Scientific, Bremen, Germany*; ²*Thermo Fisher Scientific, Bremen, Germany*; ³*ThermoFisher, San Jose, CA*
- WP 439 **Development of Vacuum Measurement and Control System for Quadrupole Mass Spectrometer**; [Li Kai](#)¹; li ming¹; ¹*NCS Testing technology Co.,Ltd, Beijing, China*
- WP 440 **Development of Universal and High Sensitivity Ion Mobility Spectrometer with APCI Ion Source for HPLC (LC-APCI-IMS)**; [Yoshinori Arita](#)¹; Akiko Imazu¹; Motohide Yasuno¹; Hiroshi Tanaka¹; Toshiya Habu¹; Yoshihito Yuasa¹; Kiyoshi Ogawa¹; ¹*Shimadzu Corporation, Kyoto, Japan*
- WP 441 **DRY Ion Localization and Locomotion (DRILL) MS Interface for Sensitivity Enhancement via Droplet Size Based Inertial Separation**; [Jung Lee](#)¹; Peter Kottke¹; Crystal L Pace²; David C Muddiman²; Alex Jonke³; Matthew P. Torres³; Andrei Fedorov¹; ¹*Georgia Institute of Technology, Atlanta, GA*; ²*North Carolina State University, Raleigh, NC*; ³*School of Biological Sciences, Georgia Institute of Technology, Atlanta, GA*
- WP 442 **Ion Manipulation Using Stacked PCB-Based Electrode Device (SPED)**; Yi-teng Hsiao¹; Szu-Wei Chou¹; [Yi-Kun Lee](#)¹; Pin-Duo Lee¹; Shih-Chieh Yang¹; Yao-Hsin Tseng¹; Chun-Yen Cheng¹; ¹*AcroMass Technologies, Inc., Hsinchu, Taiwan*
- WP 443 **Comparison of UPLC and RapidFire MS/MS Methods for Content Uniformity Analysis in Tablet-Splitting for a Narrow Therapeutic Index Drug Warfarin**; [Jiang Wang](#)¹; Haiou Qu²; Robert L Hunt²; Leanna Hengst²; Patrick J. Faustino²; Jinhui Zhang²; ¹*Food and Drug Administration - Center for Drug Evaluation and Research, Silver Spring, Md*; ²*FDA, Silver Spring, MD*
- WP 444 **Impact of Dwell Time and Ion Flux on Multiple Reaction Ion Monitoring (MRM) Measurement Precision**; [Behrooz Zekavat](#)¹; Charles Nichols¹; Anabel Fandino¹; ¹*Agilent Technologies, Santa Clara, CA*
- WP 445 **Resolution Improvement through Modulation of Collective Ion Motion and Ejection in Quadrupole Ion Trap Mass Spectrometry for Intact Protein**; [Yi-teng Hsiao](#)¹; Szu-Wei Chou¹; Shih-Chieh Yang¹; Pin-Duo Lee¹; Yi-Kun Lee¹; Yao-Hsin Tseng¹; Chun-Yen Cheng¹; ¹*AcroMass Technologies, Inc., Hsinchu, Taiwan*
- WP 446 **A Novel Mass Spectrometry-Based Analytical System for Single-Cell Proteomics and Metabolomics in Mammalian Cells**; [Yoshihiro Izumi](#)¹; Kousuke Hata¹; Kohta Nakatani¹; Takeshi Hara¹; Shohei Yamamura²; Masaki Matsumoto¹; Takeshi Bamba¹; ¹*Medical Institute of Bioregulation, Kyushu University, Fukuoka, Japan*; ²*Health Research Institute, National Institute of Advanced Industrial Science and Technology, Kagawa, Japan*
- WP 447 **Transfer of Plasma-Generated Ions into a Fourier Transform Quadrupole Ion Trap (FT-QIT) with Running RF Trapping Field**; [Yessica Brachthäuser](#)¹; Chris Heintz²; Alexander Laue¹; Michel Aliman¹; Hin Yiu Chung¹; Thorsten Benter²; ¹*Zeiss SMT GmbH, Oberkochen, Germany*; ²*University of Wuppertal, Wuppertal, Germany*
- WP 448 **Automated Tuning of an Electromagnetostatic Cell for Electron Capture Dissociation with Q-ToF Mass Spectrometers**; [Blake A. Hakkila](#)¹; Joseph C. Meeuwsen^{1,2}; Yury V. Vasil'ev^{1,2}; Joseph S. Beckman^{1,2}; Valery G. Voinov^{1,2}; ¹*e-MSion, Inc., Corvallis, OR*; ²*Oregon State University, Corvallis, OR*
- WP 449 **Rectilinear Quadrupole Ion Guides: Transmission as a Function of Mass, RF Amplitude and RF Frequency**; [Kevin Kuchta](#)¹; Luke J. Metzler²; Michael J. Van Stipdonk²; Randall E Pedder¹; ¹*Ardara Technologies, Ardara, PA*;

²*Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA*

- WP 450 **Developing a Multi-Pass Overtone Mobility Spectrometry "Ping Pong" Insert to Improve the Drift Resolution of the Waters HDMS (G1)**; [Kyle Buckley](#)¹; Marc Legris¹; Arthur Laganowsky²; David H. Russell²; David E. Clemmer¹; ¹*Indiana University, Bloomington, IN*; ²*Texas A&M University, College Station, TX*
- WP 451 **Characterization of Ion Funnel: Transmission Characteristics as a Function of Mass, RF Voltage and RF Frequency**; [Luke J. Metzler](#)¹; Kevin Kuchta²; Michael J. Van Stipdonk¹; Randall E Pedder²; ¹*Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA*; ²*Ardara Technologies L.P., Ardara, PA*
- WP 452 **Modifying the Ion Optics and Scan Sequences on a Tribrid MS to Improve Sensitivity, Duty Cycle, and Overall Instrument Ease-of-Use**; [Graeme McAlister](#)¹; Michael Goodwin¹; Lee Earley¹; Raman Mathur¹; Oliver Lange²; Romain Huguet¹; Vlad Zabrouskov¹; Mike Senko¹; ¹*Thermo Fisher Scientific, San Jose, CA*; ²*Thermo Fisher Scientific, Bremen, Germany*

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- WP 453 **A Microchannel Thermalization Inlet Design to Eliminate Impact-Induced Molecular Fragmentation in Closed-Source Mass Spectrometers**; [Brandon Turner](#)¹; Anupriya Anupriya¹; Sandra Osburn-Staker¹; Abraham De la Cruz¹; Eric T. Sevy¹; Daniel E. Austin¹; ¹*Brigham Young University, Provo, UT*
- WP 454 **Concurrent Dual Polarity Ion Mobility (IM) Separations using Traveling Wave-based Structures for Lossless Ion Manipulations (SLIM)**; [Isaac Kwame Attah](#)¹; Yehia M. Ibrahim¹; Sandilya V.B. Garimella¹; Gabe Nagy¹; Randolph V. Norheim¹; Colby E. Schimelfenig¹; Richard D. Smith¹; ¹*Pacific Northwest National Laboratory, Richland, WA*
- WP 455 **Ion Mobility Measurement using a Miniature Dual-Trap Mass Spectrometer**; [Jingjin Fan](#)¹; Xinwei Liu¹; Xiaoyu Zhou¹; Zheng Ouyang¹; ¹*Tsinghua University, Beijing, China*
- WP 456 **Combining DIUTHAME and Stigmatic-Type Mass Microscope toward Cellular Scale Imaging Mass Spectrometry**; [Tsuyoshi Hirao](#)^{1,2}; Yasuhide Naito¹; ¹*GPI, Hamamatsu, Japan*; ²*Hamamatsu Photonics K.K., Hamamatsu, Japan*
- WP 457 **High Sensitivity and Resolution IMS Separations at 100% Ion Utilization Efficiency**; [Sandilya Garimella](#)¹; Gabe Nagy¹; Yehia M Ibrahim¹; Isaac K. Attah¹; Aneesh Prabhakaran¹; Richard D. Smith¹; ¹*Pacific Northwest National Laboratory, Richland, WA*
- WP 458 **Bridging the Gap Between Gas- and Condensed-Phase Using Dual-Polarity Ion Soft Landing**; [Pei Su](#)¹; Hang Hu¹; Jonas Warneke¹; Mikhail Belov²; Gordon Anderson³; Julia Laskin¹; ¹*Purdue University, West Lafayette, IN*; ²*Spectrograph, LLC, Kennewick, WA*; ³*GAA Custom Engineering, LLC, Benton City, WA*
- WP 459 **Determination of Drugs of Abuse in Human Hair by On-Line Supercritical Fluid Extraction – Supercritical Fluid Chromatography - Mass Spectrometry**; Alison P Wicker¹; [Blair K Berger](#)¹; Tairo Ogura²; Kenichiro Tanaka²; Masayuki Nishimura³; Vivian chen³; William Hedgepeth³; Kevin A. Schug¹; ¹*University of Texas at Arlington, Arlington, TX*; ²*Shimadzu Corporation, Nakagyo-ku, Japan*; ³*Shimadzu Scientific Instruments, Inc, Innovation Center, Columbia, MD*
- WP 460 **Implementation of an Ambient-Fourier Transform-Drift Tube on an Ultra High Mass Range Orbitrap™ Mass Spectrometer for Analysis of Protein Complexes**; Sarah Sipe¹; James Sanders¹; Tobias Reinecke²; Brian H. Clowers²; [Jennifer S Brodbelt](#)¹; ¹*Department of Chemistry, University of Texas at Austin, Austin, TX*; ²*Department of Chemistry, Washington State University, Pullman, WA*



- WP 461 **Evaluation of a Novel PTR-TOFMS Setup Capable of Extremely Rapid Reagent Ion Switching;** Alfons Jordan¹; Christian Lindinger¹; Stefan Feil¹; Gernot Hanel¹; Lukas Märk¹; Philipp Sulzer¹; ¹IONICON Analytik GmbH, Innsbruck, Austria
- WP 462 **Experimental Design of a Rotor-Induced Collision Cell (RICC) to Study Molecular Fragmentation During Hypervelocity Impacts Prior to Mass Analysis;** Abraham L De la Cruz Hernandez¹; Friso Van Amerom²; Anupriya Anupriya³; Sandra Osburn-Staker⁴; Brandon Turner¹; Eric T. Sevy¹; Daniel E. Austin¹; ¹Brigham Young University, Provo, UT; ²Mini Mass Consulting, St. Petersburg, Florida; ³Intel, Portland, Oregon; ⁴University of Utah, Salt Lake City, UT
- WP 463 **Pulse Width Modulation Control of Electron Beam Intensity in Electron Capture Dissociation using Precursor Charge State Information;** Anjali Chelur¹; Suya Liu¹; Calin Bradau¹; Pavel Ryumin¹; Thomas J Binko¹; Nick Albeanu¹; Takashi Baba¹; ¹SCIEX, Concord, ON
- WP 464 **High Resolution Acceptance Phase Plane Analysis of the Rectangular and Sinusoidally Driven Linear RF Quadrupole;** Adam P. Huntley¹; Gregory F. Brabeck²; Peter T. A. Reilly¹; ¹Washington State University, Pullman, WA; ²Excellims Corporation, Acton, Massachusetts
- WP 465 **SLIMion: An Automated Framework for Performing Multi-Dimensional Parameter Optimizations of Structures for Lossless Ion Manipulations (SLIM) Using SIMION;** Ron Danehy¹; Ahmed M Hamid¹; Liulin Deng¹; John Daniel Debord¹; ¹MOBILion Systems Inc., Exton, PA
- WP 466 **A Novel Instrument Platform for the Investigation of Particle Formation from the Gas Phase;** Tina Kasper¹; Martin Hoener¹; Dimitris Papanastasiou²; Alexander Lekkas²; Diamantis Kounadis²; John Orfanopoulos²; ¹University of Duisburg, Duisburg, Germany; ²Fasmatech, Athens, Greece
- WP 467 **Covalent Modification via Ion/Ion Reactions with Ion Mobility/Mass Spectrometry Structural Analyses;** Veronica V Carvalho¹; Ian K. Webb¹; ¹IUPUI Department of Chemistry & Chemical Biology, Indianapolis, IN
- WP 468 **Development of Colinear Resonance Ionisation Spectroscopy (CRIS) for Sub-ppt quasi-IRMS Based Assays Including Carbon Dating;** Giles Edwards^{1,2}; Ben Cooper¹; Sultan Alsufyani¹; Christopher Ricketts¹; Holly Perrett¹; Cory Binnerley¹; Kieran Flanagan^{1,2}; ¹The University of Manchester, School of Physics and Astronomy, Manchester, United Kingdom; ²The Photon Science Institute, The University of Manchester, Manchester, United Kingdom
- WP 469 **Extended Path Length Ion Mobility with Structures for Lossless Ion Manipulations (SLIM) as an Ultra-Sensitive Pressure Gauge;** Gregory Webster¹; Ahmed Mohamed Hamid¹; Daniel DeBord¹; Liulin Deng¹; Kelly Wormwood¹; Anisha Yadav¹; Gordon Anderson²; ¹MOBILion Systems Inc., Exton, PA; ²GAA Custom Engineering, LLC, Benton City, WA
- WP 470 **Development of a [CID-TIMS]x[CID-TIMS]-q-CID-TOF HRMS platform for Discovery and Targeted o-mics Studies;** Mark E. Ridgeway¹; Melvin A. Park²; Francisco Fernandez Lima³; ¹Bruker Daltonics Inc., Billerica, MA; ²Bruker Daltonics Inc., Billerica, MA 01821; ³Florida International University, Miami, FL
- WP 471 **Phasing two-dimensional (2D) Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS) in both dimensions;** Ulviya Abdulkarimova¹; Marc Haegelin²; Fabrice Bray²; Anne Jeannin-Girardon¹; Pierre Collet¹; Christian Rolando²; ¹Université de Strasbourg, Strasbourg, France; ²Université de Lille, Villeneuve d'Ascq, France
- WP 472 **Neoteric Approaches to MS Instrumentation Facilitated by Simulation;** Jerome Moore; ¹Robert Nose Corporation, Lemont, IL
- WP 473 **Ruthenium Catalyzed 2e-/2H+ PCET - Characterizing the Catalyst-Substrate Interaction with High-Resolution Mass Spectrometry and Gas-Phase Vibrational Spectroscopy;** Fabian S Menges¹; Evan H Perez²; Mauricio Cattaneo²; James Mayer¹; Mark Johnson¹; ¹Yale University, New Haven, CT; ²Universidad Nacional de Tucumán, Tucumán, Argentina
- WP 474 **Improved Integration of a Separation Column to an Ion Source for Liquid Chromatography Mass Spectrometry;** Michael Fogwill¹; Angela Doneanu¹; Stephen Hattan¹; Jason Hill¹; Wade P Leveille¹; Thomas McDonald¹; Joseph Michienzi¹; ¹Waters Corporation, Milford, MA
- WP 475 **Nano-Scale HPLC System for Isocratic and Gradient Ultra-Nano HPLC Separations;** Stan Stearns¹; Jennifer Copeland¹; Huamin Cai¹; Martin Brisbin¹; Alex Plistil¹; Hal Barnett¹; ¹VICI Valco Instrument, Houston, TX
- WP 476 **Advanced analytics for regulatory science: Application of an innovative robotic sample separation system coupled with tandem mass spectrometry;** Jinhui Zhang¹; Patrick J. Faustino¹; ¹FDA, Silver Spring, MD
- WP 477 **Growing MS adoption: A "Self-Driving" Mass Spectrometer Designed for Non-MS Experts;** Maggie A. Ostrowski¹; F. Robert Ley¹; Kyle Covert¹; Kai Zhang¹; Susan Shen¹; Shane E. Tichy¹; ¹Agilent Technologies, Inc., Santa Clara, CA
- WP 478 **Automated and Simultaneous Identification and Quantification in Extractables and Leachables Analysis;** Andrew Jones¹; Tommy Saunders¹; Ashley Baeten²; Yongdong Wang³; ¹Activated Research Company, Eden Prairie, MN; ²Abbott, St. Paul, Minnesota; ³Cerno Bioscience, Norwalk, CT

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- WP 479 **Computational Chemistry and Ion Mobility – Mass Spectrometry at High Resolving Power Suggest Prototropism of Cyclic Lipopeptides;** Andréa Mccann¹; Christopher Kune¹; Johann Far¹; Philippe Massonnet^{1,2}; Philippe Jacques³; Marc Ongena³; Loic Quinton¹; Edwin De Pauw¹; ¹University of Liege, MS Lab - GIGA, MoISys Research Unit, Liege, Belgium; ²Maastricht Multimodal Molecular Imaging (M4I) Institute, Division of Imaging Mass Spectrometry, Maastricht, Netherlands; ³Terra teaching and research center, Gembloux Agro-Bio Tech, University of Liege, Gembloux, Belgium
- WP 480 **Use of DESI with IMS Enhancement in Study of Transferred Material on Paper;** Liepin Huang¹; Carrie L Hogue²; Gilbert Castillo²; ¹Corning Inc., Horseheads, NY; ²Corning Inc., Painted Post, 14870
- WP 481 **Collision Induced Unfolding Experiments to Decipher the Structural Regions of a Hybrid Monoclonal Antibody;** Thomas Botzanowski¹; Oscar Hernandez-Alba¹; Olivier Colas²; Elsa Wagner-Rousset²; Alain Beck²; Sarah Cianferani¹; ¹Laboratoire de Spectrométrie de Masse BioOrganique, Université de Strasbourg, CNRS, IPHC UMR 7178, Strasbourg, France; ²IRPF, Centre d'Immunologie Pierre-Fabre (CIPF), Saint-Julien-en-Genevois, France
- WP 482 **New High Resolution Mass Spectrometry Ion Mobility Applications in the Identification of Challenging Environmental Metabolites;** Yelena A. Adelfinskaya¹; David G McCaskill¹; Jesse L Balcer¹; Nick N Wang¹; Jeffery Gilbert¹; Michael W. Madary¹; Pete L. Johnson¹; Suresh Annangudi Palani¹; Scott A. Greenwalt¹; ¹Corteva Agriscience, Indianapolis, IN
- WP 483 **Characterisation of Intact Hemoglobin Variants Utilising a Cyclic Ion Mobility-Enabled Quadrupole Time-of-Flight (Q-cIM-oaToF) Mass Spectrometer;** Ahmad Alkawi¹; James Scrivens¹; Gillian Taylor¹; Safwan Akram¹; Martin Palmer²; Jakub Ujma²; Kevin Giles²; Jonathan P Williams²; Matthew Edgeworth³; ¹Teesside University, Middlesbrough,



- WP 484 **United Kingdom; ²Waters Corpotaion, Cheshire, United Kingdom; ³MedImmune, Granta Park, United Kingdom**
Copper Complexation Strategies for Differentiating Amino Acid Enantiomers by Ion Mobility; Emanuel Zlibut¹; Jody C. May¹; John A. McLean¹; ¹Vanderbilt University, Nashville, TN
- WP 485 **Chirality-Regulated Human Serum Albumin-Neuropeptide Interactions Revealed by Ion Mobility-Mass Spectrometry; Jiabao Guo¹; Gongyu Li²; Lingjun Li^{1,2}; ¹Department of Chemistry, University of Wisconsin-Madison, Madison, WI; ²School of Pharmacy, University of Wisconsin-Madison, Madison, WI**
- WP 486 **Structural Analysis of Phosphopeptide Conformers using ECD, TWIMS and Molecular Modelling; Anna L Simmonds¹; Andrea F Lopez-Clavijo²; Peter J Winn¹; John K Heath¹; David H. Russell³; Iain B. Styles¹; Helen J Cooper¹; ¹University of Birmingham, Birmingham, United Kingdom; ²Babraham Institute, Cambridge, United Kingdom; ³Texas A&M University, College Station, TX**
- WP 487 **Analysis of Heteroatomic Species in Weathered Crude Oil using Ion Mobility Time-of-Flight ESI-MS; Nolan Snyder¹; Feiyue Wang¹; Jake Ritchie¹; Diana Saltymakova¹; Katarzyna Polcwiartek¹; Durell S. Desmond¹; Casey Hubert²; Gary A. Stern¹; Alastair F. Smith²; ¹University of Manitoba, Winnipeg, MB; ²University of Calgary, Calgary, AB**
- WP 488 **Analysis of Gold-Molybdenum Complexes by Nano-Electrospray Ionization-Ion Mobility-Mass spectrometry; Hannah J Harbin¹; Kyle L Wilhelm¹; Dhirgam Humaidy²; Raul Villacob¹; Alice E Bruce²; Mitchell R. M. Bruce²; Touradj Solouki¹; ¹Baylor University, Waco, TX; ²The University of Maine, Orono, ME**
- WP 489 **Improvement in Quantitative Analysis of Vitamin D Metabolites in Blood using Click Derivatization Reagents Combined with LC-TimsTOF; Debin Wan¹; Xuejun Peng²; Jun yang¹; Bogdan Barnych¹; Nalin Singh¹; Bruce D Hammock¹; ¹UC Davis, Davis, CA; ²Bruker Daltonics Inc., San Jose, CA**
- WP 490 **Azobenzene Photoswitches: Observing Molecules Switching Using Ion Mobility Mass Spectrometry; Julien De Winter¹; Agostino Galanti²; Quentin Duez¹; Jérôme Cornil¹; Paolo Samori²; Pascal Gerbault¹; ¹University of Mons, Mons, Belgium; ²University of Strasbourg, Strasbourg, France**
- WP 491 **Enhanced Software for the Classification of Charge Multiplexed Collision Induced Unfolding Data; Daniel A. Polasky¹; Sugyan M. Dixit¹; Kathryn D. Kulju¹; Daniel D. Vallejo¹; Ruwan T. Kurulugama²; John C. Fjeldsted²; Brandon T. Ruotolo¹; ¹University of Michigan, Ann Arbor, MI; ²Agilent Technologies, Santa Clara, CA**
- WP 492 **The Benefit of Peptide CCS Value Prediction and Experimental Determination; Sebastian Wehner¹; Favio Salinas²; Stuart Pengelley¹; Heiko Neuweger¹; Heiner Koch¹; Anjali Alving³; Na Parra³; Greig Michael³; Juergen Cox²; Detlev Suckau¹; ¹Bruker Daltonics, Bremen, Germany; ²Max Planck Institute of Biochemistry, Martinsried, Germany; ³Bruker Daltonics Inc., Billerica, MA**
- WP 493 **Characterization of Derivatized Carbohydrates Using High Resolution Cyclic IMS and Tandem-IMS Techniques; Kristin McKenna¹; Andrew Baker²; Martin Palmer³; Dale Cooper-Shepherd³; Facundo M. Fernandez¹; ¹Georgia Institute of Technology, Atlanta, GA; ²Waters Corporation, Pleasanton, CA; ³Waters Corporation, Wilmslow, United Kingdom**
- WP 494 **Differentiating Commercial Lubricant Oils using Ion-Mobility Enabled Mass Spectrometry; Jeff Goshawk¹; Eleanor Riches¹; Caitlyn Da Costa¹; Gordon Jones¹; ¹Waters Corporation, Wilmslow, United Kingdom**
- WP 495 **Development of a Collisional Cross Section Library using Trapped Ion Mobility Spectrometry (TIMS) and Its Use in Plant Metabolomics; Mark J Schroeder^{1,2,3}; Sven W. Meyer⁴; Aiko Barsch⁴; Lloyd W. Sumner^{1,2,3}; ¹Department of Biochemistry, University of Missouri, Columbia, MO; ²Bond Life Sciences Center, University of Missouri, Columbia, MO; ³Interdisciplinary Plant Group, University of Missouri, Columbia, MO; ⁴Bruker Daltonik GmbH, Bremen, Germany**
- WP 496 **De Novo Peptide Sequencing Using TIMS- MS/MS for Amphibian Skin Peptides; Benjamin Bokor¹; Jacob Porter¹; Mario E. Gomez Hernandez¹; Alessandro Catenazzi¹; Francisco A. Fernandez-Lima¹; ¹Florida International University, Miami, FL**
- WP 497 **Post-ionization separation of isomeric cannabinoids by means of Trapped Ion Mobility-Mass Spectrometry; Arne Behrens¹; Sabrina Kröger¹; Uwe Karst¹; ¹University of Muenster, Institute of Inorganic and Analytical Chemistry, Muenster, Germany**
- WP 498 **Atmospheric Pressure Ion-Mobility MS with a Low Entrance Potential; William P. McMahon¹; Joseph E. Lesniewski¹; Kaveh Jorabchi¹; ¹Georgetown University, Washington, DC**
- WP 499 **Trapped Ion Mobility Spectrometry and Surface-Induced Dissociation (TIMS-SID) on a 15 T FT-ICR for Structural Characterization of Native Protein Complexes; Erin Panczyk^{1,2}; Arpad Somogyi^{2,3}; Mark E. Ridgeway⁴; Melvin A. Park⁴; Vicki H. Wysocki^{1,2,3}; ¹Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH; ²Resource for Native MS Guided Structural Biology, The Ohio State University, Columbus, OH; ³Campus Chemical Instrument Center, Mass Spectrometry and Proteomics Facility, The Ohio State University, Columbus, OH; ⁴Bruker Daltonics Inc., Billerica, MA**
- WP 500 **Exploring the Conformational Space of Growth Hormone-Releasing Hormone Analogs using Dopant Assisted Trapped Ion Mobility Spectrometry; Javier Moreno¹; Kevin Jeanne Dit Fouque¹; Francisco Fernandez-Lima¹; ¹Florida International University, Miami, FL**

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- WP 501 **Direct LC/MS Analysis Method of Surfactants Contained in Antibody Drugs Using a Polymer-Based Reversed Phase Column; Leah Sullivan¹; Junji Sasuga¹; Hiroki Takenaka¹; Eiji Kagawa¹; Ron Benson¹; ¹Shodex, Showa Denko America, Inc., New York, NY**
- WP 502 **Mutant KRas Protein and Tryptic Peptides Separation and Characterization Using Enhanced Fluidity Liquid Chromatography Coupled with Tandem Mass Spectrometry; Juan Bian; ¹The Ohio State University, Columbus, OH**
- WP 503 **Ultra-fast Capillary-Flow LC-MS Profiling of Complex Biological Matrices: Applicable to Large Sample Cohorts; Oleksandr Boychenko¹; Jenny Ho²; Christopher Pynn¹; ¹Thermo Fisher Scientific, Germering, Germany; ²Thermo Fisher Scientific, Hemel Hempstead, United Kingdom**
- WP 504 **The Characterization of Column Heating Effect in Nano-Flow Liquid Chromatography Mass Spectrometry (nanoLC-MS)-Based Proteomics; Linhui Zhai¹; Bolin Li¹; Hao Hu¹; Fang Guo²; Ping Liu¹; Minjia Tan¹; ¹Shanghai Institute of Materia Medica, Chinese Academy of Sciences, Shanghai, China; ²Shanghai Easymass Co., Ltd., Shanghai, China**
- WP 505 **Characterization of the Merck Sample Collection by UPLC-MS And Evaluation of the Data Using Virscidian; Wilfredo Pinto; Merck, Rahway, NJ**
- WP 506 **An Updated Perspective on Deconvoluting Chimeric MS/MS Spectra by LC and Precursor Isolation and Their Subsequent Assignment by CharmERT; Manuel I. Villalobos Solis^{1,2}; Richard J. Giannone¹; Robert L. Hettich¹; Paul E. Abraham¹; ¹Oak Ridge National Laboratory, Oak Ridge, TN; ²University of Tennessee, Knoxville, TN**



- WP 507 **Rapid Separation of Reduced Antibody Chains by Size Exclusion Chromatography Coupled to Electro spray Mass Spectrometry**; John H. Robinson¹; John O. Hui¹; Iain D. G. Campuzano¹; ¹Amgen Inc., Thousand Oaks, CA
- WP 508 **Instrument Performance Evaluation and Tracking Using a Quality Control Standard for Proteomics Laboratory**; Shenheng Guan^{1,2}; Jonathan Krieger²; Leanne Wybenga-Groot²; Bin Ma³; Michael F. Moran^{2,4}; ¹University of Waterloo, Waterloo; ²SPARC BioCentre, Hospital for Sick Children, Toronto, Ontario; ³University of Waterloo, Waterloo, ON; ⁴University of Toronto, Toronto, ON
- WP 509 **Characterization of the Activity and Kinetics of Guanine Deaminase**; Justin Godinho¹; Ben Libert¹; Barry Boyes¹; ¹Advanced Materials Technology, Wilmington, DE
- WP 510 **A new LC-MS Approach for Synthetic Peptide Characterization and Impurity Profiling**; Asish Chakraborty¹; Nilini Nilini Ranbaduge¹; Ying Qing Yu¹; ¹Waters Corporation, Milford, MA
- WP 511 **Becoming Street-Smart in the CDMO Space: Utilization of Multiple Technologies to Harmonize Release and Characterization Assays for non-mAb Proteins**; Irina Perdivara¹; Margo Wilson¹; Clara Smith¹; ¹Fujifilm Diosynth Biotechnologies, Morrisville, NC
- WP 512 **Intact Analysis of Biopharmaceuticals by Hydrophobic Interaction/Reversed Phase 2D-LC/MS System**; sandeep kondaveeti¹; Dat Phan¹; Bob Giuffrè¹; Gregory Staples²; Andrew Coffey³; Suma Ramagiri¹; Priya Jayaraman¹; Jin Zhang¹; ¹Agilent Technologies, Inc., Wilmington, DE; ²Agilent Technologies, Inc., Santa Clara, CA; ³Agilent Technologies, Churuch Stretton, United Kingdom
- WP 513 **A Quantitative Compliant Multi Attribute Methodology (MAM) LC/MS workflow**; Zoe Zhang¹; Sean McCarthy²; Elliott Jones¹; Todd Stawicki²; ¹Sciex, Redwood City, CA; ²Sciex, Framingham, MA
- WP 514 **A Sensitive Microflow LC/MS/MS Method for the Analysis of Corticosteroids in Human Plasma**; Ting Liu¹; Wenhai Jin¹; Daniel K Blake²; ¹Sciex, Shanghai, China; ²SCIEX, Warrington, United Kingdom
- WP 515 **Homology-Based Peptide Retention Time Prediction for Proteomic RP HPLC-MS Applications**; Oleg V. Krokhin¹; Vic Spicer¹; ¹University of Manitoba, Winnipeg, MB
- WP 516 **Temperature-Specific Peptide Retention Time Prediction for nano-RP-HPLC in Proteomic Applications**; Carina Villacres¹; Benilde Mizero²; Vic Spicer³; Rosa Viner⁴; Julian Saba⁵; Bhavin Patel⁶; Sergei Snovid⁶; Penny Jensen⁶; Andreas Huhmer⁴; Oleg V. Krokhin^{2,3,7}; ¹Manitoba Centre for Proteomics and Systems Biology, University of Manitoba, Winnipeg, Manitoba; ²Department of Chemistry, University of Manitoba, Winnipeg, MB; ³Manitoba Centre for Proteomics and Systems Biology, University of Manitoba, Winnipeg, MB; ⁴Thermo Fisher Scientific, San Jose, CA; ⁵Thermo Fisher Scientific, Mississauga, ON; ⁶Thermo Fisher Scientific, Rockford, IL; ⁷Department of Internal Medicine, Winnipeg, MB
- WP 517 **Peptide Retention Time Prediction for TMT-Labeled Peptides in RP-HPLC for Proteomic Applications**; Benilde Mizero¹; Carina Villacres²; Vic Spicer²; Rosa Viner³; Julian Saba; Bhavin Patel⁴; Sergei Snovid⁴; Penny Jensen⁴; Andreas Huhmer³; Oleg V. Krokhin²; ¹Department of Chemistry, University of Manitoba, Winnipeg, MB; ²Manitoba Centre for Proteomics and Systems Biology, University of Manitoba, Winnipeg, Manitoba; ³ThermoFisher, San Jose, CA; ⁴Thermo Fisher Scientific, Rockford, IL
- WP 518 **Simultaneous Extraction of Proteins, Lipids, and Metabolites for Integrated-omics Approaches for Low Tissue Sampling Volumes**; Luke T. Richardson¹; Amy N. W. Schnelle¹; Fabrizio Donnaruma²; Michael E. Pettit¹; Shubhneet Warar¹; Nicholas M. von Waaden¹; Kermit K. Murray²; Touradj Solouki¹; ¹Baylor University, Waco, TX; ²Louisiana State University, Baton Rouge, LA
- WP 519 **A Comparative Analysis of Two Sample Preparation Methods for the Multi-Omic Analysis of Proteins, Lipids, and Metabolites**; Melissa R Pergande^{1,2}; Sheher Banu Mohsin²; Limian Zhao³; Stephanie M Cologna¹; ¹University of Illinois at Chicago, Chicago, IL; ²Agilent Technologies, Wood Dale, IL; ³Agilent Technologies, Inc., Wilmington, DE
- WP 520 **A Robotic System for High Throughput Isolation of Phospholipids from Non-Polar Lipids**; Hui Gyu Park¹; Jeffery G. McDonald²; Bonnie M. Thompson²; Gonçalo Vale²; Tom Brenna¹; ¹University of Texas at Austin, Austin, TX; ²University of Texas Southwestern Medical School, Dallas, Texas
- WP 521 **Phospholipid Removal from Protein Precipitated Plasma Using In-Line Sample Preparation (ILSP)**; Sharon Lupo¹; Randy Romesberg¹; Xiaoning Lu¹; ¹Restek, Bellefonte, PA
- WP 522 **Study of Co-Extracted Matrix Impurities on Coated Solid Phase Microextraction Devices During Short Extractions Out of Plasma**; Olga I. Shimelis¹; Katherine K. Stenerson¹; Teresa Marsala¹; Emily R. Barrey¹; Hugh Cramer¹; Cory Muraco¹; ¹MilliporeSigma, Bellefonte, PA
- WP 523 **A Sensitive LC-MS/MS Method for Quantitation of Free and Liposomal Doxorubicin in Dog Plasma**; Sheng Wang¹; Jing Huang¹; Yifan Wang¹; Lele Yu¹; Xiaoying Jin¹; Dawei Zhou²; ¹Lab Testing Division of WuXi AppTec, Inc., Suzhou Site, Suzhou, China; ²WuXi AppTec, Cranbury, NJ
- WP 524 **LC-MS/MS Method for Determining Cannabidiol in Complex Matrices with a Dual Column-Switching Strategy**; Ze Li¹; Peng Wang¹; ¹WuXi AppTec, Plainsboro, NJ
- WP 525 **Determination of Tetramethylammonium Hydroxide in Serum by micro Solid Phase Extraction Coupled to Liquid Chromatography-Tandem Mass Spectrometry**; Chung-Yu Chen¹; Chia-Ying Lin¹; Cheng-Chieh Yen²; Maw-Rong Lee¹; ¹National Chung-Hsing University, Taichung, Taiwan; ²Chung Shan Medical University, Taichung, Taiwan
- WP 526 **Development and Implementation of Ultra-Trace Level Detection by LC/MS/MS for Quantitation of Thyroxine Isomers and Metabolites for in-vitro Toxicology Screening**; Jeremy McFadden¹; Mercedes Biven¹; David Robbins²; Jessica LaRocca¹; Audrey Lehman¹; Bethany Hannas¹; David Hills²; ¹Corteva Agriscience, Indianapolis, IN; ²Eurofins Lancaster Laboratories Professional Scientific Services, Lancaster, PA
- WP 527 **Automating the Analysis of Estrogens in Plasma using a Multi-Purpose Auto-Sampler Coupled to Liquid Chromatography Triple Quadrupole Mass Spectrometry**; Mary Blackburn; Thermo Fisher Scientific, San Jose, CA
- WP 528 **Evolution of Sample Preparation: Workflow Simplification Utilizing Sample Hold-Up Technology in Forensic and Clinical Analyses**; Rhys Jones¹; Adam Senior¹; Helen Lodder¹; Lee Williams¹; Geoff Davies¹; Katie-Jo Teehan¹; Alan Edgington¹; Steve Jordan¹; Claire Desbrow¹; Paul Roberts¹; ¹Biotage GB Limited, Cardiff, United Kingdom
- WP 529 **Determination of Optimal Sample Size with Microelution without Dry Down Using Solid Phase Extraction for a Drugs of Abuse Panel**; Jillian Neifeld¹; Jeremy Smith¹; Stephanie Marin¹; Mohamed Youssef¹; Elena Gairloch¹; ¹Biotage, Charlotte, NC
- WP 530 **A new device for direct QuEChERS salts extraction: Application to Drugs of Abuse in Blood, Urine and Oral Fluid**; Tiphaine Robin¹; Stephane Moreau²; Franck Saint-Marcoux¹; Etienne Maout^{3,3}; ¹CBRS, Limoges, France; ²Shimadzu Europa GmbH, Duisburg, Germany; ³shimadzu france, Paris, France

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- WP 518 **Simultaneous Extraction of Proteins, Lipids, and Metabolites for Integrated-omics Approaches for Low Tissue Sampling Volumes**; Luke T. Richardson¹; Amy N. W. Schnelle¹; Fabrizio Donnaruma²; Michael E. Pettit¹;



- WP 531 **UHPLC-MS/MS Analysis of Neonicotinoids and their Metabolites in Plant Tissues and Pollen by Modified QuEChERS**; Viet D Dang¹; Maura J Hall¹; Ed George²; David J. Borts¹; ¹Iowa State University, Ames, IA; ²ThermoFisher Scientific, San Jose, CA
- WP 532 **Determination of Pesticides in Edible Oils by GC-MS/MS**; Euan Ross¹; Jd De-Alwis¹; Simon Hird¹; Kenneth Rosnack²; ¹Waters, Wilmslow, United Kingdom; ²Waters Corporation, Milford, MA
- WP 533 **Determination of Pesticides in Dog Collars by On-line Supercritical Fluid Extraction – Supercritical Fluid Chromatography - Mass Spectrometry**; William Hedgepeth¹; Yuka Fujita²; ¹Shimadzu Scientific Instruments, Inc, Columbia, MD; ²Shimadzu Scientific Instruments, Inc., Columbia, Maryland
- WP 534 **Future Directions of Extractable and Leachable (E/L) Analysis from Automated Sample Preparation using online SPE and Online Solvent Mixing**; David A Weil¹; James Pyke²; Michael Woodman¹; Gosia Medrecki³; Melissa R Pergande⁴; ¹Agilent Technologies, Wood Dale, IL; ²Agilent Technologies, Santa Clara, CA; ³Agilent Technologies, Wood Dale, IL; ⁴University of Illinois at Chicago, Chicago, IL
- WP 535 **Overcoming Recovery Challenges in Hemolyzed Samples for the Determination of Propafenone and 5-Hydroxy Propafenone by LC-MS/MS**; Vinicio Vasquez¹; Milton Furtado¹; Mingluan Chen¹; Anahita Keyhani¹; ¹Altasciences, Laval, QC
- WP 536 **Development and Validation of LC-MS/MS Method for Determining Temozolomide in Mouse Brain Following Intra-Cerebral Microdialysis**; Raghavi Kakarla¹; Kimberly Yacoub¹; Baochuan Guo¹; ¹Cleveland State University, Cleveland, OH
- WP 537 **Mass Spectrometry Based Analysis of Permethylated N-Glycans Purified and Separated using Microgradient Device**; Pavel Rehulka¹; Martina Zahradnikova²; Lukas Uhrík²; Helena Rehulkova¹; Rudolf Nenutil²; Lenka Hernychova²; Milos V. Novotny³; ¹Faculty of Military Health Sci., Univ. of Defence, Hradec Kralove, Czech Republic; ²Regional Centre for Applied Molecular Oncology, Masaryk Memorial Cancer Institute, Brno, Czech Republic; ³Department of Chemistry, Indiana University, Bloomington, IN
- WP 538 **Automating Metabolic Stability Assays and Analyses using a Robotic Autosampler and LC/MS/MS Platform**; Fred D. Foster¹; John R. Stuff¹; Laurel A. Verarelli¹; Jacqueline A. Whitecavage¹; ¹Gerstel, Inc., Linthicum, MD
- WP 539 **Comparison of SPE Protocols for Phospholipid Removal in Basic Analyte Bioanalytical Quantitation**; Melvin Blaze Muttikal Thomas¹; Thomas H Walter¹; Kenneth Berthelette¹; Bonnie A Alden¹; Donna Osterman¹; Kevin Wyndham¹; ¹Waters Corporation, Milford, MA
- WP 540 **Cleanup of Pharmaceutical Drugs in Biological Fluids by Automated microSPE Prior to LC/MS**; Raquel Gonzalez de Vega¹; Simin Maleknia¹; Matthew Diplock¹; Andrew Minett²; Philip Doble¹; ¹University of Technology Sydney, Sydney, Australia; ²Eprep Pty Ltd, Mulgrave, Australia
- WP 541 **Blowing Analytical Precision and Accuracy out of the Water – microSPE of Explosives**; Matthew Diplock¹; Raquel Gonzalez de Vega¹; Philip Doble¹; Andrew Minett²; ¹University of Technology Sydney, Sydney, Australia; ²Eprep Pty Ltd, Mulgrave, Australia
- WP 542 **Fully Automated Determination of Phosphatidylethanol 16:0/18:1 and 16:0/18:2 in Dried Blood Spots**; Marc Joel Luginbuehl¹; Stefan Gaugler²; Wolfgang Weinmann¹; ¹Institute of Forensic Medicine Bern, Bern, Switzerland; ²CAMAG, Muttenz, Switzerland
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- WP 543 **Mechanism of Prostaglandin E2 Accumulation in Amniotic Fluid during Human Labor**; Toshiaki Okuno¹; Nanase Takahashi¹; Takehiko Yokomizo¹; ¹Department of Biochemistry, Juntendo University School of Medicine, Tokyo, Japan
- WP 544 **Screening New Reagents for the Paternò-Büchi Reactions for Lipid Analysis by Mass Spectrometry**; Jing Zhao¹; Xiaobo Xie¹; Yu Xia¹; ¹Tsinghua University, Beijing, China
- WP 545 **Investigating Enzymatic Lipase Activity via Contained-Electrospray Ionization (ESI) Mass Spectrometry as a Function of Secondary Organic Aerosol (SOA) Evolution**; Mickey M. Rogers¹; Benjamin J. Burris¹; Abraham K. Badu-Tawiah¹; ¹The Ohio State University, Columbus, OH
- WP 546 **Top-Down Shotgun Lipidomics Analysis with Ultra-High Resolution Orbitrap Mass Spectrometry**; Kai Schuhmann¹; Konstantin Nagornov²; Anton Kozhinov²; Yury Tsybin²; Andrej Shevchenko¹; ¹MPI-CBG, Dresden, Germany; ²Spectroswiss Sàrl, Lausanne, Switzerland
- WP 547 **Quantitative Analysis of Trans-Fatty Acids in Humans**; Heather C Kuiper¹; Na Wei¹; Emily J Mueller¹; Sarah W Kingsley¹; Hubert W Vesper¹; ¹CDC, Atlanta, GA
- WP 548 **Analysis of Oxidized Cardiolipins by Solid Phase Extraction and LC/MS**; Gaoyuan Liu¹; Richard W Gross²; ¹Washington University in Saint Louis, Saint Louis, MO; ²Washington University School of Medicine, St. Louis, MO
- WP 549 **Acute-phase Serum Lipidome Alterations in a Rodent Model of Closed Head Traumatic Brain Injury**; Scott Hogan¹; Kyle Milligan²; Michelle LaPlaca²; Facundo M Fernandez¹; ¹Georgia Institute of Technology, School of Chemistry and Biochemistry, Atlanta, Georgia; ²Georgia Institute of Technology, Department of Biomedical Engineering, Atlanta, Georgia
- WP 550 **Comparative Analysis of Nutritional Lipids from Marine Sources by Supercritical Fluid Chromatography with Tandem Mass Spectrometry**; Greg Winter¹; Paolo Lecchi¹; Craig Mallon¹; Dominik Burger¹; ¹DSM, Columbia, MD
- WP 551 **Serum Lipidomics of Pregnant African American Women Exposed to Environmental Toxicants**; Anna A Ivanova¹; Kristal Maner-Smith¹; Dana Boyd Barr¹; Anne L Dunlop¹; Eric A Ortlund¹; ¹Emory University, Atlanta, GA
- WP 552 **Analysis of Very Long Chain Fatty Acids by Supercritical Fluid Chromatography-Mass Spectrometry**; Paolo Lecchi¹; Gregory Winter¹; Dominik Burger¹; Srujana Beeram¹; ¹DSM Nutritional Products, Columbia, MD
- WP 553 **Triglyceride Precursor Pool Enrichment and de novo Lipogenesis in Plasma Lipoproteins Probed by Stable-Isotope GC/MS-MIDA Methodology Using Multiple Tracer-Administration Protocols**; Sergiu P. Paliu¹; Grace M. Jones¹; Mariel Dologmandin¹; Zachary Woodward¹; David Doud¹; Jean-Marc Schwarz^{1,2}; ¹Touro University California, Vallejo, CA; ²University of California, San Francisco (UCSF), San Francisco, CA
- WP 554 **Discovery of Novel LPA-Binding Proteins Using a Chemical Proteomic Method**; Xuejiao Dong¹; Yinsheng Wang¹; ¹UC Riverside, Riverside
- WP 555 **Effect of Matrix Type and Storage Conditions on Lipid Profiles of Clinical Blood Samples**; Rahul Deshpande¹; Kaitlyn Scola¹; Tim Wood¹; ¹Greenwood Genetic Center, Greenwood, SC
- WP 556 **Lipid profiling of Chromochloris zofingiensis in Photoautotrophic and Heterotrophic Cultures**; Yuntao Hu^{1,2}; Melissa S Roth²; Katherine Louie^{1,3}; Benjamin Bowen^{1,3}; Krishna Niyogi²; Trent Northen^{1,3}; ¹Lawrence Berkeley Laboratory, Berkeley, CA; ²University of California, Berkeley, Berkeley, CA; ³Joint Genome Institute, Walnut Creek, CA



- WP 557 **Lipidomic Analyses of Wild Type, Knock-Out, S508D-, and S508A-CEACAM1 Hepatocarcinoma Cells;** Gabriel B Gugiu^{1,2,3}; Jennifer Chean^{1,2}; Chang Chen^{1,2}; John E Shively^{1,2}; ¹City of Hope, Duarte, CA; ²Beckman Research Institute, Department of Molecular Imaging and Therapy, Duarte, CA; ³Beckman Research Institute, Department of Shared Resources, Mass Spectrometry and Proteomics Core Facility, Duarte, CA
- WP 558 **High Speed Untargeted Lipidomics and Metabolomics LC-MS/MS workflows with Parallel Accumulation Serial Fragmentation (PASEF);** Ulrike Schweiger-Hufnagel¹; Aiko Barsch¹; Sven W. Meyer¹; ¹Bruker Daltonics, Bremen, Germany
- WP 559 **The Regulation of the Molecular Structural Diversity of Mitochondrial Cardiolipins in Mouse Tissues;** Gregor Oemer¹; Jakob Koch²; Mohammed Tauqeer Alam³; Marie-Luise Edenhofer²; Sabrina Sailer⁴; Carolina Doerrier⁵; Ernst R Werner⁴; Katrin Watschinger⁴; Erich Gnaiger⁶; Johannes Zschocke²; Markus A Keller²; ¹Division of Human Genetics, Medical University of Innsbruck, Innsbruck, Austria; ²Division of Human Genetics, Medical University of Innsbruck, Innsbruck, Austria; ³Division of Biomedical Sciences, Warwick Medical School, University of Warwick, Warwick, United Kingdom; ⁴Division of Biological Chemistry, Biocenter, Medical University of Innsbruck, Innsbruck, Austria; ⁵Oroboros Instruments Corporation, Innsbruck, Austria
- WP 560 **Fatty Liver is More than Neutral Lipid Accumulation: An Analysis of Human Non-Alcoholic Fatty Liver by Shotgun Lipidomics;** Olga Vvedenskaya¹; Oskar Knittelfelder¹; Eduardo Jacobo Miranda Ackerman¹; Josch Pauling²; Judith Wodke³; Jochen Hampe⁴; Andrej Shevchenko⁵; ¹Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany; ²Technische Universität München, Freising, Germany; ³Humboldt University, Berlin, Germany; ⁴Dresden University Clinic, Dresden, Germany; ⁵Max Plank Institute for Molecular Cell Biology and Genetics, Dresden, Germany
- WP 561 **Mass Spectrometric Study on the Source of Error in Quantification of Free Fatty Acids;** Hyejin Park¹; Tae-Young Kim¹; ¹School of Earth Sciences and Environmental Engineering, Gwangju Institute of Science and Technology, Gwangju, South Korea
- WP 562 **Trapped Ion Mobility Spectrometry (TIMS) and Parallel Accumulation Serial Fragmentation (PASEF) for Nanoflow LC-MS/MS-Based Lipidomics;** Catherine G. Vasilopoulou¹; Karolina Sulek²; Andreas-David Brunner¹; Sven W. Meyer³; Ulrike Schweiger-Hufnagel³; Ningombam Sanjib Meitei⁴; Matthias Mann^{1,2}; Florian Meier¹; ¹Max Planck Institute of Biochemistry, Martinsried, Germany; ²NNF Center for Protein Research University of Copenhagen, Copenhagen, Denmark; ³Bruker Daltonik GmbH, Bremen, Germany; ⁴PREMIER Biosoft, Palo Alto, CA
- WP 563 **Lipidomics of Dolphin Serum to Assess Physiological and Ecological Changes Following the Deepwater Horizon Oil Spill;** Michael P. Napolitano^{1,2}; Maggie Broadwater¹; Tracey B. Schock^{2,3}; Ryan Takeshita⁴; Terri K. Rowles⁵; Lori H. Schwacke⁶; ¹National Oceanic and Atmospheric Administration, Charleston, SC; ²Hollings Marine Laboratory, Charleston, SC; ³National Institute of Standards and Technology, Charleston, SC; ⁴National Marine Mammal Foundation, Boulder, CO; ⁵National Oceanic and Atmospheric Administration, Silver Spring, MD; ⁶National Marine Mammal Foundation, Charleston, SC
- WP 564 **Sample Preparation Effects on Retinal Lipid Analysis by MALDI Imaging and LC-MS Technologies;** Ankita Kotnala; Vanderbilt University, Nashville, TN
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- WP 565 **MxP® Quant 500 Kit – Novel Standardized Metabolomics/Lipidomics Analysis Tool for Comprehensive Targeted Profiling;** Hai Pham Tuan¹; Ulf Sommer¹; Svenja Heischmann¹; Doreen Kirchberg¹; Xenia Iwanowa¹; Radu Talmazan¹; Barbara Wolf¹; Martin Buratti¹; Rosa Argamasilla Martinez¹; Cornelia Röhring¹; Therese Koal¹; ¹BIOCRATES Life Sciences AG, Innsbruck, Austria
- WP 566 **New Features and Functions of the Old “Mustard Oil Bomb” in Single Cell-Types;** Shweta Chhajed¹; Craig Dufresne²; Nathalia Tello^{1,3}; Alice Harmon^{1,4,5}; Sixue Chen^{1,4,5,6}; ¹Department of Biology, University of Florida, Gainesville, FL; ²Thermo Fisher Scientific, West Palm Beach, FL; ³SF2UF Bridge Program, University of Florida, Gainesville, FL; ⁴Plant Molecular and Cellular Biology, University of Florida, Gainesville, FL; ⁵Genetics Institute, University of Florida, Gainesville, FL; ⁶Interdisciplinary Center for Biotechnology Research, University of Florida, Gainesville, FL
- WP 567 **Effects of Acute Ambient PM2.5 Exposure on Heart in C57BL/6J Diet-Induced Obesity Mouse Model;** Yuanjuan Song¹; Yanhao Zhang¹; Zenghua Qi²; Ruijin Li³; Zongwei Cai¹; ¹Hong Kong Baptist University, Hong Kong, China; ²Guangdong University of Technology, Guangzhou, China; ³Shanxi University, Taiyuan, China
- WP 568 **Meta-Analysis of Targeted Metabolomics Data from Heterogeneous Biological Samples Provides Insights into Metabolite Dynamics;** Ho-Joon Lee¹; Daniel Kremer¹; Peter Sajjakulnukit¹; Li Zhang¹; Costas Lyssiotis¹; ¹University of Michigan Medical School, Ann Arbor, MI
- WP 569 **Targeted Multi-OMICS: Rapid Plasma Profiling of a Bladder and Lung Cancer Human Cohort;** Sarah Lennon¹; Billy J Molloy¹; Lee A Gethings¹; Robert S Plumb²; Andrew Peck²; ¹Waters corporation, Wilmslow, United Kingdom; ²Waters Corporation, Milford, MA
- WP 570 **An Improved Isotope-Labeling Chemical Derivatization – LC/MRM-MS Method for Reliable Quantitation of >70 FAs in Human Serum;** Jun Han^{1,2}; Kieran Atkinson¹; Evan Dyson-Loewen¹; Mia Frier¹; Juncong Yang¹; John Ducas³; Robin Ducas³; Erin Weldon⁴; Tom Jelic⁴; R. Antony Shaw⁵; Christoph H. Borchers^{1,6,7,8}; ¹University of Victoria-Genome BC Proteomics Centre, Victoria, BC; ²Division of Medical Sciences, University of Victoria, Victoria, BC; ³Faculty of Medicine, Department of Cardiology, University of Manitoba, Winnipeg, Manitoba; ⁴Faculty of Medicine, Department of Emergency Medicine, University of Manitoba, Winnipeg, Manitoba; ⁵National Research Council of Canada, Winnipeg, Manitoba; ⁶Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC; ⁷Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; ⁸Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC
- WP 571 **Quantification of Polar Metabolites in Urine using an Automated Parallel Derivatization Strategy and LC-SWATH-MS;** Guenter Boehm¹; Maria Fernanda Cifuentes Girard²; David Ruscio³; Renzo Picononi¹; Gerard Hopfgartner³; ¹CTC Analytics AG, Zwingen, Switzerland; ²Life Sciences Mass Spectrometry, Department of analytical and Inorganic Chemistry, University of Geneva, Geneva, Switzerland; ³Life Sciences Mass Spectrometry, Department of analytical and Inorganic Chemistry, University of Geneva, Geneva, Switzerland
- WP 572 **Isotope-Labeled Metabolic Flux Analysis of the Gut Microbiota-Driven Carnitine Metabolism;** Hsin-bai Zou¹; Fang-Wei Kuo²; Qiang Lyu³; Hsin-Yuan Chang³; Cheng-Chih Hsu³; Wei-Kai Wu⁴; ¹Department of Chemistry, National Taiwan University, Taipei, Taiwan; ²Institute of



- food science and technology, taipei, Taiwan; ³Department of Chemistry, National Taiwan University, Taipei, Taiwan; ⁴Department of Internal Medicine, National Taiwan University Hospital Bei-Hu Branch, Taipei, Taiwan, taipei, Taiwan
- WP 573 **Multiplexed High Throughput LC-MS/MS Method for Targeted Metabolites and Neurotransmitters from Central Nervous System;** Juho Heininen¹; Tapio Kotiaho¹; Anu Vaikkinen¹; Risto Kostianen¹; ¹University of Helsinki, Helsinki, Finland
- WP 574 **Derivatisation of Central Metabolites in SUIT-2 Cells Using 2-bromo-1-(4-dimethylamino-phenyl)-ethanone Enables LC-MS/MS Energy-State Analysis;** Cornelius C W Willacey¹; Martijn Naaktgeboren¹; Edinson Lucumi Moreno¹; Alida S D Kindt¹; Daan van der Es²; Ronan M T Fleming¹; Amy C Harms¹; Thomas Hankemeier¹; ¹Analytical BioSciences and Metabolomics, Systems Biomedicine and Pharmacology, Leiden Academic Centre for Drug Research, Leiden University, Leiden, Netherlands; ²Medicinal Chemistry, Drug Discovery and Safety, Leiden Academic Centre for Drug Research, Leiden University, Leiden, The Netherlands, Leiden, Netherlands
- WP 575 **Assessment of the Microbiota Metabolome and Its Role in Cardiovascular Diseases;** Tuan Hai Pham¹; Ulf Sommer¹; Svenja Heischmann¹; Barbara Wolf¹; Fadi Abdi¹; Therese Koal¹; ¹BIOCRATES Life Sciences AG, Innsbruck, Austria
- WP 576 **Quantitative Comparison of the Suppression between HILIC and Reverse Phase Chromatography;** Lucas Veillon¹; John N Weinstein¹; Phil Lorenzi¹; Felice A de Jong²; Chris Beecher²; ¹MD Anderson Cancer Center, Houston, TX; ²IROA Technologies LLC, Bolton, MA
- WP 577 **5-plex iDileu Enabled Neurotransmitter Absolute Quantitation in the Crustacean Nervous System;** Qinjingwen Cao¹; Gongyu Li¹; Amanda R. Buchberger¹; Lingjun Li¹; ¹University of Wisconsin-Madison, Madison, WI
- WP 578 **Rapid Automated Absolute Quantification of Metabolites Using Polly QuantFit to Understand Tumor Nutrient Availability;** Abhishek Jha¹; Avijit Zutishi²; Raghav Sehgal²; Shubham Agarwal²; Taranjot Singh²; Shefali Lathwal²; Swetabh Pathak²; Alex Muir³; Caroline Lewis⁴; Mark Sullivan³; Matthew G. Vander Heiden³; ¹Elucidata, Cambridge, MA; ²Elucidata, Delhi, India; ³Massachusetts Institute of Technology, Cambridge, MA; ⁴Whitehead Institute, Cambridge, MA
- WP 579 **Simultaneous Analysis of Steroids and Lipids in Serum Employing Liquid Chromatography-Ion Mobility Spectrometry-Mass Spectrometry Analysis;** Alana Rister¹; Katie L Bidne¹; Jennifer R Wood¹; Eric D. Dodds¹; ¹University of Nebraska - Lincoln, Lincoln, NE
- WP 580 **Direct Quantification of Polyamines in Arabidopsis thaliana seedlings by LC-MS/MS;** Masoud Zabet Moghaddam¹; parvin mirzaei²; mohamed Fokar²; Yehia Mechref³; ¹Texas Tech University, Box 43132 Lubbock, TX; ²Texas Tech University, Lubbock, TX; ³Texas Tech University, Lubbock
- WP 581 **Innovative One-Step Protocol for Producing Deuterium-Labeled Metabolites and Their Use for Quantitative LC-HRMS-Based Targeted Metabolomics;** Annelaure Damont¹; Yu Min Kiw¹; Kathleen Rousseau¹; Sophie Feuillastre²; Grégory Pieters²; Christophe Junot³; François Fenaille¹; ¹Service de Pharmacologie et Immunoanalyse (SPI), Laboratoire d'Etude du Métabolisme des Médicaments (LEMM), CEA, INRA, Université Paris-Saclay, MetaboHUB-IDF, Gif-Sur-Yvette, France; ²Service de Chimie Bio-organique et de Marquage, Laboratoire de Marquage au Tritium, Département Médicaments et Technologies pour la Santé, Institut Joliot, CEA, Université Paris-Saclay, Gif-Sur-Yvette, France; ³Service de Pharmacologie et Immunoanalyse (SPI), Département Médicaments et Technologies pour la Santé, Institut Joliot, CEA, INRA, Université Paris-Saclay, MetaboHUB-IDF, Gif-Sur-Yvette, France
- WP 582 **Reovirus-Induced Alterations in the Metabolome of M1 and M2 Macrophages;** Michael Giacomantonio¹; Patrick J Murphy¹; Barry Kennedy¹; Shashi Gujar^{1,2}; ¹Department of Pathology, Dalhousie University, Halifax, NS, Canada, Halifax, NS; ²Department of Microbiology and Immunology, Dalhousie University, Halifax, NS, Canada, Halifax, NS, Canada, Halifax, NS
- WP 583 **Profiling of Bile Acids, Histidine, and Histamine in Gastric Juice by LC-MS/MS Combined with Serial Derivatization: Diagnosis of Gastric Cancer;** Wonwoong Lee¹; Jinhee Um¹; Keon-hee Ko¹; Bong Chul Chung²; Jongki Hong¹; ¹Kyung Hee University, Seoul, South Korea; ²Korea Institute of Science and Technology, Seoul, South Korea
- WP 584 **Rapid LC-MS/MS Method for Targeted Quantitation of Human Performance Metabolites in Saliva;** Ethan M McBride¹; Richard J Lawrence¹; Kirstin McGee¹; Phillip M Mach¹; Paul S Demond²; Michael W Busch²; John W Ramsay³; Erika K Hussey³; Trevor Glaros¹; Elizabeth S Dhummakupt¹; ¹Research and Technology Directorate, Research Development & Engineering Command (RDECOM) Edgewood Chemical Biological Center (ECBC), Aberdeen Proving Ground, MD; ²Excet, Inc., Springfield, VA; ³U.S. Army Natick Soldier Research, Development & Engineering Center, Natick, MA
- WP 585 **Spatial Distribution of Ractopamine Residues in Bovine muscle;** Valerie Lindstrom¹; Haley E Davis¹; Jacqueline M Chaparro¹; Keith E Belk¹; Jessica E. Prenni¹; ¹Colorado State University, Fort Collins, CO
- WP 586 **Improving the Accuracy of Endogenous tZ-Type Cytokinins Determination by Elucidation of the Fragmentation Mechanism;** Peiyong Xin¹; Jinfang Chu¹; ¹National Center for Plant Gene Research (Beijing), Institute of Genetics and Developmental Biology, Chinese Academy of Sciences, Beijing, China
- WP 587 **Measurement of Metabolites in Feces of Japanese Rock Ptarmigans by LC-MS/MS;** Takanari Hattori¹; Yukari Oka¹; Shuichi Kawana¹; Koretsugu Ogata¹; Sayaka Tsuchida^{2,3}; Atsushi Kobayashi⁴; Yoshiaki Nakamura⁵; Hiroshi Nakamura⁶; ¹Shimadzu Corporation, Kyoto, Japan; ²Kyoto Prefectural University, Kyoto, Japan; ³Chubu University, Kasugai, Japan; ⁴Toho University, Tokyo, Japan; ⁵Hiroshima University, Hiroshima, Japan; ⁶Nakamura Hiroshi International Institute for Ornithology, Nagano, Japan
- WP 588 **Rapid Throughput Quantitation of Carboxylic Acid Metabolites Using UHPLC/QqQ-MS to Monitor Diet and the Microbiome;** Diane Tu¹; Carol Stroble¹; Matthew J. Amicucci¹; Gege Xu¹; Jennifer T Smilowitz¹; Carlito B Lebrilla¹; ¹University of California, Davis, Davis, CA
- WP 589 **A Critical Look at Highly Multiplexed Targeted Metabolomics: Data Quality Effects from Large Target Lists;** Robert Pepin¹; Mathew Ellenberger¹; Daniel Rafferty^{1,2}; ¹University of Washington, Seattle, WA; ²Fred Hutchinson Cancer Research Center, Seattle, WA
- WP 590 **Simultaneous Detection of Tricarboxylic Acid Cycle Intermediates using LC-MS/MS with a Synergi® Fusion-RP HPLC Column;** Xianrong (Jenny) Wei¹; Ryan Splitstone¹; Sean Orłowicz¹; ¹Phenomenex, Torrance, CA
- WP 591 **Comparative Metabolomics of Staphylococcus aureus by HPLC-DAD-MS/MS;** Gerson D. López¹; Chad Leidy¹; Chiara Carazzone¹; ¹Universidad de los Andes, Bogotá D.C, Colombia
- WP 592 **Development of a UPLC-MS/MS Method to Quantitate Process-Induced Nitrogen Compounds and their Metabolites in Urine Samples;** Yi-Chen Sun¹; Hsin-Chang Chen¹; ¹Institute of Food Safety and Health, National Taiwan University, Taipei, Taiwan



- WP 593 **Analysis of Endogenous Steroid Hormones in Urine Using High-Resolution LC-MS; Lancia N.F. Darville-bowleg¹; Min Liu¹; Jayden Cline¹; Yessica C. Martinez-Monta¹; Shannan Rich²; John Koomen¹; Lusine Yaghjian²; Kathleen M Egan¹; ¹Moffitt Cancer Center, Tampa, FL; ²University of Florida, Gainesville, FL**
- WP 594 **Gut Microbial and Hepatic Metabolism of the Hop Flavonoid, Xanthohumol, in Humans; Wenbin Wu¹; Ines L Paraiso¹; Ralph Reed¹; Jeffrey Morr  ²; Jan F. Stevens¹; ¹Department of Pharmaceutical Sciences, Linus Pauling Institute, Oregon State University, Corvallis, Oregon; ²Department of Chemistry, Oregon State University, Corvallis, Oregon**
- WP 595 **Fit-for-Purpose Quantitative LC-MS and CE-MS Metabolomics Methods to Inform Alzheimer's Research; Kendra J. Adams¹; J. Will Thompson¹; W. Kirby Gottschalk¹; Joan G. Wilson¹; M. Arthur Moseley¹; Carol A. Colton¹; ¹Duke University School of Medicine, Durham, NC**
- WP 596 **A Novel and Comprehensive Steroid Assay Including Thyroxin Compounds Using Small Volume Human Serum or Plasma Samples; Gregory Byram¹; Chris Vanselow²; Patrick Fitzgerald¹; Catherine Paige Riley³; Stacy Tremintin²; Oliver Fiehn¹; ¹UC Davis West Coast Metabolomics Center, Davis, CA; ²Thermo Fisher Scientific, San Jose, CA; ³Thermo Fisher Scientific, West Palm Beach, FL**
- WP 597 **Probing the Altered Microbiome of ASD for Metabolic Clues; Emily R. Sekera¹; Troy D. Wood¹; Heather L. Rudolph¹; ¹University at Buffalo, Buffalo, NY**
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- WP 598 **Untargeted Metabolomics Profiling of Longitudinal Urine Samples Collected from Individual Participant of Integrated Personalized Omics Profiling (iPOP) Project; Songjie Chen¹; Liang Liang¹; Yuqin Dai²; Michael Snyder¹; ¹Stanford University, Stanford, CA; ²Agilent, Santa Clara, CA**
- WP 599 **Using Mass Spectrometry-Based Metabolomics to Explore Polyphenol Profile Diversity among Different Lentil Seed Coat Colors and Patterns; Fatma M. Ellessawy¹; Derek Wright¹; Albert Vandenberg¹; Anas El-Aneed¹; Randall W. Purves^{1,2}; ¹University of Saskatchewan, Saskatoon, SK; ²Canadian Food Inspection Agency, Saskatoon, SK**
- WP 600 **Correcting Metabolomic Data for Source Variances Using IROA; Fei Tang¹; Felice de Jong²; Chris Beecher²; Markos Leggas¹; ¹University of Kentucky, Lexington, KY; ²IROA Technologies LLC, Bolton, MA**
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- WP 602 **A Metabolomics Study into during Infection with Influenza Virus by HRAM Q-TOF Analysis; Emily Armitage¹; Jonathan Swann²; Mick Bailey³; Ian D Wilson²; Neil J Loftus¹; ¹Shimadzu MS/BU, Manchester, United Kingdom; ²Imperial College London, Department of Surgery and Cancer, United Kingdom; ³School of Veterinary Sciences, University of Bristol, Bristol, United Kingdom**
- WP 603 **Using IROA-Based Internal Standard Normalization to Minimize Non-IROA Metabolite Variation; Chris Beecher¹; Felice de Jong²; ¹IROA Technologies, Chapel Hill, NC; ²IROA Technologies LLC, Bolton, MA**
- WP 604 **Regaining the ASHES: Finding Chemical 'Clues' to Mitigate the Impact OF Ash Dieback; John D Sidda¹; Christine M Sambles²; Lijiang Song¹; Murray R Grant¹; ¹University of Warwick, Coventry, United Kingdom; ²University of Exeter, Exeter, United Kingdom**
- WP 605 **Proteometabolomics of Bortezomib Resistance in Multiple Myeloma; David C. Koomen¹; Joy D. Guingab-Cagmat²; Paula S. Oliveira¹; Bin Fang¹; Min Liu¹; Eric A. Welsh¹; Mark B. Meads¹; Tuan Nguyen¹; Laurel E. Meke²; Steven A. Eschrich¹; Timothy J. Garrett²; John M. Koomen¹; Kenneth H. Shain¹; ¹H. Lee Moffitt Cancer Center, Tampa, FL; ²University of Florida, Gainesville, FL**
- WP 606 **Untargeted Metabolomics of Bumble Bee Cold Tolerance Using Stacked Injection of Biphasic Extraction with LC-MS/MS; Mitchell Helling¹; Kennan J. Oyen¹; Michael E. Dillon¹; Franco Basile¹; ¹University of Wyoming, Laramie, WY**
- WP 607 **Methanol Quenching Versus Flash Freezing for Metabolomics Profiling of Wheat Leaves; Marie J. Andales¹; Linxing Yao²; Corey D. Broeckling¹; Kaitlyn Maloley¹; ¹Proteomics & Metabolomics Facility, Colorado State University, Fort Collins, CO; ²Proteomics and Metabolomics Facility of Colorado State University, Fort Collins, CO**
- WP 608 **A Metabolomic SWATH-MS Approach Applied to PBMCs from First Psychotic Episode Patients; Margarida Coelho¹; Vera M Mendes¹; C  tia Santa¹; Manuel Coroa²; Sofia Moraes²; In  s Baldeiras²; Nuno Madeira²; Antonio Macedo²; Bruno Manadas¹; ¹Center for Neuroscience and Cell Biology, Cantanhede, Portugal; ²Psychiatry department, CHUC, Coimbra, Portugal**
- WP 609 **Development and Application of a Novel Metabolomics Platform Based on Capillary Electrophoresis Coupled with a High-Resolution Mass Spectrometry; Kazunori Sasaki¹; Hitoshi Sagawa¹; Makoto Suzuki¹; Kaori Abe¹; Satoshi Ito²; Tsutomu Negama²; Moon-Il Kang¹; Kenjiro Kami¹; ¹Human Metabolome Technologies, Tsuruoka, Japan; ²Sekisui Medical Company, Chuo-ku, Japan**
- WP 610 **Comparison of Data-Dependent Acquisition Methods on an Orbitrap ID-X; Kevin Y Cho¹; Fuad J Naser¹; Michaela Schwaiger-Haber¹; Miriam Sindelar¹; Gary J Patti¹; ¹Washington University in St. Louis, St. Louis, MO**
- WP 611 **A Systematic Approach to Development of Analytical Scale and Microflow-based LC-MS Metabolomics Methods to Support Drug Discovery and Development; Sarah Geller¹; Harvey Lieberman¹; Alla Kloss¹; Alexander R Ivanov²; ¹Sanofi, Waltham, MA; ²Department of Chemistry and Chemical Biology, Northeastern University, Boston, MA**
- WP 612 **Metabolomics Analysis of Respirofermentative Phenotypes in a Crabtree-Positive and -Negative Yeast; April Miguez¹; Mark Styczynski¹; ¹Georgia Institute of Technology, Atlanta, GA**
- WP 613 **Separation and Analysis of Low Molecular Weight Organic Acid Metabolites by Mixed-Mode Chromatography Coupled to Mass Spectrometry; Kerri Smith¹; Paul D Rainville¹; ¹Waters Corporation, Milford, MA**



- WP 614 **Quantitative Metabolomics, Histology and Clinical Pathology Using the Exact Same Tissue Sample: Two-for-One Analyses for Biomarker Discovery;** Dorothea Y. Mung¹; Stephen L. Carrithers²; Richard T. Coughlin²; Dean A. Troyer³; Liang Li⁴; ¹Nova Medical Testing Inc., Edmonton, AB; ²Lagrange Scientific LLC, Pewee Valley, KY; ³Eastern Virginia Medical School, Norfolk, VA; ⁴University of Alberta, Edmonton, AB
- WP 615 **MDM2 Copy Number Aberrations Alter Ceramide Glycosylation in Liposarcoma Tumors, Impacting Drug Response;** Andrew Patt¹; Bryce Demoret¹; Andrew Patterson²; Philip Smith²; Ewy Mathe¹; James Chen¹; ¹The Ohio State University, Columbus, OH; ²Pennsylvania State University, State College, PA
- WP 616 **Analysis of Volatile Organic Profiles in Stem Cells by Comprehensive Two-Dimensional Gas Chromatography with Time-of-Flight Mass Spectrometry;** Christopher A. Heist¹; Jean-marie D. Dimandja²; Milad Navaei¹; ¹Georgia Tech Research Institute, Atlanta, GA; ²Georgia Institute of Technology, Department of Mechanical Engineering, Atlanta, GA
- WP 617 **Stable Isotope Label-Supported IM-QRAI Methods for Metabolomics;** Max Feuerstein¹; Ruwan T. Kurulugama²; John C. Fjeldsted²; Tim Causon¹; Stephan Hann¹; ¹Institute of Analytical Chemistry, Department of Chemistry, University of Natural Resources and Life Sciences (BOKU), Vienna, Austria; ²Agilent Technologies, Inc., Santa Clara, CA
- WP 618 **Integrating 4D Peak Picking of LC-TIMS-MS/MS Data into GNPS Feature Based Molecular Networking for Metabolomics and Lipidomics Analysis;** Florian Zubeil¹; Nikolas Kessler¹; Heiko Neuweger¹; Sven W. Meyer¹; Ulrike Schweiger-Hufnagel¹; Aiko Barsch¹; ¹Bruker Daltonik GmbH, Bremen, Germany
- WP 619 **Robust and Sensitive Untargeted Microflow Metabolomics with OptiFlow™ Turbo V Source;** Khatereh Motamedchaboki¹; Carmal Carmal²; Lekha Sleno³; Vivaldy Prinville³; ¹Sciex, Redwood City, CA; ²SCIEX, Concord, ON; ³Universite du Quebec a Montreal, Montreal, Québec
- WP 620 **Development of 4-Channel Chemical Isotope Labeling LC-MS for Comprehensive Profiling of the Human Tear Metabolome;** Kevin Hooton¹; Gavin SW Tan^{2,3,4,5}; Lei Zhou^{2,4,5}; Liang Li⁶; ¹Nova Medical Testing Inc., Edmonton, AB; ²Singapore Eye Research Institute, Singapore, Singapore; ³Singapore National Eye Center, Singapore, Singapore; ⁴Duke-NUS Medical School, Singapore, Singapore; ⁵National University of Singapore, Singapore, Singapore; ⁶University of Alberta, Edmonton, AB
- WP 621 **HILIC-HR-MS for (untargeted) Metabolomics in Microorganisms – the Optimal Method for Polar Compounds in an Industrial Setting?;** Leon Coulier¹; Wouter Coppes¹; Raymond Ramaker¹; Sandra Pous-Torres¹; ¹DSM Biotechnology Center, Delft, Netherlands
- WP 622 **Nutrient Addition Effect on Four Setaria Accessions in Marginal Soil: Deciphering Plant-Ectorrhizosphere's Relationships under Nutrient Limitation;** Matthew J. Peterson¹; Pubudu P. Handakumbura¹; Zachary R. Russell¹; Christer Jansson¹; Young-Mo Kim¹; Sarah J. Fansler¹; Montana L. Smith¹; Jason G. Toyoda¹; Rosalie K. Chu¹; Bryan A. Stanfill¹; Steven C. Fransen²; Kim K. Hixson¹; Stephen J. Callister¹; ¹Pacific Northwest National Laboratory, Richland, WA; ²Washington State University Irrigation Agriculture Research and Extension Center, Prosser, WA
- WP 623 **Unifying Ionization Efficiencies: Quantitative Comparison of Diverse Data Sets and Validation of Prediction Models;** Piiia Liigand¹; Jaanus Liigand¹; Karl Kaupmees¹; Anneli Kruve¹; ¹University of Tartu, Institute of Chemistry, Tartu, Estonia
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- WP 624 **Investigation of the Formation and Structure Characteristics of miR-92a G-quadruplex by ESI-MS;** Min Xi^{1,2}; Jiang Zhou¹; Yizhou Li²; ¹College of Chemistry and Molecular Engineering, Peking University, Beijing, China; ²School of Pharmaceutical Sciences, Chongqing University, Shapingba, China
- WP 625 **Nucleotide Composition Analysis of Unknown Synthetic Oligo Products;** Roger G Moore¹; Denise A Keen¹; Piotr Swiderski¹; Marcin Kortylewski¹; Markus Kalkum¹; ¹City of Hope, Duarte, CA
- WP 626 **Compliant-Ready Workflow for Mass Confirmation Of Oligonucleotide and Related Impurities;** Andrew Tudor¹; Maria Basanta-sanchez²; Alessio Zammataro³; Barry Dyson³; Laetitia Denbigh³; ¹waters, Wilmslow, United Kingdom; ²Waters Corporation, Pleasanton, CA; ³Waters Corporation, Wilmslow, United Kingdom
- WP 627 **Binding of Phenanthroline-Neomycin Conjugates with Different G-Quadruplex DNA Investigated by ESI Mass Spectrometry and Isothermal Titration Calorimetry;** Mandeep Singh¹; Vanessa Marie Range¹; Ryan Hekman¹; Craig Vierra¹; Liang Xue¹; ¹University of the Pacific, Stockton, CA
- WP 628 **DNA/RNA Adducts Formation from Bisphenol F 3,4-Quinone Metabolite;** Wang Xiaoxiao¹; Zhao Hongzhi²; Cai Zongwei²; ¹State Key Laboratory of Environmental and Biological Analysis, Department of Chemistry, Hong Kong Baptist University, Hong Kong, China; ²State Key Laboratory of Environmental and Biological Analysis, Department of Chemistry, Hong Kong Baptist University, HongKong, China
- WP 629 **Automatic Top-Down Spectral Annotation of Modified Oligonucleotides;** Maria Basanta-sanchez¹; Iggy Kass²; Catalin Doneanu²; ¹Waters Corporation, Pleasanton, CA; ²Waters Corporation, Milford, MA
- WP 630 **Discovery and Identification of an Unknown DNA Adduct in HeLa Cells Exposed to Colibactin-Producing E.coli using Untargeted DDA-CNL/MS3 Adductomic Analysis;** Peter W Villalta¹; Matthew R Wilson²; Yindi Jiang²; Alessia Stornetta¹; Paul D Boudreau²; Andrea Carra¹; Caitlin A Brennan³; Eunyoung Chun³; Lizzie Ngo⁴; Leona D Samson⁴; Bevin P Engelward⁴; Wendy S Garrett^{3,5,6}; Emily P Balskus²; Silvia Balbo^{1,7}; ¹University of Minnesota Masonic Cancer Center, Minneapolis, Minnesota; ²Department of Chemistry and Chemical Biology, Harvard University, Cambridge, Massachusetts; ³Department of Immunology and Infectious Diseases and Department of Genetics and Complex Diseases, Harvard T. H. Chan School of Public Health, Boston, Massachusetts; ⁴Department of Biological Engineering, MIT, Cambridge, Massachusetts; ⁵Broad Institute of MIT and Harvard, Cambridge, Massachusetts; ⁶Department of Medical Oncology, Dana-Farber Cancer Institute, Boston, Massachusetts; ⁷Division of Environmental Health Sciences, University of Minnesota, Minneapolis, Minnesota
- WP 631 **Method Development for Metabolite and Impurity Profiling of Oligonucleotide Therapeutics;** Kaoru Karasawa¹; Lyle Burton²; Eva Duchoslav²; ¹SCIEX, Shinagawa-ku, Japan; ²SCIEX, Concord, ON
- WP 632 **Comparison between ISD by MALDI Tof and CID by ESI ion trap FTICR of NF-κB Decoy Oligodeoxynucleotide and its metabolites;** Zenzaburo Tozuka¹; Akihiro Kunisawa²; Junko Iida²; Ryuichi Morishita³; Shohei Shioyama⁴; ¹Grad. Sch. Pharm. Sci./Osaka University, Suita, Osaka, Japan, Suita, Japan; ²Anal. Innov. Res. Lab. Grad. Sch. Eng./Osaka University, Suita, Japan; ³Grad. Sch. Med. Sci./Osaka University, Suita, Japan; ⁴JCL Bioassay Corporation, Nishiwaki, Japan
- WP 633 **Study of the Reduction of Azidothymidine (AZT) Using Electrochemistry Coupled to a Mass Spectrometer;**



- WP 634 Raquel Teijeiro¹; Francesca Cogliandro¹; Elvira Gomez¹; Jef Rozenski¹; ¹Rega Institute, Leuven, Belgium
Identification and Characterization of Urinary Nucleosides using Compound Discoverer 3.0 and Fragment Identification Search (FISH); Robert Ross¹;
 Ruoxia Zhao¹; Ningxi Yu¹; Andrew Wood¹; Manasses Jora¹; Ralf Tautenhahn²; Patrick A Limbach¹; ¹University of Cincinnati, Cincinnati, OH; ²Thermo Fisher Scientific, San Jose, CA
- WP 635 **A Method for the Automated Determination of Early Eluting Oligonucleotide Drug Impurities Using IP-RPLC HRMS; Stilianos G. Roussis¹**; Claus Rentel¹; ¹Ionis Pharmaceuticals, Inc., Carlsbad, CA
- WP 636 **Comparison of an Automated versus Manual SPE Sample Preparation Method for Improved Throughput during siRNA LC-MS Analysis; Babak Basiri¹**; Thuy Tran¹; Mark Boggeri²; Mei Han¹; Fang Xie¹; Brooke Rock¹; ¹Amgen Inc., South San Francisco, CA; ²Tecan SP, Inc., Baldwin Park, CA
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- WP 638 **A Highly Selective and Sensitive Analytical Method Using LC-MS/MS for Phosphorothioate Oligonucleotides; Yasuko Tsukazaki¹**; Naoto Senda¹; Mariko Harada-Shiba²; Fumito Wada²; Noriyuki Iwasaki³; Kaoru Karasawa³; ¹Shin Nippon Biomedical Laboratories, Ltd., Tsukuba, Japan; ²National Cerebral and Cardiovascular Center Research Institute, Suita, Japan; ³SCIEX, Shinagawa-ku, Japan
- WP 639 **Charge Deconvolution and Automatic Sequence Matching for Oligonucleotides; Wilfred Tang¹**; Marshall Bern¹; Rose D Lawler¹; James Moore¹; David Garby²; Nicholas Skizim²; ¹Protein Metrics Inc., Cupertino, CA; ²GreenLight Biosciences, Inc., Medford, MA
- WP 640 **Detection of the Altered tRNA Modification Profiles in Primary and Metastatic Melanoma by LC-MS; Congliang Sun¹**; Zalfa Abdel-Malek¹; Patrick A Limbach¹; Balasubrahmanyam Addepalli¹; ¹University of Cincinnati, Cincinnati, OH
- WP 641 **Strategies for Bioanalysis of an Oligonucleotide and Chain-Shorted Metabolites from Human Plasma Employing LC-UV/MS/MS Detection; Ying Peng¹**; Noah Post²; Moo-young Kim¹; Shabana Khatr²; Shannon Hall²; Fumin Li¹; ¹PPD, Middleton, WI; ²Ionis Pharmaceuticals, Inc., Carlsbad, CA
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- WP 642 **Glycoproteomic Analysis using 213 nm Ultraviolet Photodissociation Mass Spectrometry; Edwin Escobar¹**; Jennifer S Brodbelt¹; ¹University of Texas at Austin, Austin, TX
- WP 643 **Simultaneous Glyco- and Phosphopeptide Enrichment by Phytic Acid-Modified Titanium(IV) Immobilized Metal Affinity Chromatography (PA-Ti-IMAC); Dylan Nicholas Tabang¹**; Yusi Cui¹; Jillian Johnson²; Lingjun Li^{1,2}; ¹Department of Chemistry, University of Wisconsin, Madison, WI; ²School of Pharmacy, University of Wisconsin, Madison, WI
- WP 644 **Identification of Glutamic Acid Isomers Produced During Deamidation Through RDD Diagnostic Fragments; Jacob W Silzel¹**; Yana Lyon¹; Dylan Riggs¹; Ryan R. Julian¹; ¹UC Riverside, Riverside, CA
- WP 645 **Evaluation of an Automated, Acidic pH Protein Digestion for Reduced Levels of Artificial Deamidation in Biotherapeutic Peptide Mapping Studies; Tom Buchanan¹**; Ken Cook¹; Sara Carillo²; Silvia Millan Martin²; Dan Bach Kristensen³; Kevin Meyer⁴; Marc Geunder⁵;
 Rowan Moore¹; ¹Thermo Fisher Scientific, Runcorn, United Kingdom; ²National Institute for Bioprocessing Research and Training, Dublin, Ireland; ³Symphogen, Ballerup, Denmark; ⁴Perfinity, West Lafayette, Indiana; ⁵Thermo Fisher Scientific, Reinach, Switzerland
- WP 646 **Proteomic Analysis of Arginine-Rich RNA Binding Proteins by Electron Transfer Dissociation Mass Spectrometry; Sean R Kundinger¹**; Isaac Bishof¹; Duc M. Duong¹; Nicholas T. Seyfried¹; ¹Emory University, Atlanta, GA
- WP 647 **Quantitative Proteomic Analysis of Histone-PTMs in Breast Cancer Stem Cells by Multiple Reaction Monitoring; Seung Ju Moon¹**; Byoung-Kyu Cho¹; Nu-Ri Im¹; Eugene C. Yi¹; ¹Department of Molecular Medicine and Biopharmaceutical Sciences, Graduate School of Convergence Science and Technology, Seoul National University, Seoul, South Korea
- WP 648 **Novel Rabbit Monoclonal Antibodies for Profiling of Ser/Thr O-GlcNAc modified proteins; Matthew D. Fry¹**; Rami Najjar¹; Yiyang Zhu¹; Devin K Schweppe²; Steven Gygi²; Matthew P Stokes¹; ¹cell Signaling Technology, Danvers, MA; ²Harvard Medical School, Boston, MA
- WP 649 **Combining Proteomics Strategies to Study Polyglutamylated Peptides for Tubulin Analysis; Thibault Chaze¹**; Mathieu Dupré¹; Elise Warter²; Serge Bonnefoy²; Jujimon A.s³; Carsten Janke³; Philippe Bastin²; Mariette Matondo¹; Julia Chamot-Rooke¹; ¹Mass Spectrometry for Biology Unit, Institut Pasteur, CNRS USR2000, Paris, France; ²Trypanosome Cell Biology Unit, Institut Pasteur, INSERM U1201, Paris, France; ³Regulation of Microtubule Dynamics and Functions Unit, Institut Curie, CNRS UMR3348, Orsay, France
- WP 650 **Delineation of Glycopeptides and D-Amino Acid Containing Peptides (DAACPs) with Variant PTM Structure or Localization by High-Resolution FAIMS and ETD; Matthew A Baird¹**; Alexandre A Shvartsburg¹; ¹Wichita State University, Wichita, KS
- WP 651 **Large-Scale Profiling of Mannose-6-phosphate Glycoproteome from Human Cells by Ti(IV)-IMAC; Dangling Wang¹**; Junfeng Huang²; Yuan Liu²; Yusi Cui¹; Jillian Johnson²; Lingjun Li^{1,2}; ¹Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706; ²School of Pharmacy, University of Wisconsin-Madison, Madison, WI 53705
- WP 652 **Optimized EThcD Fragmentation Method for Confirmation of Isoaspartic Acid Peptides; Raghothama Chaerkady¹**; Ben Niu¹; Keith Rickert¹; Sonja Hess¹; ¹MedImmune, Gaithersburg
- WP 653 **Expanding the Glycoforms Detected in Complex Glycopeptide Datasets; Katalin F. Medzihradzsky¹**; Peter R. Baker²; Adam Pap¹; Zsuzsanna Darula¹; Robert Chalkley²; ¹Biological Research Centre of the Hungarian Academy of Sciences, Szeged, Hungary; ²UCSF, San Francisco, CA
- WP 654 **Highly Efficient and Precise Glycoproteomic Analysis with Intelligent Technology; Weiqian Cao¹**; Wenfeng Zeng²; Mingqi Liu¹; Chao Liu²; Biyun Jiang¹; Pan Fang¹; Huali Shen¹; Simin He²; Pengyuan Yang¹; ¹Fudan University, Shanghai, China; ²Institute of Computing Technology, Chinese Academy of Sciences, Beijing, China
- WP 655 **A Novel, Fast Post Translational Modification Localization Algorithm for Targeted DIA Outperforming DDA on a Controlled Sample Set; Oliver M Bernhardt¹**; Christian D. Kelstrup²; Tejas Gandhi¹; Lynn Verbeke¹; Alexander Hogrebe³; Dorte B. Bekker-Jensen²; Jesper V. Olsen³; Lukas Reiter¹; ¹Biognosys AG, Schlieren, Switzerland; ²Novo Nordisk Foundation Center for Protein Research, Faculty of Health and Medical Sciences, University of Copenhagen, Copenhagen, Denmark; ³Novo Nordisk Foundation Center for Protein Research, Faculty



- of Health and Medical Sciences, University of Copenhagen, Copenhagen, Denmark
- WP 656 **Finding the Sweet Spot in SAX-ERLIC Mobile Phase for Simultaneous Enrichment of Glyco and Phosphopeptides**; Yusi Cui¹; Ka Yang²; Dylan Nicholas Tabang²; Junfeng Huang²; Weiping Tang²; Lingjun Li²; ¹University of Wisconsin-Madison, Madison, WI; ²University of Wisconsin, Madison, Madison, WI
- WP 657 **RDD-MS Reveals the Isomerization Rate of Amyloid Beta and a Novel Cause for Alzheimer's Disease**; Ryan R. Julian¹; Dylan Riggs¹; Tyler Lambeth¹; ¹University of California, Riverside, Riverside, CA
- WP 658 **Verification of Sulfotyrosine and 4-Hydroxyproline in Biotherapeutics**; Oksana Tyshchuk¹; Christoph J. Gstöttner²; Dennis Funk³; Simone Simone Nicolardi²; Stefan Frost³; Felix Schumacher³; Manfred Wuhrer²; Michael Molhoj³; Vincent Larraillet³; ¹Roche Diagnostics GmbH, Penzberg, Germany; ²Leiden University Medical Center, Center for Proteomics and Metabolomics, Leiden, Netherlands; ³Roche Pharmaceutical Research and Early Development (pRED), Roche Innovation Center Munich, Germany
- WP 659 **Integrated Mass Spectrometry Method Development for Arginine methylation Analysis**; Chao Peng¹; Ping wu²; ¹National Center for Protein Science (Shanghai), Institute of Biochemistry and Cell biology, SIBS, CAS, Shanghai, China; ²National facility for Protein Science, Shanghai, China
- WP 660 **Comparison of Enrichment Strategies for In-Depth Proteomics Analysis of ADP-Ribosylation Sites**; Alexandra F. Stripp¹; Sara C. Larsen¹; Ivo A. Hendriks¹; Michael L. Nielsen¹; ¹Novo Nordisk Foundation Center for Protein Research, Faculty of Health and Medical Sciences, University of Copenhagen, Copenhagen, Denmark
- WP 661 **Investigating Crosstalk between endogenous SUMOylation and ADP-Ribosylation in the Cellular Response to Oxidative Stress**; Ivo A. Hendriks¹; Michael L. Nielsen¹; ¹Novo Nordisk Foundation Center for Protein Research, Faculty of Health and Medical Sciences, University of Copenhagen, Copenhagen, Denmark
- WP 662 **Identification and Quantitation of Phosphopeptide Positional Isomers using Trapped Ion Mobility Spectrometry and PASEF**; Chris Adams¹; Michael Krawitzky¹; Katherine Tran²; Baozhen Shan²; Zac Anderson²; Charles Farnsworth³; Matthew P Stokes³; Kimberly Lee³; Shourjo Ghose⁴; Matthew Willetts⁴; Gary Kruppa⁴; ¹Bruker Daltonics, San Jose, CA; ²Bioinformatics Solutions Inc., Waterloo, ON; ³Cell Signaling Technology, Danvers, MA; ⁴Bruker Daltonics Inc., Billerica, MA
- WP 663 **Characterization and Discrimination of Sulfopeptides and Phosphopeptides in Positive Mode Mass Spectrometry**; Maia Kelly¹; Justin Lawrie¹; Jiantao Guo¹; Eric D. Dodds¹; ¹University of Nebraska - Lincoln, Lincoln, NE
- WP 664 **Supercharging of Palmitoylated Peptides for Improved Electron Capture/Transfer Dissociation Tandem Mass Spectrometry**; Nhat H.V. Le¹; John E. Crellin¹; Gabriela Grigorean¹; Brent R. Martin¹; Kristina Hakansson¹; ¹University of Michigan, Ann Arbor, MI
- WP 665 **Direct Identification and Site-Specific Profiling of S-Palmitoylation by Liquid Chromatography/Tandem Mass Spectrometry**; John E. Crellin¹; Nicholas B. Borotto¹; Kristina Hakansson¹; Brent R. Martin¹; ¹University of Michigan, Ann Arbor, MI
- WP 666 **Identification of γ -Carboxyglutamic Acid Modified Proteins in Triple Negative Breast Cancer Cells by Immunocapture and Data Dependent nanoLC-MS/MS**; James McCardle^{1,2}; Sarah Beaudin²; Leila Kokabee²; JoEllen Welsh^{1,2}; ¹School of Public Health, Rensselaer, NY; ²University at Albany-SUNY, Rensselaer, NY 12144
- WP 667 **Identification of Human Chorionic Gonadotropin Glycoforms in Two Populations Using Improved Bottom-Up Analysis**; Nicolas Eskenazi¹; Chiara Giangrande¹; Joëlle Vinh¹; ¹SMBP, ESPCI, PSL University, Paris, France
- WP 668 **Identifying the Range of Protein Post-Translational Modifications that have Temporal Rhythms in the CAM Plant Kalanchoe**; Cheng Chen¹; Paul Abraham^{1,2}; Robert Hettich^{1,2}; ¹University of Tennessee, Knoxville, TN; ²Oak Ridge National Laboratory, Oak Ridge, TN
- WP 669 **Comprehensive Profiling of ADP-Ribosylation Sites Using Complementary Proteolytic Digestion and Precursor Fragmentation Strategies**; Sara C Larsen¹; Ivo A. Hendriks¹; Michael L. Nielsen¹; ¹University of Copenhagen NNF CPR, Copenhagen N, Denmark
- WP 670 **Unstructured Regions are Hotspots of Arginine Dimethylation in Neurodegeneration-Linked Proteins**; Jeremy D. O'Connell¹; Janos Demeter¹; Marcus Kelly¹; Nancie A. Mooney¹; Ran Cheng¹; Peter K. Jackson¹; ¹Stanford University, Palo Alto, CA
- WP 671 **Screening Spectra from Dimethylated Peptides Improve the Identification Rate of SUMOylation Sites by Orbitrap Mass Spectrometer**; Fu-An Li¹; Yu-Hsiang Cheng¹; ¹Institute of Biomedical Sciences, Academia Sinica, Taipei, Taiwan
- WP 672 **Database Search Strategies for Sulfopeptide Identification**; Hye Kyong Kweon¹; Andy T. Kong²; Katherine E. Hersberger¹; Shijiao Huang¹; Yanzhuang Wang¹; Alexey I. Nesvizhskii²; Philip C. Andrews¹; Kristina Hakansson¹; ¹University of Michigan, Ann Arbor, MI; ²University of Michigan Medical School, Ann Arbor, MI
- WP 673 **Assessment of Chromatographic Separation and Fragmentation Behavior of Isobaric Phosphopeptides Using Data Independent Acquisition Mass Spectrometric Approaches**; Christian A Doerig¹; Ludovic Gillet¹; Ulrike Kusebauch²; Dave Lee³; Robert L Moritz²; Anthony D Whetton^{3,4}; Paola Picotti¹; Ruedi Aebersold^{1,5}; ¹Department of Biology, Institute of Molecular Systems Biology, ETH Zurich, Zurich, Switzerland; ²Systems Biology, Seattle, WA; ³Stoller Biomarker Discovery Centre, University of Manchester, Manchester, United Kingdom; ⁴The School of Medical Sciences and Manchester Academic Health Sciences Centre, University of Manchester, Manchester, United Kingdom; ⁵Faculty of Science, University of Zurich, Zurich, Switzerland
- WP 674 **Pinpointing Isomerization Sites in Human Lens Crystallin using IMS-MS**; Hoi Ting Wu¹; Ryan R. Julian¹; ¹University of California, Riverside, Riverside, CA
- WP 675 **Identification of Cross-Linked Peptides and Oxidation Products in Lysozyme Subjected to Photo-Oxidation and Peroxyl Radical Oxidation**; Michele Mariotti¹; Eduardo Fuentes-Lemus²; Camilo López Alarcón²; Per Häggglund³; Michael Jonathan Davies³; ¹University of Copenhagen, Copenhagen, Denmark; ²University of Chile, Santiago, Chile; ³University of Copenhagen, Copenhagen, Denmark

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- WP 676 **Blood Brain Barrier (BBB) Penetration of Pituitary Adenylate Cyclase-Activating Polypeptide (PACAP) Glycosylated Peptides by 'Shotgun Microdialysis' Coupled with LC-MS3**; Chenxi Liu¹; Mitchell J Bartlett²; Christopher Robert Apostol¹; Lajos Szabo¹; Robin Polt¹; Torsten Falk²; Michael L Heien¹; ¹Department of Chemistry and Biochemistry, The University of Arizona, Tucson, Arizona; ²Department of Neurology, The University of Arizona, Tucson, Arizona
- WP 677 **Targeted Quantification of Detergent-Insoluble RNA-Binding Proteins in Alzheimer's Diseases**; Qi Guo¹; Eric B Dammer¹; maotian zhou¹; Marla Gearing¹; James J.



- Lah¹; Allan I. Levey¹; Nicholas Seyfried¹; ¹Emory University, Atlanta, GA
- WP 678 **Quantification of a Novel Peptide, CPT31, in Rat and Monkey Plasma by LC-MS;** China Y. Lim¹; Sarah Meghan Kriger¹; Brandon Wilcock¹; Vamshi Manda¹; Brett Welch²; Erik Kish-Trier³; Scott Reuschel¹; Troy Voelker¹; ¹Covance, Salt Lake City, UT; ²Navigen, Inc., Salt Lake City, UT; ³ARUP Laboratories, Salt Lake City, UT
- WP 679 **A Comparison Between MRM and PRM for the Quantitation of LEAP2 in Serum;** Chelsea C. Boo¹; Ranjitha Gaddipati¹; Joseph S. Grimsby¹; Sonja Hess¹; ¹MedImmune, Gaithersburg, MD
- WP 680 **Developing a Targeted Method for Monitoring Cytosolic Iron-Sulfur Cluster Assembly Pathway;** Xiaorui Fan¹; William D. Barshop¹; Ajay A. Vashisht^{1,2}; Stephanie Leal³; James A. Wohlschlegel¹; ¹UCLA, Los Angeles, CA; ²The Genomics Institute of the Novartis Research Foundation, San Diego, CA; ³California State University-Long Beach, Long Beach, CA
- WP 681 **Sub-Picogram Level Quantitation of Desmopressin in Small Volumes of Human Plasma Using a Trap-Elute Micro LC-MS System;** Rahul Baghla¹; Khatereh Motamedchaboki¹; Remco van Soest¹; Lei Xiong¹; ¹Sciex, Redwood City, CA
- WP 682 **A Potential Reference Measurement Procedure for Quantification of α -Synuclein in Biological Fluids;** Julia Mateyka¹; Adam Cryar¹; Giles Drinkwater¹; Milena Quaglia¹; Guglielmo Verona²; Vittorio Bellotti²; Sylvain Lehmann³; ¹LGC Group, Teddington, United Kingdom; ²UCL, London, United Kingdom; ³CHU Montpellier, Montpellier, France
- WP 683 **A Software Platform for Peptide Synthesis Quality Control by both LC-free MALDI-TOF and LC-ESI-QTOF Molecular Weight Determination;** Anjali Alving¹; Eckhard Belau²; Waltraud Evers²; Anja Resemann²; Wulff Niedner²; Detlev Suckau²; ¹Bruker Daltonics Inc., Billerica, MA; ²Bruker Daltonics, Bremen, Germany
- WP 684 **Factors that Influence the Recovery of Hydrophobic Peptides during LC-MS Sample Handling;** Moon Chul Jung¹; Kim Haynes¹; Markus Wanninger¹; ¹Waters Corporation, Milford, MA
- WP 685 **Absolute Quantification of Targeted Host Cell Proteins (HCPs) in Biotherapeutics by Liquid Chromatography-Multiple Reaction Monitoring (LC-MRM) Method;** Baibhav Rawal¹; Xnliu Gao²; Yan-Hui Liu²; ¹Merck & Co., Kenilworth, NJ; ²Merck & Co. Inc., Kenilworth, New Jersey
- WP 686 **Sequential Windowed Acquisition of Reporter Masses for Quantitation-First Proteomics;** William D. Barshop¹; Hee Jong Kim¹; Shima Rayatpisheh¹; James A. Wohlschlegel¹; ¹University of California Los Angeles, Los Angeles, CA
- WP 687 **Gonadotropin-Releasing Hormones (GnRH) Quantitation in Brain and Plasma by LC-HRMS/MS;** Claudio Medana¹; Federica Dal Bello¹; Michael Zorzi¹; Elisa Pastorello¹; Paolo Giacobini²; ¹University of Turin, Torino, Italy; ²Inserm, Lille, France
- WP 688 **Developing Fit-for-Purpose LC-MS Based Quantitative Assays to Support Drug Discovery Activities for Cyclic Peptides;** Rena N Zhang¹; Michelle R Robinson²; Komal Kedia²; Daniel Spellman²; ¹Merck & Co., Inc, West Point, PA; ²Merck & Co., Inc., West Point, PA
- WP 689 **Detecting Low Abundance Proteins in the Complex Background of the Cochlea by Mass Spectrometry;** Miguel Ramirez; ^{Northwestern University, Chicago, IL}
- WP 690 **Quantification and Evaluation of Sample Preparation Techniques in the Determination of Dynorphin Opioid Peptides by LC-MS/MS (MRM);** Karthik Chandu¹; Tony L Sahley²; Michael D Hammonds²; Masaru Miyagi³; David J Anderson⁴; ¹Cleveland State University, Cleveland, OH; ²School of Health Sciences; Cleveland State University, Cleveland, OH; ³Department of Pharmacology; Case Western Reserve University, Cleveland, OH; ⁴Department of Chemistry; Cleveland State University, Cleveland, OH
- WP 691 **The Role of the Cytoplasmic Capping Enzyme on the Proteome Diversity;** Bernice A. Agana¹; Sophie R. Harvey¹; Daniel R. Schoenberg¹; Vicki H. Wysocki¹; ¹The Ohio State University, Columbus, OH
- WP 692 **Assay of Human Insulin by Liquid Chromatography High Resolution Mass Spectrometry;** Kui Zeng¹; Jingyue Yang¹; Connie Ruzicka¹; ¹FDA, Saint Louis, MO
- WP 693 **Retention Time Correction Method Utilizing Unspecified Peaks in MS Scans;** Philip M Remes¹; Ping Yip¹; Romain Huguet¹; ¹Thermo Fisher Scientific, San Jose, CA
- WP 694 **Targeted Top-down Mass Spectrometry for Characterization and Quantitation of Crustacean Hyperglycemic Hormones (CHHs) and CHH Precursor-Related Peptides;** Yang Liu¹; Gongyu Li¹; Lingjun Li¹; ¹University of Wisconsin-Madison, Madison, WI
- WP 695 **Investigations of *Caenorhabditis elegans* egl-3 Mutants Reveal an Important Role in Neuropeptide Processing and a Significant Impact on Nociceptive Responses;** Bruno Nkambeu¹; Jennifer Ben Salem^{1,2}; Dina N Arvanitis²; Francis Beaudry¹; ¹Université de Montréal, St-Hyacinthe, QC; ²Institut des Maladies Métaboliques et Cardiovasculaires, INSERM UMR1048, Toulouse, France
- WP 696 **Development of a high throughput hybrid MS assay for human insulin in clinical samples, using surrogate matrices;** Michael A. Blackburn¹; Stuart McDougall¹; Stephen Gray¹; ¹Arcinova, Northumberland, United Kingdom
- WP 697 **Verification of the Bladder Cancer Biomarker Candidates in Clinical Urine Specimens by a SISCAPA-MRM Assay;** Yi-Ting Chen¹; Meng-Kai Chou¹; Yung-Chin Hsiao¹; Ying-Hsu Chang²; Chien-Lun Chen²; Jau-Song Yu¹; Yu-Sun Chang¹; ¹Chang Gung University, Taoyuan, Taiwan; ²LinKou Chang Gung Memorial Hospital, Taoyuan, Taiwan
- WP 698 **Podocalyxin and Podocin Multiplex Urine Analysis using Tandem Mass Spectrometry for the Evaluation of Podocyturia in Patients;** Tristan Martineau¹; Michel Boutin¹; Anne-Marie Côté¹; Daniel Bichet²; Bruno Maranda¹; Christiane Auray-Blais¹; ¹Université de Sherbrooke, Sherbrooke, QC; ²Hôpital du Sacré-Cœur, Université de Montréal, Montréal, QC
- WP 699 **A Comparative Study on Peptide Quantitation between Traditional LC-MS/MS and microLC-MS/MS for Discovery DMPK;** Yuanqiang Su¹; Meijuan He¹; Xinxin Wen¹; Xiaotong Li¹; Cheng Chen¹; Weimin Hu¹; Weiqun Cao¹; Lili Xing¹; Xin Zhang¹; Yi Tao¹; ¹WuXi AppTec, Shanghai, China
- WP 700 **Towards Turnkey Targeted Proteomics Solutions using Internal Standard Triggered Acquisitions on Modified Orbitrap Mass Spectrometers;** Sebastien Gallien^{1,2}; Aaron S. Gajadhar³; Bhavin Patel⁴; Markus Kellmann⁵; Tabiwang N. Arrey⁵; Alexander Harder⁶; Romain Huguet³; Graeme McAlister³; Derek Bailey³; Shannon Eliuk³; Emily I. Chen¹; Yue Xuan⁵; Andreas Huhmer³; ¹Thermo Fisher Scientific, Precision Medicine Science Center, Cambridge, MA; ²Thermo Fisher Scientific, Paris, France; ³Thermo Fisher Scientific, San Jose, CA; ⁴Thermo Fisher Scientific, Rockford, IL; ⁵Thermo Fisher Scientific, Bremen, Germany
- WP 701 **Comparison of Targeted Proteomics Approaches on a TIMS-Q-TOF;** Antoine Lesur¹; Pierre-Olivier Schmit²; Joseph Longworth¹; Gunnar Dittmar¹; ¹LIH, Luxembourg Institute of Health, Strassen, Luxembourg; ²Bruker Daltonique S.A., Wissembourg, France
- WP 702 **Targeted Membrane Protein Quantification for Therapeutic Target Identification;** Lei Guo; Sanofi, Cambridge, MA



- WP 703 **Development of a Very Sensitive LC-MS Assay to Quantitate Ultra Low Levels of GLP-1 Targeted Peptide Mimetics;** Jennifer Luong¹; Jeremy Brassard¹; Alyssa Kabat¹; Eric Schniederer²; Allysen Meymaris¹; Steven Wiltshire¹; Jakal Amin¹; ¹Charles River Laboratories, Worcester, MA; ²ProLynx LLC, San Francisco, CA
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- WP 704 **In-situ Chemical X-linking MS for Antibody-tractable Antigen identification;** Kang Hyun Kim¹; Jung Hyeon Lee²; Seung Ju Moon¹; Kristine M. Kim²; Eugene C. Yi¹; ¹Department of Molecular Medicine and Biopharmaceutical Sciences, Graduate School of Convergence Science and Technology, Seoul National University, Seoul, South Korea; ²Division of Biomedical Convergence, College of Biomedical Science, Kangwon National University, Chuncheon, South Korea
- WP 705 **Multiplexed TMT-Based Interactomics Reveals Coordination of Proteostasis Network Remodeling and Mechanisms of Protein Quality Control;** Madison T Wright¹; Lars Plate¹; ¹Vanderbilt University, Nashville, TN
- WP 706 **Revealing the Molecular Makeup of Rationally Designed Heterologomeric Assemblies of Stable Protein 1;** Nicholas Demarais; University of Auckland, Auckland, New Zealand
- WP 707 **Thyroglobulin as a Model for Analysis of Protein Quality Control Dynamics;** Madison T. Wright¹; Lars Plate¹; ¹Vanderbilt University, Nashville, TN
- WP 708 **TRIM28 as a Candidate Mutant p53 Interacting Partner in Cancer Cells;** Mariel R Mendoza¹; Katherine Alexander¹; Enrique Lin Shiao¹; Charly Ryan Good¹; Benjamin A. Garcia¹; Shelley L. Berger¹; ¹University of Pennsylvania, Philadelphia
- WP 709 **Analysis of the Lysosomal Membrane Interactome via Cross-Linking Mass-Spectrometry;** Jasjot Singh¹; Srigayatri Ponnaiyan¹; Fatema Akter¹; Dominic Winter¹; ¹University of Bonn - Institute of Biochemistry and Molecular Biology, Bonn, Germany
- WP 710 **FBXO11 Network Identifies Novel Disease-Relevant Interaction with the Ubiquitin-Specific Protease USP28;** Jonathan St-Germain¹; Etienne Coyaud¹; Estelle Laurent¹; Faith Yeung¹; Brian Raught¹; ¹Princess Margaret Cancer Centre, Toronto, ON
- WP 711 **Chaperone Activation and Client Binding of a 2-Cysteine Peroxiredoxin as Determined by Crosslinking Combined with MS and Cryogenic Electron Microscopy;** Karl A. T. Makepeace^{1,2}; Filipa Teixeira^{3,4,5,6}; Eric Tse⁷; Helena Castro^{4,5}; Ben A. Meinen^{4,8}; Leslie B. Poole⁹; James C. Bardwell^{3,8}; Ana M. Tomás^{4,5,6}; Evgeniy V. Petrotchenko¹⁰; Daniel R. Southworth⁷; Ursula Jakob³; Christoph H. Borchers^{1,2,10,11}; ¹University of Victoria-Genome BC Proteomics Centre, Victoria, BC; ²Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC; ³Department of Molecular, Cellular, and Developmental Biology, Ann Arbor, Michigan; ⁴i3S - Instituto de Investigação e Inovação em Saúde, Universidade do Porto, Porto, Portugal; ⁵IBMC - Instituto de Biologia Molecular e Celular, Universidade do Porto, Porto, Portugal; ⁶ICBAS - Instituto de Ciências Biomédicas Abel Salazar, Universidade do Porto, Porto, Portugal; ⁷Department of Biochemistry and Biophysics, Institute for Neurodegenerative Diseases, University of California, San Francisco, CA; ⁸Howard Hughes Medical Institute, University of Michigan, Ann Arbor, Michigan; ⁹Wake Forest Baptist Medical Center, Winston-Salem, NC; ¹⁰Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; ¹¹Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC
- WP 712 **Mass Spectrometry-Based Protein Footprinting Probes the Conformational Changes during Aβ42 Aggregation upon Binding to Novel Small Molecule Inhibitors;** Saketh Chemuru¹; George Mathai²; Jong Hee Song¹; Michael L Gross¹; ¹Washington University, St.Louis, MO; ²Sacred Heart College, Cochin, India
- WP 713 **On the Possibility of an Idiosyncratic Role of Heparin as Anticoagulant: in vitro Deactivation of Factor Xa via Heparin-Assisted Autolysis;** Chendi Niu¹; Cedric E. Bobst¹; Sergey Savinov¹; Igor A. Kaltashov¹; ¹University of Massachusetts Amherst, Amherst, MA
- WP 714 **Native Top Down Analysis of 184-218 kDa Protein Complexes Reveals the First Pentameric Viral Fibrils;** Matthew V. Holt¹; Tao Wang¹; Nicolas Leon Young¹; ¹Baylor College of Medicine, Houston, TX
- WP 715 **Rapid and Automatable Desalting of Protein Complexes by Size Exclusion Chromatography for On-line Detection by Native Mass Spectrometry;** Zachary VanAernum^{1,2}; Florian Busch^{1,2,3}; Benjamin J. Jones^{1,2}; Mengxuan Jia^{1,2}; Vicki Wysocki^{1,2,3}; ¹Department of Chemistry and Biochemistry, The Ohio State University, Columbus, Ohio; ²Resource for Native Mass Spectrometry Guided Structural Biology, Columbus, OH; ³Campus Chemical Instrument Center, The Ohio State University, Columbus, Ohio
- WP 716 **Investigating the Glycan Ligands of Siglecs through MS-Based Shotgun Glycomics;** Heajin Park¹; Elena N Kitova¹; Jaesoo Jung¹; Emily Rodrigues¹; Matthew S. Macauley¹; John Klassen¹; ¹University of Alberta, Edmonton, AB
- WP 717 **A Cross-Linking-Aided IP/MS Workflow Reveals Extensive Intracellular Trafficking in Time-Resolved, Signal-Dependent EGFR Proteome;** Yue Chen¹; Mei Leng¹; Yankun Gao²; Jongmin Choi¹; Dongdong Zhan²; Jun Qin^{1,2}; Sung Yun Jung¹; Yi Wang^{1,2}; ¹Department of Biochemistry and Molecular Biology, Baylor College of Medicine, Houston, TX; ²National Center for Protein Sciences (Beijing), State Key Laboratory of Proteomics, Institute of Lifeomics, Beijing, China
- WP 718 **Characterization of Essential Reprogramming Factors' Interaction Partner Dynamics during Cellular Reprogramming towards Pluripotency through Multiple Optimized Proteomics Approaches;** Weixian Deng¹; William Barshop¹; ¹UCLA, Los Angeles, CA
- WP 719 **Tandem Ion Mobility Coupled with Mass Spectrometry for Gas Phase Protein Unfolding Studies;** LeRoy B. Martin¹; Martin Palmer²; Dale A Cooper-Shepherd²; James I Langridge²; ¹Waters Corporation, Beverly, MA; ²Waters Corporation, Wilmslow, United Kingdom
- WP 720 **Characterization of Protein Biotinylation Sites by Peptide-Based Immunoaffinity Enrichment;** Yiyang Zhu¹; Matthew D. Fry¹; Alissa J. Nelson¹; Jianmin Ren¹; Vicky Yang¹; Michael C. Palazzola¹; Charles L. Farnsworth¹; Matthew P. Stokes¹; Kimberly A. Lee¹; ¹Cell Signaling Technology, Danvers, MA
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- WP 721 **Integrated Quantitative Proteomics in Cardiac Regeneration for Cardiac Systems Biology;** Trisha Tucholski¹; Ling Gao²; Kyle Brown¹; Yanlong Zhu¹; Jake Melby¹; Jianyi Zhang²; Ying Ge¹; ¹University of Wisconsin, Madison, WI; ²University of Alabama at Birmingham, Birmingham, AL
- WP 722 **A "GeLC-MS"-Based Method for Label-Free Quantitative Proteomics of Bronchoalveolar Lavage Fluid following Diisocyanate Exposure;** Brandon F. Law¹; Chen-Chung Lin¹; Justin M. Hettick¹; ¹NIOSH, Morgantown, WV
- WP 723 **Exploring Egg Characteristics of Striped Bass;** Taufika Islam Williams¹; Cara Kowalchuk¹; Jesse Fischer¹; Benjamin J. Reading¹; ¹North Carolina State University, Raleigh, NC



- WP 724 **Development of Label Free Quantitative Method for Proteomics and its Validation through Interlab Study;** Ki Na Yun^{1,2}; Geul Bang^{1,3}; Gun Wook Park¹; Heeyoun Hwang¹; Hongkyeong Jung¹; Hye-Jung Kim⁴; Eugene Lee⁵; Yong-In Kim⁵; Jeong Hee Moon⁶; Sungho Yun⁷; Jong Shin Yoo¹; Jin Young Kim¹; ¹Biomedical Omics Group, Korea Basic Science Institute, Cheongju, South Korea; ²Department of Chemistry, Sogang University, Mapo-gu, South Korea; ³College of Pharmacy, Korea University, Jochiwon, South Korea; ⁴New Drug Development Center, KBIO Osong Medical Innovation Foundation, Cheongju, South Korea; ⁵Korea Research Institute of Standards and Science, Yuseong-gu, South Korea; ⁶Disease Target Structure Research Center, KRIBB, Yuseong-gu, South Korea; ⁷Drug and disease target research team, Korea Basic Science Institute, Cheongju, South Korea
- WP 725 **Isotope Dilution Mass Spectrometry for Quantification of Influenza Proteins in Various Influenza Virus Preparations and Vaccines;** Wanda I Santana¹; Lidoshka Marc¹; Hans C Cooper¹; John R Barr¹; Tracie L Williams¹; ¹Centers for Disease Control and Prevention, Atlanta, GA
- WP 726 **A Proteomic-Based Pathway Analysis Identifies Bmi1 as a Potential Modulator for Tumor Growth and Invasion in Triple Negative Breast Cancer;** JungHun Lee¹; Bobae Shim²; Hyeyoon Kim^{1,2}; Han Suk Ryu²; Dohyun Han¹; ¹Proteomics core facility, Biomedical Research Institute, Seoul National University Hospital, Seoul, South Korea; ²Department of Pathology, Seoul National University Hospital, Seoul National University College of Medicine, Seoul, South Korea
- WP 727 **Proteomics Investigation of Induced Obstructive Sleep Apnea (OSA) in Rat Atria using Mass Spectrometry;** Devika Channaveerappa¹; Jacob C. Lux¹; Madhuri Jayathirtha¹; Cristiana Dumbraveanu¹; Brian K. Panama²; Costel C. Darie¹; ¹Clarkson University, Potsdam, NY; ²Masonic Medical Research Laboratory, Utica, NY
- WP 728 **Quantitative Proteomics of Acetomicrobium hydrogeniformans OS1: Converting Glucose to H₂;** Janine Y. Fu¹; Lauren Cook¹; Farzaneh Sedighian¹; Matthew Maune²; Ralph S. Tanner²; Michael J. McNerney²; Joseph A. Loo¹; Robert P. Gunsalus¹; Rachel R. Ogorzalek Loo¹; ¹University of California Los Angeles, Los Angeles, CA; ²University of Oklahoma, Norman, OK
- WP 729 **A Comprehensive Characterization of Proteome in Sz. Pombe DJ-1 Homologs: a Preliminary Study;** aline De Lima Leite^{1,2}; Kaleb Jones¹; Eli Riekeberg¹; Mark Wilson^{1,2}; Robert Powers^{1,2,3}; ¹University of Nebraska Lincoln, Lincoln, NE; ²Nebraska Center for Integrated Biomolecular Communication, University of Nebraska-Lincoln, Lincoln, Nebraska; ³Redox Biology Center, University of Nebraska-Lincoln, Lincoln, Nebraska
- WP 730 **Meltome Atlas – Thermal Proteome Stability across the Tree of Life;** Anna Jarzab¹; Nils Kurzawa²; Thomas Hopf³; Matthias Moerch⁴; Jana Zecha¹; Niels Leijten⁵; Eva Musiol⁶; Melanie Maschberger³; Gabrielle Stoehr³; Charlotte Daly¹; Tobias Schmidt¹; Julia Mergner¹; Britta Spanier⁷; Angel Angelov⁴; Thilo Werner⁸; Marcus Bantscheff⁸; Mathias Wilhelm¹; Martin Klingenspor⁶; Simone Lemeer⁹; Wolfgang Liebl⁴; Hannes Hahne³; Mikhail Savitski¹⁰; Bernhard Kuster¹; ¹Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; ²Genome Biology Unit, EMBL Heidelberg, Heidelberg, Germany; ³OmicScouts GmbH, Freising, Germany; ⁴Department of Microbiology, Technical University of Munich, Freising, Germany; ⁵Netherlands Proteomics Center, Utrecht, Netherlands; ⁶Chair of Molecular Nutritional Medicine, Technical University of Munich, Freising, Germany; ⁷Molecular Nutrition Unit, Technical University of Munich, Freising, Germany; ⁸Cellzome, a GSK company, Heidelberg, Germany; ⁹Netherlands Proteomics Center, Utrecht, Netherlands; ¹⁰Genome Biology Unit, EMBL Heidelberg, Heidelberg, Germany
- WP 731 **Doxorubicin-Induced Changes in the HLA Peptidome Determined using Tandem Mass Tags;** Patrick Murphy¹; Prathyusha Konda¹; Joao A. Paulo²; Heiko Schuster³; Daniel J Kowalewski³; Youra Kim¹; Derek R Clements¹; Michael Giacomantonio¹; Stefan Stevanović³; Steven P Gygi²; Shashi Gujar¹; ¹Dalhousie University, Halifax; ²Harvard Medical School, Boston, MA; ³Tuebingen University, Tuebingen, Germany
- WP 732 **Various Gonadotrohin Amounts Have Different Influence on the Secretom of human Granulosa and KGN Cells;** Tanja Panic-Jankovic¹; Ulrike Resch²; Goran Mitulovic¹; ¹Medical University of Vienna, Vienna, Austria; ²Medical University of Vienna, Vienna, Austria
- WP 733 **Quantitative Analysis of Chromatin Bound Metabolic Enzymes by High Resolution Mass Spectrometry;** Katja Parapatics¹; Jung-Ming George Lin^{2,3}; Sara Sdelci²; Andre C. Müller²; Stefan Kubicek^{2,3}; ¹CeMM-Research Center for Molecular Medicine of the Austrian Academy of Sciences, Vienna, Austria; ²CeMM-Research Center for Molecular Medicine of the Austrian Academy of Sciences, Vienna, Austria; ³Christian Doppler Laboratory for Chemical Epigenetics and Antiinfectives, CeMM Research Center for Molecular Medicine of the Austrian Academy of Sciences, Vienna, Austria
- WP 734 **Data Analysis for Accurate Label-Free Quantitation: Detection of and Correction for Co-Eluting Peptides;** Wenzhu Zhang¹; Brian T. Chait¹; ¹The Rockefeller University, New York, NY
- WP 735 **Optimizing Injection Time Predictions to Improve Isobaric Reagent Reporter Ion Yield during Multiplexed Quantitative Proteomic Experiments;** Craig Braun¹; Ryan Kunz¹; Alison Erickson¹; Steven P Gygi²; Brian Erickson¹; ¹IQ Proteomics LLC, Cambridge, MA; ²Harvard Medical School, Boston, MA
- WP 736 **Reporter Ion Cross-Channel Signals in TMT Multiplexing for the Carrier/Reference Strategy;** Paul Stemmer¹; Nicholas J. Carruthers¹; Joseph A Caruso¹; David M. Lubman²; Zhijing Tan²; ¹Wayne State University, Detroit, MI; ²University of Michigan, Ann Arbor, MI
- WP 737 **MRM Based Characterization of the Effect of HIV Infection and Methamphetamine Exposure on Human Monocyte Derived Macrophages;** Sarah C. Zieschang¹; Shulei Lei¹; Emma Harwood¹; Katarzyna Lech^{1,2}; Spencer Marshall Jaquet¹; Brenda Morsey¹; Howard S. Fox¹; Pawel Ciborowski¹; ¹University of Nebraska Medical Center, Omaha, NE; ²Faculty of Chemistry, Warsaw University of Technology, Warsaw, Poland
- WP 738 **MS Based Proteomics Reveals Differentially Regulated Proteins in Temozolomide Resistant Glioma;** Milan V. Teraiya^{1,2}; Helene Perreault¹; Vincent C. Chen³; ¹University of Manitoba, Winnipeg, MB; ²Brandon University (Visiting Student), Brandon, Manitoba; ³Brandon University, Brandon, Manitoba
- WP 739 **Quantitative Proteomics of Differential Protein Expression in USP24 Depleted Systems;** Joanne Y. Chan^{1,2}; John Le²; Lihua Jiang¹; Ruiqi Jian¹; Michael Snyder¹; Feng Gong²; ¹Stanford University, Stanford, CA; ²University of Miami Miller School of Medicine, Miami, FL
- WP 740 **Targeted Proteomic Analysis of Small GTPases in Murine Adipogenesis;** Yen-Yu Yang¹; Ming Huang²; Yinsheng Wang²; ¹University of California Riverside, Riverside, CA; ²University of California, Riverside, Riverside, CA
- WP 741 **A Filter-Assisted Approach for Rapid Proteomic Sample Quality Estimation;** Jair T Montford¹; Wenjing Peng¹; Jingfu Zhao¹; Aiyang Yu¹; Yehia Mechref¹; ¹Texas Tech University, Lubbock, TX



- WP 742 **Proteomic Analysis of Plasma – Sample Preparation and Multiplexing Workflows for Relative Quantitation;** Sergei Snovida¹; Yen-Chun Lai²; Amarjeet Flora¹; Ryan D. Bomgarden¹; John C Rogers¹; ¹*Thermo Fisher Scientific, Rockford, IL*; ²*Indiana University School of Medicine, Indianapolis, IN*
- WP 743 **Benchmark Instrument for Performing Hands-Free, Standardized Sample Preparation for Quantitative Proteomic Analyses;** Greg A. Foster¹; Woong Kim¹; Ryan D. Bomgarden²; Suzanne M. Smith²; Daniel Lopez-Ferrer¹; ¹*Thermo Fisher Scientific, San Jose, CA*; ²*Thermo Fisher Scientific, Rockford, IL*
- WP 744 **A Standardized Workflow for Tandem Mass Tags™ (TMT™) Based Proteomic Quantification Yields Improved Performance, Reproducible Quantitation, and Throughput Efficiency;** Aaron Robitaille¹; Ryan D. Bomgarden²; Amarjeet Flora²; Sergei Snovida²; Rosa Viner¹; Daniel Lopez-Ferrer¹; Andreas Huhmer¹; John C Rogers²; ¹*Thermo Fisher Scientific, San Jose, CA*; ²*Thermo Fisher Scientific, Rockford, IL*
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- WP 745 **High-Throughput Quantitative Measurement of Acetylsalicylic Acid, Salicylic Acid and Omeprazole in Human Plasma using LC-MS/MS;** Jingduan Chi¹; Fumin Li¹; ¹*PPD Inc, Madison, WI*
- WP 746 **Multivariate Approach to On-Line Supercritical Fluid Extraction – Supercritical Fluid Chromatography - Mass Spectrometry Method Development;** Alison P. Wicker¹; Kenichiro Tanaka²; Masayuki Nishimura³; Vivian Chen³; Tairo Ogura²; William Hedgepeth³; Kevin A. Schug¹; ¹*University of Texas at Arlington, Arlington, TX*; ²*Shimadzu Corporation, Nakagyo-ku, Japan*; ³*Shimadzu Scientific Instruments, Inc, Innovation Center, Columbia, MD*
- WP 747 **Electrochemistry-Assisted Absolute Quantitation by Mass Spectrometry;** Pengyi Zhao¹; Hao Chen¹; ¹*New Jersey Institute of Technology, Newark, NJ*
- WP 748 **Development and Validation of a Simple and Rugged LC-MS/MS Method to Measure 17-Desacetyl Norgestimate in Human Plasma;** Nick Peng¹; Ben Gaboury¹; Ardeshir Khadang¹; ¹*Axis Clinicals, Dilworth, MN*
- WP 749 **High Throughput MS Testing of APX001A in Rat Tissues;** China Y. Lim¹; Nidhi Jaiswal¹; Ben Johnson¹; Lucie Loukotkova¹; Robert Mansbach²; Karen J. Shaw²; Scott Reuschel¹; Troy Voelker¹; ¹*Covance, Salt Lake City, UT*; ²*Amplify Pharmaceuticals, San Diego, CA*
- WP 750 **Determination of Latanoprost and Latanoprost Free Acid in Plasma by LC-MS/MS Using Electrospray and UniSpray;** Matej Simek^{1,2}; Tereza Foglová¹; Petr Šulc¹; Martina Hermannová¹; Vladimír Velebný¹; ¹*Contipro, Dolní Dobruč, Czech Republic*; ²*Palacký University, Olomouc, Czech Republic*
- WP 751 **Overcoming Challenges to Develop a Robust Method for Quantifying Urinary Mono-Hydroxylated Polycyclic Aromatic Hydrocarbons (OH-PAHs) by On-Line SPE-LC-MS;** Yuesong Wang¹; Erin N. Pittman¹; Debra A. Trinidad¹; Hei Sio Ao¹; Antonia M. Calafat¹; Julianne C. Botelho¹; ¹*CDC, Atlanta, GA*
- WP 752 **Development and Validation of an Analytical Method for Quantitation of Emtricitabine, Tenofovir, and Efavirenz in Mouse Tissues by UPLC-MS/MS;** Jennifer A. Gilliam¹; Melanie A. Rehder Silinski¹; Brenda L. Fletcher¹; Reshan A. Fernando¹; Veronica G. Robinson²; Suramya Waidyanatha²; ¹*RTI International, Research Triangle Park, NC*; ²*Division of the National Toxicology Program, NIEHS, Research Triangle Park, NC*
- WP 753 **Ultrasensitive Quantification of Fluticasone Propionate and Salmeterol from Human Plasma Using UPLC/MS/MS;** Michael D Jones¹; Nikunj Tanna¹; ¹*Waters Corporation, Milford, MA*
- WP 754 **Development of a Rapid Method for the Quantification of Fidaxomicin from Biological Samples;** Anthony Haag^{1,2}; Kathleen M Hoch^{1,2}; Sigmund J Haidacher^{1,2}; ¹*Baylor College of Medicine, Houston, TX*; ²*Texas Children's Hospital, Houston, Texas*
- WP 755 **Analysis of Propylene Glycol in Rat Plasma after Derivatization using Liquid Chromatography Coupled with Tandem Mass Spectrometric Detection (LC-MS/MS);** Changyu Quang¹; William C. Nethero¹; Donald B. Giroux¹; Liam Moran¹; Elizabeth A Groeber¹; ¹*Charles River, Ashland, OH*
- WP 756 **Delivery Efficiency of Aerosolized Epoprostenol to the Lung through a Mechanical Ventilator Circuit;** Paul S. Soma¹; Nicholas J. Wallbillich¹; Jhaymie L. Cappiello²; Gary L. Glish¹; ¹*University of North Carolina at Chapel Hill, Chapel Hill, NC*; ²*Duke University Hospital, Durham, NC*
- WP 757 **Trace Level Analysis of Dithiothreitol in Complex Proteins by LC/MS/MS Analysis;** Jeffrey M. Selenka¹; Christopher G. Ciptadaya¹; Thomas Leitzinger¹; Jie Ding¹; ¹*PPD, Middleton, WI*
- WP 758 **A Rapid and Sensitive LC-MS/MS Method for Quantitative Analysis of GSK-3 Inhibitors in Mouse Plasma;** Ruhan Wei¹; David Wald²; Aimin Zhou¹; ¹*Cleveland State University, Cleveland, OH*; ²*Case Western Reserve University, Cleveland, OH*
- WP 759 **Using Labeling Probes and Isotope Tagging for Detection and Quantification of Short Chain Fatty Acids by LCMS in Biological Samples;** Rikard Fristedt; *Chalmers University of Technology, Gothenburg, Sweden*
- WP 760 **Investigation of Structure-Dependent Detection Limits for Phthalates, Nitrosamines, Alkylphenols and Aminoglycosides Extracted from Complex Sample Matrix Using LC-MS/MS;** Peijun Tu; *Intertek, Allentown, PA*
- WP 761 **Quantification of Tapentadol and Metabolites in Urine by Liquid Chromatography-Mass Spectrometry;** Suraj Saraswat¹; Kamisha L Johnson-Davis^{1,2}; ¹*ARUP Institute for Clinical and Experimental Pathology, Salt Lake City, UT*; ²*University of Utah Health Sciences Center, Department of Pathology, Salt Lake City, UT*
- WP 762 **Development of a Sensitive and Rugged LC(HILIC)-MS/MS Method for Pantothenic Acid in Human Plasma and Whole Blood Samples;** Xiaodong Zhu¹; Jingguo Huo¹; Thomas Lloyd¹; Edward Wells¹; ¹*Worldwide Clinical Trials, Austin, TX*
- WP 763 **Method Validation for the Determination of Novel Psychoactive Substances in Human Urine by Liquid Chromatography/High Resolution Mass Spectrometry;** Amber Awad¹; Ana Celia Grenier¹; Lawrence J Andrade¹; ¹*Dominion Diagnostics, North Kingstown, RI*
- WP 764 **A Fast and Simple Analysis of a Wide Range of Polar Compounds in Spent Media using Ultivo LC/TQ;** Jennifer Cottine Hitchcock¹; Jordy J. Hsiao¹; Yanan Yang¹; ¹*Agilent Technologies, Santa Clara, CA*
- WP 765 **Separation Efficiencies of PFP Columns in Reversed Phase Chromatography;** Koji Suzuki¹; Hiroshi Oikawa¹; Nozomi Murayama¹; Hiromi Miyagawa¹; Masatoshi Akitake¹; Bruno Ogawa¹; Natsuki Saotome¹; Yukio Otsuka¹; Hideo Matsuoka¹; Atsushi Sato¹; ¹*GL Sciences, Saitama, Japan*
- WP 766 **Quantitative Variability of Fat-Soluble Vitamins, Hormones, and Mycotoxin Content in Caged, Cage-Free, free-Range, Pasture Raised, and Home Raised chicken eggs;** Jamie L. York¹; Kevin A. Schug¹; ¹*The University of Texas at Arlington, Arlington, TX*
- WP 767 **LC/MS/MS Analysis for Restricted Chemicals in Textiles;** Tetsuo Tanigawa¹; Natsuyo Asano²; Jun Watanabe²; Yin Ling Chew¹; Jun Xiang Lee¹; Jie Xing¹; Zhaoqi Zhan¹; ¹*Shimadzu (Asia Pacific) Pte Ltd., Singapore, Singapore*; ²*Shimadzu Corporation, Nakagyo-ku, Japan*



- WP 768 **Modified Mass Barcoded AuNPs Signal Amplification for the Detection of Amphetamines with Laser Desorption Ionization Time-of-Flight Mass Spectrometer;** Liu-ti Wang¹; He-Hsuan Hsiao¹; ¹*Department of Chemistry, National Chung Hsing University, Taichung City, Taiwan*
- WP 769 **A HILIC-MS Method to Quantitate a Phospholipid Adjuvant for Vaccines;** Bin Deng¹; Carol Claus¹; Eric Yang¹; ¹*Sanofi Pasteur, Toronto, ON*
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- WP 770 **Untargeted Profiling of Toxicologically Relevant Metabolites: Case Study of Reactive Aldehydes;** Loïc Mervant^{1,2}; Robin Costantino³; Jean-François Martin³; Laurent Debrauwer³; Françoise Guéraud²; Emilien L. Jamin³; ¹*MetaboHUB-MetaToul, Toulouse, France*; ²*Toxalim (Research Centre in Food Toxicology) University of Toulouse, INRA, Toulouse, France*; ³*MetaboHUB-MetaToul, Toulouse, France*
- WP 771 **Optimization of Collision Cell Potentials for Analysis of Opiates and their Glucuronyl Metabolites in a Triple Quadrupole Mass Spectrometer;** Bennett Kalafut¹; Jianyun Zhao¹; Harald Oser¹; ¹*Thermo Fisher Scientific, San Jose, CA*
- WP 772 **Glucuronide Hydrolysis Optimization for Drugs Screening in Urine Using LDTD-MS/MS at 8 seconds per sample;** Serge Auger¹; Pier-Luc Plante²; Jean Lacoursière¹; Pierre Picard¹; ¹*Phytronix Technologies, Quebec, QC*; ²*Université Laval, Quebec, Quebec*
- WP 773 **Quantitative Swab Touch Spray Mass Spectrometry for Oral Fluid Drug Testing;** Nicolas M. Morato¹; Valentina Pirro¹; Patrick W. Fedick¹; Stuart A. Kushon²; R. Graham Cooks¹; ¹*Purdue University, West Lafayette, IN*; ²*Neoteryx, Torrence, CA*
- WP 774 **Urine Pain Panel Drug Screen for 42 Analytes with Enzyme Hydrolysis and an Internal Hydrolysis Indicator in Each Patient Sample;** Stephen D Merrigan¹; Gwendolyn A McMillin^{1,2}; ¹*ARUP Institute for Clinical and Experimental Pathology, Salt Lake City, UT*; ²*University of Utah Health Sciences Center, Department of Pathology, Salt Lake City, UT*
- WP 775 **Advancing Forensic DUID Screening with Mass Spectrometry;** Oscar Cabrices¹; Pierre Negri²; Dean Fritch³; Melanie Stauffer³; Nadine Koenig³; Derrick Schollenberger³; Jennifer Gilman³; Adrian Taylor⁴; ¹*SCIEX, Redwood Shores, CA*; ²*SCIEX, Redwood City, CA*; ³*Health Network Laboratories, Allentown, PA*; ⁴*SCIEX, Concord, ON*
- WP 776 **Streamlining Unknown Screening for Postmortem Analysis;** Adrian Taylor¹; Oscar Cabrices²; Xiang He²; Dean Fritch³; Nadine Koenig³; Melanie Stauffer³; Derrick Schollenberger³; ¹*SCIEX, Concord, ON*; ²*SCIEX, Redwood Shores, CA*; ³*Health Network Laboratories, Allentown, PA*
- WP 777 **Monitoring the Human Serum Albumin Adductome for Contact Allergens;** Lorena Ndreu¹; Alister James Cumming²; Johan Eriksson¹; Margareta Törnqvist¹; Isabella Karlsson¹; ¹*Department of Analytical Chemistry and Environmental Sciences (ACES), Stockholm University, Stockholm, Sweden*; ²*Department of Biochemistry and Biophysics, Stockholm University, Stockholm, Sweden*
- WP 778 **Mass Spectrometric Identification and Estrogenic Potential of cyclic Phenone Metabolites Formed in *in vitro* Assays with Fish Liver Slices;** Jose Serrano¹; Richard C Kolanczyk²; Mark A Tapper²; Barbara R Sheedy²; Tylor J Lahren²; Patricia A Kosian²; Alena Kubatova³; ¹*USEPA.ORD/NHEERL, Duluth, MN*; ²*USEPA.ORD/NHEERL, Duluth, Minnesota*; ³*University of North Dakota Department of Chemistry, Grand Forks, North Dakota*
- WP 779 **UHPLC-nanoESI-MSn Method for Quantification of DNA Adducts from Meat Carcinogens Implicated in Colorectal Cancer;** Dmitri Konorev¹; Lihua Yao¹; Robert Turesky¹; ¹*Masonic Cancer Center, U of MN, Minneapolis*
- WP 780 **Evaluating the Tolerance Mechanism of Zebrafish Embryo to Spermidine Carbon Quantum Dots by Proteomics Analysis;** YuJu Chen¹; Pang-Hung Hsu²; Han-Jia Lin²; ¹*National Yang-Ming University, Taipei, Taiwan*; ²*National Taiwan Ocean University, Keelung, Taiwan*
- WP 781 **Presumptive and Definitive Analysis of Urine Antidepressants by Prelude LX-4 MD™ and Sciex 4500 LC-MS/MS;** Anita Dermartirosian¹; Edith Shahbol¹; Karin Thomassian¹; Shaun Rezaei¹; Asad Shah¹; ¹*Quest Diagnostics, Inc., Valencia, CA*
- WP 782 **Quantitation of Total Carbamazepine and Carbamazepine Epoxide in Serum/Plasma on HPLC-MS/MS;** Diane Ly¹; Kamisha L. Johnson-Davis^{1,2}; ¹*ARUP Institute for Clinical and Experimental Pathology, Salt Lake City, UT*; ²*University of Utah Health Sciences Center, Department of Pathology, Salt Lake City, UT*
- WP 783 **Toxicological and Biochemical Changes Induced by Sub-Acute Exposure of Wistar Rats to Silver Nanoparticles using Soft Landing Ion Mobility Instrument;** Subhayu Nayek¹; Guido F. Verbeck¹; ¹*University of North Texas, Denton, TX*
- WP 784 **Small Molecules Automated Extraction from Human Breast Milk Using the Extrahera and the EVOLUTE Express CX Prior to LC-MS/MS Analysis;** Mohamed Yousef¹; Stephanie Marin¹; Jillian Neifeld¹; Jeremy Smith¹; Mario Merida¹; Elena Gairloch¹; ¹*Biotage, Charlotte, NC*
- WP 785 **Quantitative Proteomic Analysis of Cardiac Endothelial Cells Treated with Doxorubicin;** Xinzhu Pu¹; Steve Nick^{1,2}; Matthew Turner¹; Laura Bond¹; Kenneth Cornell¹; ¹*Boise State University, Boise, ID*; ²*University of Arizona, Tucson, AZ*
- WP 786 **Effects of DDE/Dieldrin on the Steroid Hormone Profile in Largemouth Bass (*Micropterus Salmoides*) Plasma;** Mohammad-Zaman Nouri¹; Kevin J. Kroll¹; Nancy D. Denslow¹; ¹*Department of Physiological Sciences and Center for Environmental and Human Toxicology, University of Florida, Gainesville, FL*
- WP 787 **Alternative Forensic Matrices: Evaluation of Simplified Workflow for Drugs of Abuse Extraction from Nail Samples Prior to LC-MS/MS Analysis;** Katie-Jo Teehan¹; Lee Williams¹; Rhys Jones¹; Geoff Davies¹; Adam Senior¹; Helen Lodder¹; Alan Edgington¹; Steve Jordan¹; Claire Desbrow¹; Paul Roberts¹; ¹*Biotage GB Limited, Cardiff, United Kingdom*
- WP 788 **Using a LC/MSD XT Single Quadrupole and HILIC-Z Column for Sensitive and Reliable Detection of Potential Genotoxic Impurities;** Patrick M Batoon¹; Kyle Covert²; ¹*Agilent Technologies Inc., Santa Clara, CA*; ²*Agilent Technologies, Inc., Santa Clara, CA*
- WP 789 **Method Validation for Trace Phentermine in the Presence of High Methylamphetamine Concentration and Other Analytes in Human Urine by LC-MS/MS;** Jianmei Wang¹; Jeremy Delao¹; ¹*Spectrum Diagnostic Laboratories, Arlington, TX*



THURSDAY POSTERS

Set up all Thursday posters
7:00 - 8:00 am

Odd-numbered posters present
10:30 - 11:30 am PLUS 12:30 - 2:30 pm

Even-numbered posters present
10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

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

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AMBIENT IONIZATION: APPLICATIONS II 001-032

- ThP 001 **Molecular Profiling of Cyanobacteria under Environmental Stimuli Using Laser Ablation Electrospray Ionization Coupled with Ion Mobility Separation Mass Spectrometry**; Jessica Vasconcelos¹; Sylwia A Stopka²; Boniek G Vaz¹; Akos Vertes²; ¹Federal University of Goias, Goiania, Brazil; ²George Washington University, Washington, DC
- ThP 002 **Accelerated Energetic Syntheses through the Use of Confined Volume Systems Generated by Ambient Ionization Sources**; Patrick W Fedick; Naval Air Warfare Center, Weapons Division, Research Department, Chemistry Division, China Lake, CA
- ThP 003 **Highly Sensitive and Rapid Screening for Pesticides using Direct Analysis in Real Time Triple Quadrupole Mass Spectrometry**; He Cui¹; Yongyi Jiang²; Kerry Song³; Xiuzhen Yin^{1,4}; Tingting Han²; Jiale Xu³; Xiaokun Duan³; Charles C. Liu³; ¹Qingdao Customs District, Qingdao, China; ²Qingdao Future Test, Qingdao, China; ³ASPEC Technologies, Beijing, China; ⁴Qingdao University of Science and Technology, Qingdao, China
- ThP 004 **Detection of Ricin and Abrin Toxin by Laboratory-Based and Portable Direct Analysis in Real-Time Mass Spectrometry (DART-MS)**; Jennifer W Sekowski¹; Debora Van Der Riet-van Oeveren²; Ad De Jong²; Alex Fidler²; Paul S Demond¹; Jacquelyn V Harris¹; Daan Noort²; ¹U.S. Army RDECOM Chemical & Biological Center, Aberdeen Proving Ground, MD; ²The Netherlands Organization, Rijswijk, Netherlands
- ThP 005 **Solvent-Assisted Paper Spray Ionization Mass Spectrometry (SAPSI-MS) for the Analysis of Biomolecules and Biofluids**; Alessandro Quaranta¹; Nicoló Riboni¹; Hitesh V Motwani¹; Nicklas Österlund¹; Astrid Gräslund¹; Federica Bianchi²; Leopold L Ilag¹; ¹Stockholm University, Stockholm, Sweden; ²University of Parma, Parma, Italy
- ThP 006 **Improved Sensitivity for Saccharides via In-Source Derivatization Using Coaxial Contained Electrospray Mass Spectrometry**; Derik R. Heiss^{1,2}; Abraham K. Badu-Tawiah³; ¹The Ohio State University, Columbus, OH; ²Battelle Memorial Institute, Columbus, OH; ³The Ohio State University, Columbus, OH
- ThP 007 **Cross-Continental, Multisite Round Robin REIMS Study for the Evaluation of REIMS Fundamentals and Technology**; Julia Balog¹; Pierre-Maxence Vaysse²; Tiffany Porta Siegel²; Martin Kaufmann³; Ala Amgheib⁴; Viktoria Varga¹; Andras Marton¹; Steven D Pringle⁵; John Rudan³; Ron M. A. Heeren²; Zoltan Takats⁴; ¹Waters Research Center, Budapest, Hungary; ²Maastricht Multimodal Molecular Imaging (M4I) Institute, Division of Imaging Mass Spectrometry, Maastricht, Netherlands; ³Queen's University, Kingston, ON; ⁴Imperial College, London, United Kingdom; ⁵Waters Corporation, Wilmslow, United Kingdom
- ThP 008 **Molecular Characterization of Terminal Structures for Polycarbonates Using a Thermal Desorption/Pyrolysis DART-MS**; Kenichi Yoshizawa¹; Chikako Takei¹; Sayaka Nakamura²; Hiroaki Sato²; ¹BioChromato, Inc., Fujisawa, Japan; ²National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan
- ThP 009 **Improved Rapid Untargeted Screening Method for Veterinary Drug Residues in Animal Tissues Using Liquid Microjunction Surface Sampling Probe Mass Spectrometry**; Laura Burns¹; David J. Borts^{1,2}; ¹Interdepartmental Toxicology Program, Iowa State University, Ames, Iowa; ²Department of Veterinary Diagnostic & Production Animal Medicine, Iowa State University, Ames, IA



- ThP 010 **Flavor release monitoring using direct analysis in real-time mass spectrometry on differentiate with respect to time;** Motoshi Sakakura¹; Teruhisa Shiota¹; Takehito Sagawa²; ¹AMR, Inc., Tokyo, Japan; ²S&B foods Inc., Tokyo, Japan
- ThP 011 **Revealing Photo-Thermal Stability of Pharmaceuticals and the Degradation Mechanism by Microwave Plasma Torch Mass Spectrometry;** Shuanglong Wang¹; Wei Liu¹; Huanwen Chen¹; ¹East China University of Technology, Nanchang, China
- ThP 012 **Electroextraction (EE) Coupled with Paper Spray Mass Spectrometry (PS-MS) for Selective and Sensitive Analyses of Target Analytes in Complex Samples;** Rodinei Augusti¹; Victoria Silva Amador¹; Juliane Soares Moreira¹; Denise Versiane Monteiro de Sousa¹; Ricardo Mathias Orlando¹; ¹Federal University of Minas Gerais, Belo Horizonte, Brazil
- ThP 013 **A Robust, Long-Lasting Microspray Metal Emitter with Nanospray Sensitivity for Proteomics;** Sau Lan Staats¹; Anna Stoltzfus¹; Andris Suna¹; ¹Phoenix S & T, Inc, Chadds Ford, PA
- ThP 014 **Quantitative Analysis of Linezolid in Human Plasma by DART-MS and its Application to a Pharmacokinetic Study;** Lei Yin^{1,2,3}; Yixuan Feng^{1,2}; Jin Tong^{1,2}; Zhiqiong Guo^{1,2}; Yuyao Zhang^{1,2}; Xiaokun Duan⁴; Lifeng Xu⁴; Charles C. Liu⁴; Jingkai Gu^{*1,2}; ¹Jilin University, Changchun, China; ²Beijing Institute of Modern Drug Metabolism, Beijing, China; ³University of Arizona, Tucson, AZ; ⁴ASPEC Technologies, Beijing, China
- ThP 015 **Reaction Acceleration at the Surface of Droplets;** Yangjie Li¹; Zhenwei Wei¹; Yong Liu²; R. Graham Cooks¹; ¹Department of Chemistry, Purdue University, West Lafayette, IN; ²Merck & Co., Inc., Rahway, NJ
- ThP 016 **A Comparative Profiling of DHA-rich Oil Products by DESI and DART Mass Spectrometry;** Kerry Song¹; Jiale Xu¹; Wen Zhou²; Jiang Zhou²; Wei Chen¹; Xiaokun Duan¹; Charles C. Liu¹; ¹ASPEC Technologies, Beijing, China; ²Peking University, Beijing, China
- ThP 017 **Repeatability and Practicality of PESI/MS/MS-Based *in vivo* Real-Time Monitoring System for Hepatic/Brain Metabolites in Living Mice;** Kei Zaitu^{1,2}; Yumi Hayashi^{1,3}; Tasuku Murata⁴; Kazumi Yokota⁴; Tomomi Ohara²; Hitoshi Tsuchihashi²; Akira Ishii²; Koretsugu Ogata⁴; Hiroshi Taninata⁴; ¹In Vivo Real-Time Omics Laboratory, Institute for Advanced Research, Nagoya University, Nagoya, Japan; ²Department of Legal Medicine and Bioethics, Nagoya University Graduate School of Medicine, Nagoya, Japan; ³Pathophysiological Laboratory Sciences, Department of Radiological and Medical Laboratory Sciences, Nagoya University Graduate School of Medicine, Nagoya, Japan; ⁴Shimadzu Corporation, Kyoto, Japan
- ThP 018 **Using Rapid Evaporative Ionisation Mass Spectrometry (REIMS) to Improve Efficiency and Add Capability in Pharmaceutical R&D;** Paul Abu-Rabie; GSK R&D, Stevenage, United Kingdom
- ThP 019 **Pre-Concentration and a Special Scan Function for More Sensitive and Stable Ambient Ionization Mass Spectrometry;** Taoqing Wang¹; Linfan Li²; Mengtian Li¹; Huishan Li¹; Jae C Schwartz²; Anyin Li¹; Nicolas Heath¹; ¹University of New Hampshire, Durham, NH; ²Thermo Fisher Scientific, San Jose, CA
- ThP 020 **Coated Blade Spray-High-Resolution Mass Spectrometry: A Versatile Tool for Sample Profiling and Screening of Controlled Substances in Complex Matrices;** German Augusto Gómez-ríos¹; Robert Cody²; Nathaly Reyes-garcés¹; Frances Carroll¹; Gary Stidsen¹; David Bell¹; ¹Restek Corporation, Bellefonte, PA; ²JEOL USA, Inc., Peabody, MA
- ThP 021 **Extractable Analysis of Heart Stem Using HPLC Q-ToF Mass Spectrometry Coupled with High Resolution Database and Library;** Chang Jiang; , Chengdu, China
- ThP 022 **Ion-Neutral Complex Mediated Benzyl Cation Transfer and Proton Transfer of Protonated Benzyl Phenyl Sulfone in the Gas Phase;** Yin Qi; Zhejiang University, Hangzhou, China
- ThP 023 **Rapid Characterization of Saponins in Ginseng Species Roots by Liquid Extraction Surface Analysis Mass Spectrometry;** Mei Tian¹; Yuanguai Yang¹; Linnan Li¹; Li Yang^{1,2}; Xiaokun Duan³; Kerry Song³; Shujie Zou³; Echo Jia³; Charles.C Liu³; Zhengtao Wang^{1,2}; ¹Shanghai University of Traditional Chinese Medicine, Shanghai, China; ²Shanghai R&D Center for Standardization of Chinese Medicines, Shanghai, China; ³ASPEC Technologies, Beijing, China
- ThP 024 **Analysis of Immunosuppressant Drugs directly from Whole Blood using PaperSpray Technology;** Cornelia Leonie Boeser¹; Neloni R. Wijeratne¹; Mary L. Blackburn¹; ¹Thermo Fisher Scientific, San Jose, CA
- ThP 025 **Sticky Paper Spray Ionization for Analysis of Powdered Analyte Grains;** Praneeth Hettikankanange¹; Grant Klingler¹; Mason Laikupu¹; Daniel Austin¹; ¹Brigham Young University, Provo, UT
- ThP 026 **Mechanistic Study of Organometallic Reactions by On-line Mass Spectrometry Monitoring System;** Xin Yan; Texas A&M University, College Station, TX
- ThP 027 **Strain-Level Differentiation of Bacteria by Paper Spray Mass Spectrometry;** Casey A. Chamberlain¹; Vanessa Y. Rubio¹; Timothy J. Garrett¹; ¹University of Florida, Gainesville, FL
- ThP 028 **Areca Alkaloids Measured from Buccal Cells Using DART-MS Serve as Accurate Biomarkers for Betel Nut Chewing;** Adrian Franke¹; Laura Biggs²; Joanne Y. Yew³; Jennifer F Lai⁴; ¹Univ of Hawaii Cancer Ctr, Honolulu, HI; ²University of Guam, Mangilao, Guam; ³Pacific Biosciences Research Center, University of Hawaii, Honolulu, Hawaii; ⁴University of Hawaii Cancer Center, Honolulu, Hawaii
- ThP 029 **Microdroplet Fusion Chemistry for Charge State Reduction in Synthetic and Biological Polymers via Bipolar Dual Spray;** John R Stutzman¹; Ryan M Bain¹; Sebastian Hagenoff²; William Hunter Woodward¹; John P O'Brien³; Michael Lesniak¹; ¹The Dow Chemical Company, Midland, MI; ²The Dow Chemical Company, Stade, Germany; ³The Dow Chemical Company, Lake Jackson, TX
- ThP 030 **Application of the Micro Flow Ion Source with Cartridge Columns for Fast LC-MS/MS Analysis of Vitamin D Metabolites;** Tomasz Bienkowski¹; Michał Szumski^{1,2}; Irmina Tomaszewska¹; Konrad Piotr Kowalski¹; Przemysław Kalicki¹; Michał Książkiewicz¹; ¹MS Ekspert Sp. z o.o, Gdańsk, Poland; ²Nicolaus Copernicus University, Torun, Poland
- ThP 031 **Quality Control Aspects of the REIMS Technology;** Andras Denes Marton¹; Richard Schäffer¹; Viktoria Varga¹; Tamas Karancsi¹; Lajos Godorhazy¹; Steven D Pringle²; Julia Balog^{1,3}; ¹Waters Research Center, Budapest, Hungary; ²Waters Corporation, Wilmslow, United Kingdom; ³Imperial College, London, United Kingdom
- ThP 032 **SpiderMass Real-Time, Mini Invasive Analysis of Cancer: Towards *in vivo* Molecular Diagnostics of the Future;** Nina Ogrinc¹; Philippe Saudemont¹; Yves-Marie Robin²; Julia Balog³; Dominique Tierny⁴; Jean-Pascal Gimeno¹; Zoltan Takats⁵; Michel Salzet¹; Isabelle Fournier¹; ¹PRISM Inserm U1192 - University of Lille, Villeneuve D'ascq Cedex, France; ²Pathology Department, Centre Oscar Lambret, Lille, France; ³Waters Research Center, Budapest, Hungary; ⁴OCR, Villeneuve d'Ascq, France; ⁵Imperial College London, London, United Kingdom

**AMBIENT IONIZATION: FUNDAMENTALS AND INSTRUMENTATION**
033-059

- ThP 033 **Unique Ion/Molecule Chemistry of N-Alkanes in the Flowing Atmospheric Pressure Afterglow Ionization Source;** Brian Molnar¹; Sunil P Badal¹; Jacob T Shelley¹; ¹*Rensselaer Polytechnic Institute, Troy, NY*
- ThP 034 **Visualization of Charged Droplets – Ambient Gas Interactions and Entrainment Flows in Nanoelectrospray;** Joel Chapman¹; Peter Kottke¹; Andrei Fedorov¹; ¹*Georgia Institute of Technology, Atlanta, GA*
- ThP 035 **Wire Desorption-Glow Discharge/Electrospray Ionization/Mass Spectrometry for Rapid Characterization of Compounds with a Broad Range of Polarity and Boiling Point;** Yuanlong Wang¹; Junsheng Zhang¹; Lin Liu¹; Liping Huang¹; Jentae Shiea²; Wenjian Sun¹; ¹*Shimadzu Research laboratory (Shanghai) Co. Ltd., Shanghai, China*; ²*Department of Chemistry, National Sun Yat-sen University, Kaohsiung, Taiwan*
- ThP 036 **Direct Mass Spectrometry Analysis Using In-Capillary Dicationic Ionic Liquid-Based *in situ* Dispersive Liquid-Liquid Microextraction and Sonic-Spray Ionization;** Yueguang Lv¹; Qiang Ma¹; ¹*Chinese Academy of Inspection and Quarantine, Beijing, China*
- ThP 037 **The Effects of Gas Flows and Discharge Pulse on Explosives Detection Using a Dielectric Barrier Discharge Ionization Source;** Vadym Berkout; *Smiths Detection, Edgewood, MD*
- ThP 038 **Atmospheric Pressure Dark-Current Argon Discharge Ionization with Comparable Performance to Direct Analysis in Real Time Mass Spectrometry;** Teruhisa Shiota¹; Kanako Sekimoto²; Motoshi Sakakura²; Mitsuo Takayama²; ¹*AMR, Inc., Tokyo, Japan*; ²*Yokohama City University, Yokohama, Japan*
- ThP 039 **Sampling and Ionization Process in Scanning Probe Electrospray Ionization;** Yoichi Otsuka¹; Bui Kamihoriuchi¹; Aya Takeuchi¹; Futoshi Iwata²; Takuya Matsumoto¹; ¹*Osaka University, Toyonaka, Japan*; ²*Shizuoka University, Hamamatsu, Japan*
- ThP 040 **Inlet Ionization for High Speed Mass Spectrometry;** Ellen Inutan^{1,2}; Chuping Lee¹; Eric Davis¹; Georgios Makris¹; Frank Yenchick¹; Robert Roose¹; Sarah Trimpin^{1,3}; ¹*Wayne State University, Detroit, MI*; ²*MSU-Illigan Institute of Technology, Illigan City, Philippines*; ³*Cardiovascular Research Institute, Wayne State University School of Medicine, Detroit, MI*
- ThP 041 **Surface Acoustic Wave Nebulization (SAWN) and Charge Independent Nano Electromechanical Mass Sensing (NEMS-MS) of Multi Mega-Dalton Particles;** Szu-Hsueh Lai¹; Bogdan Vysotskyi²; Luis A Cubero Montealegre²; Martial Defoort²; Kavya Clement¹; Mohammad Abdul Halim¹; Sergio Dominguez-Medina¹; Sebastien Hentz²; Christophe Masselon¹; ¹*Univ. Grenoble Alpes, CEA, Inserm, BIG-BGE, Grenoble, France*; ²*Univ. Grenoble Alpes, CEA, LETI, Grenoble, France*
- ThP 042 **An Optimized Jet Nebulization Geometry for LCMS;** Chuck Jolliffe¹; Harikrishnan Sukumar¹; Marius Radu¹; Reza Javahery¹; ¹*PerkinElmer Inc., Woodbridge, ON*
- ThP 043 **Fast Screening of Pesticides in Foods and Agricultural Products with Probe Electrospray Ionization (PESI) Tandem Mass Spectrometry;** Zhenhe Chen¹; Satoshi Yamaki¹; Jing Dong¹; Yuki Hashi²; Naoki Hamada¹; ¹*Shimadzu (China) Co., LTD., Beijing, China*; ²*Shimadzu (China) Co., LTD., Shanghai, China*
- ThP 044 **Liquid Ionization with High-Repetition Rate μ J-Laser-Induced Airborne Plasma for Direct Mass-Spectrometric Analysis;** Yi You¹; Andreas Bierstedt¹; Sebastian van Wasen¹; Gaby Bosc-Bierne¹; Michael G. Weller¹; Jens Riedel¹; ¹*Federal Institute for Materials Research and Testing (BAM), Berlin, Germany*
- ThP 045 **Solvent Assisted Surface Probe-Nanoelectrospray: A Modular Liquid-Extraction Based Tool for Combined Top-Down & Bottom-Up Proteomic Surface Analysis;** Raul Villacob¹; Luke T. Richardson¹; Matthew Mulloy¹; Touradj Solouki¹; ¹*Baylor University, Waco, TX*
- ThP 046 **Laser Desorption REIMS – the Fundamentals and How they Dictate Applications and Automation;** Emrys A Jones¹; Daniel Simon²; Tamas Karancsi²; Danielle McDougall³; Csaba Hajdu²; Richard Schaffer²; Julia Balog²; Steven D Pringle⁴; Zoltan Takats⁵; ¹*Waters, Wilmslow, United Kingdom*; ²*Waters Research Center Kft., Budapest, Hungary*; ³*Manchester Institute of Biotechnology, University of Manchester, United Kingdom*; ⁴*Waters Corporation, Wilmslow, United Kingdom*; ⁵*Imperial College, London, United Kingdom*
- ThP 047 **Systematic CFD Study of Gas Transport in a Desorption Cell Coupling AFM and AP MS in a Multimodal Imaging Platform;** Matthias Lorenz¹; Ryan Wagner²; Roger Proksch²; Olga S Ovchinnikova³; ¹*University of Tennessee / Oak Ridge National Laboratory, Oak Ridge, TN*; ²*Oxford Instruments, Santa Barbara, CA*; ³*Oak Ridge National Laboratory, Oak Ridge, TN*
- ThP 048 **An Interface for Reproducible, Multi-shot Direct Analysis of Solid-phase Microextraction Samples;** G. Asher Newsome¹; Alba Alvarez-Martin¹; Gwénaëlle Kavich¹; ¹*Smithsonian Institution Museum Conservation Institute, Suitland, MD*
- ThP 049 **Internal Energy Deposition in Infrared Matrix-Assisted Laser Desorption Electrospray Ionization with and without the Use of Ice as a Matrix;** Anqi Tu¹; David C. Muddiman^{1,2}; ¹*FTMS Laboratory for Human Health Research, Department of Chemistry, North Carolina State University, Raleigh, NC*; ²*Molecular Education, Technology, and Research Innovation Center (METRIC), North Carolina State University, Raleigh, NC*
- ThP 050 **Two-Laser Ablation Electrospray Ionization Mass Spectrometry;** Kelcey B. Hines¹; Remilekun O. Lawal¹; Fabrizio Donnarumma¹; Kermit K. Murray¹; ¹*Louisiana State University, Baton Rouge, LA*
- ThP 051 ***in vivo* Analysis of Plant Sap by Direct Sampling and Capillary Microsampling Electrospray Ionization Mass Spectrometry;** Tina Tran¹; Laith Z. Samarah¹; Akos Vertes¹; ¹*George Washington University, Washington, DC*
- ThP 052 **Key Factors Influencing Nano-Electrospray Ionization Efficiency of Tryptic Peptides from Fused Silica Emitters During Reversed-Phase Liquid Chromatography Separations;** Joshua A Silveira¹; Gary Schultz²; Wei Wei³; Aran Paulus³; Eloy R. Wouters³; ¹*Thermo Fisher Scientific, San Jose, CA*; ²*Munson Technology, Ithaca, NY*; ³*Thermo Fisher Scientific, San Jose, CA*
- ThP 053 **The Effect of High Mass Resolving Power by Involving Sample Morphology in Linear TOF;** Yi-Hong Cai; *Genomics Research Center Academia Sinica, Taipei, Taiwan*
- ThP 054 **Characterization of a Novel Plasma-Ionization Source for Real-Time Breath Analysis;** Christopher Gongar¹; Michael Wei¹; Robin H.J Kemperman¹; Richard A. Yost¹; ¹*University of Florida, Gainesville, FL*
- ThP 055 **Reactions and Fragmentation in a Microwave Plasma Jet Ambient Ionization Source;** Kenyon Evans-Nguyen¹; Abigail Smola¹; Kayla M Whitehouse¹; Tiffany Matyja¹; Micheala Le Gendre¹; ¹*University of Tampa, Tampa, FL*
- ThP 056 **Strategies to Improve Protein Analysis by Desorption Electrospray Ionization;** Andre Venter¹; Elahe Honarvar¹; Roshan Javanshad¹; Tara Maser¹; Frank Martin Beranek¹; ¹*Western Michigan University, Kalamazoo, MI*
- ThP 057 **Development of a Cryo-Stage for LESA Mass Spectrometry – Towards Truly Native Surface Sampling of Proteins;** Bin Yan¹; Adam J. Taylor¹; Josephine Bunch^{1,2};



- ¹National Physical Laboratory, Teddington, United Kingdom; ²Imperial College, London, United Kingdom
- ThP 058 **Trace Level Detection of Gas Impurities Using Atmospheric Pressure Ionization Mass Spectrometry;** Gregory Thier¹; Luke Kephart¹; Brian Regel¹; ¹Extrel CMS, Pittsburgh, PA
- ThP 059 **Investigation of Gas Flow Effects and Space Charge in Atmospheric Pressure Interfaces;** Philipp Krah¹; Laurent Bernier¹; Stephan Rauschenbach²; Julius Reiss¹; ¹Technical University Berlin, Berlin, Germany; ²University of Oxford, Oxford, United Kingdom
- CARBOHYDRATES II**
060-085
- ThP 060 **High-Throughput Clinical Glycomics with Ultra High Resolution MALDI-FTICR-MS Reveals Pancreatic Cancer Disease Signatures;** Gerda C.M. Vreeker¹; Randa g.h. Sawires¹; Simone Nicolardi¹; Marco R. Bladergroen¹; Jan Nouta¹; Wilma E. Mesker¹; Yuri E.M. van der Burgt¹; Rob A.E.M. Tollenaar¹; Manfred Wuhrer¹; ¹Leiden University Medical Center, Leiden, Netherlands
- ThP 061 **Automatically Glycan Structural Determination with Logically Derived Sequence Tandem Mass Spectrometry;** Chi-kung Ni¹; Shih-Pei Huang¹; Chia Yen Liew¹; Hsu-Chen Hsu¹; ¹Academia Sinica, Taipei, Taiwan
- ThP 062 **Discrimination of Glycan Epimers via Generation of Unique Parent-Structure-Dependent Product Ions by Free Radical Chemistry and Mass Spectrometry;** Jinshan Gao¹; Kimberly Fabijanczuk¹; Kaylee Gaspar¹; Rayan Murtada¹; ¹Montclair State University, Montclair, NJ
- ThP 063 **Laser Induced Fluorescence Imaging of the Electropray for Quantitative N-Glycosylation Analysis of Monoclonal Antibodies by Capillary Electrophoresis – Mass Spectrometry;** Andras Guttman; Sciex, Brea, CA
- ThP 064 **A Multi-Dimensional HPLC-MS Method for Heparin/Heparan Sulfate Oligosaccharide Fraction;** Hao Liu¹; Apoorva Joshi²; Pradeep Chopra²; Geert-Jan Boons^{2,3}; Joshua S Sharp⁴; ¹University of Mississippi, Oxford, MS; ²University of Georgia, Athens, GA; ³Utrecht University, Utrecht, Netherlands; ⁴University of Mississippi, Oxford, MS
- ThP 065 **Structure Modeling of Isomeric Ions of Pyridinylboronic Esters of Momo-, Di- and Oligosaccharides from IMS Q-TOF and Tandem Mass Spectrometry;** Jun J Hu¹; Qidi Wu¹; Chengyi Xie¹; ¹Ningbo University, Ningbo, China
- ThP 066 **Development of a Multiplatform Mass Spectrometry-Based Workflow for the In-Depth Structural Elucidation of Oligosaccharides and Polysaccharides;** Juan J Castillo¹; Ace G Galermo²; Matthew J Amicucci³; Eshani Nandita³; Carlito B Lebrilla³; ¹University of Davis, Davis, CA; ²University of California, Davis, Davis, CA; ³UC Davis, Davis, CA
- ThP 067 **Detailed Glycosylation Analysis: Leukemic KG1a Cells as a Case Study Using Sequential Mass Spectrometry;** David Ashline¹; Vernon Reinhold¹; ¹University of New Hampshire, Durham, NH
- ThP 068 **Definitive Structural Assignment of Isomeric Glycans by Trapped Ion Mobility-Electronic Excitation Dissociation Tandem Mass Spectrometry;** Juan Wei¹; Yang Tang¹; Mark E. Ridgeway²; Pengyu Hong³; Catherine E. Costello¹; Cheng Lin¹; ¹Boston University, Boston, MA; ²Bruker Daltonics Inc., Billerica, MA; ³Brandeis University, Waltham, MA
- ThP 069 **Automated Identification and Quantitation of 2-AA Derivatized N-Glycans from Infliximab Using UHPLC-Orbitrap-MS Analysis with SimGlycan Software;** Ningombam Sanjib Meitei^{1,2}; Himani Gupta²; Arun Apte¹; Phil Widdowson³; Silvia Millán⁴; Sara Carillo⁴; Jonathan Bones⁴; Rowan Moore³; ¹PREMIER Biosoft, Palo Alto, CA; ²PREMIER Biosoft, Indore, India; ³Thermo Fisher Scientific, Hemel Hempstead, United Kingdom; ⁴National Institute for Bioprocessing Research and Training, Dublin, Ireland
- ThP 070 **Characterization of Glycan Isomers Using Magnetic Carbon Nanoparticles as a MALDI Co-Matrix;** Alireza Banazadeh¹; Mona Goli¹; Wenjing Peng¹; Reed Nieman¹; Hans Lischka¹; Yehia Mechref¹; ¹Texas Tech University, Lubbock, TX
- ThP 071 **Isomeric Linkage Determination of Sialic acid on O-Glycopeptides Using O-Protease and LC-MS/MS;** Jieqiang Zhong¹; Yifan Huang¹; Wenjing Peng¹; Yehia Mechref¹; ¹Texas Tech University, Lubbock
- ThP 072 **Deciphering Key Protein Binding Elements within Short- and Medium-Length Heparin Oligomers Using Multidimensional Chromatography Followed by MS Analysis;** Cedric Bobst¹; Igor A. Kaltashov¹; ¹University of Massachusetts Amherst, Amherst, MA
- ThP 073 **Analysis of the CHO-S Glycocalyx via Electrospray Ionization with Tandem Mass Spectrometry;** Amanda J Pearson¹; Elyssia S. Gallagher²; ¹Baylor University, Waco, TX; ²Baylor University, Waco
- ThP 074 **A Novel Approach Coupling Electrophoresis with Mass Spectrometry for Identification and Characterization of Multicomponent Glycosaminoglycan Drugs;** Anran Sheng¹; Xiaohui Xu¹; Lianli Chi¹; ¹Shandong university, Qingdao, China
- ThP 075 **Simultaneous Determination of 18 Monosaccharide Using High Performance Anion-Exchange Chromatography Coupled with Pulsed Amperometric Detection and Tandem Mass Spectrometry;** Feng Feng¹; Feng Zhang¹; ¹Institute of Food Safety, Chinese Academy of Inspection and Quarantine, Beijing, China
- ThP 076 **Precise Sequencing of Glycosaminoglycan Tetrasaccharides by Reversed Phase Ion Pairing LC/MS and MSn Spectra Matching;** Qing Guo¹; Vernon Reinhold¹; ¹University of New Hampshire, Durham, NH
- ThP 077 **LC-MS/MS Approach for the Exploration of Glycosylation as a Gatekeeper for Successful Xeno Transplantation;** Myung Jin Oh^{1,2}; Nari Seo^{1,2}; Jaekyoung Ko^{1,2}; Jinyoung Park^{1,2}; Xi-jun Yin³; Jjin-dan Kang³; Hyun Joo An^{1,2}; ¹Chungnam national university, Daejeon, South Korea; ²Asia-Pacific Glycomics Reference Site, Daejeon, South Korea; ³Yanbian University, Yanji, China
- ThP 078 **GlyLipSILC – Glycolipid Stable Isotope Labeling in Cell Cultures;** Andrew Cho¹; Wenjing Peng¹; Yifan Huang¹; Yehia Mechref¹; ¹Texas Tech University, Lubbock, TX
- ThP 079 **Investigation of Ganglioside Isomers to Reveal the Biological Mechanism of Breast Cancer Brain Metastasis Using Nano-ZIC-HILIC-LC-MS;** Yifan Huang¹; Jieqiang Zhong¹; Wenjing Peng¹; Yehia Mechref¹; ¹Texas Tech University, Lubbock, TX
- ThP 080 **Relative Quantification of Glycans in Yeast Using Metabolic Isotope Labeling with Isotopic Glucose by Mass Spectrometry;** Jae-min Lim¹; Ji-yeon Kim²; Soo-hyun Choi²; ¹Changwon National University, Changwon, South Korea; ²Changwon National University, Changwon, South Korea
- ThP 081 **Post-Column Chiral Addition Method for the Separation and Resolution of Common Monosaccharides;** Zachary Wooke¹; Gabe Nagy¹; Lauren Barnes¹; Matthew Laing¹; Nicola L. B. Pohl¹; ¹Indiana University Bloomington, Bloomington, IN
- ThP 082 **Multiplex Stable Isotope Dimethyl Labeling Coupled with MALDI-MS for Quantitative N-Glycomics;** He Zhu¹; Cheng Ma¹; Peng George Wang¹; ¹Georgia State University, Atlanta, GA
- ThP 083 **An Investigation of Ion Adduction for Enhancing Trisaccharide Isomer Separation and Collision Cross Section Identification through TWIMS Analysis;** Jessica Minnick¹; Eric D. Dodds¹; ¹University of Nebraska - Lincoln, Lincoln, NE
- ThP 084 **Separation and Identification of Sulfated Glycosaminoglycans in Urine using Capillary**

**Electrophoresis and Tandem Mass Spectrometry;**

Patience Sanderson¹; Xiaorui Han²; Fuming Zhang²; Robert Linhardt²; I. Jonathan Amster¹; ¹University of Georgia, Athens, GA; ²Rensselaer Polytechnic Institute, Troy, NY

- ThP 085 **A Method for the Rapid Determination of Polysaccharide Structures;** Eshani Nandita¹; Matthew J. Amicucci¹; Ace G. Galermo¹; Juan J. Castillo¹; Carlito B. Lebrilla¹; ¹UC Davis, Davis, CA

DATA-DEPENDENT ACQUISITION

086-092

- ThP 086 **Deep Quantitative Phosphoproteomics by Data Independent Acquisition Mass Spectrometry;** Reta Birhanu Kitata¹; Chia-Feng Tsai²; Pei-Yi Lin¹; Wai-Kok Choong³; Yun-Chien Chang¹; Bo-Shiun Chen^{1,4}; Alexey I. Nesvizhskii⁵; Ting-Yi Sung³; Yu-Ju Chen¹; ¹Institute of Chemistry, Academia Sinica, Taipei City, Taiwan; ²Pacific Northwest National Laboratory, Richland, WA; ³Institute of Information Science, Academia Sinica, Taipei City, Taiwan; ⁴Department of Chemistry, National Taiwan University, Taipei City, Taiwan; ⁵Department of Computational Medicine and Bioinformatics and Department of Pathology, Ann Arbor, Michigan
- ThP 087 **Machine Learning on SpectroMine Results Applied to an Efficient Large-Scale Library Generation Experiment;** Lynn Verbeke¹; Jan Muntel¹; Timothy Man¹; Tejas Gandhi¹; Aljaz Baumkircher¹; Oliver M. Bernhardt¹; Ian Lienert¹; Roland Bruderer¹; Lukas Reiter¹; ¹Biognosys AG, Schlieren, Switzerland
- ThP 088 **Identification of Off-Target Protein-Small Molecule Interactions Using Cellular Thermal Shift Assay (CETSA) and Phase-Constrained Spectrum Deconvolution (ΦSDM) MS Data Acquisition;** Clifford Phaneuf¹; Antonius Koller²; Konstantin Aizikov³; Dmitry Grinfeld³; Arne Kreutzmann³; Daniel Mourad³; Oliver Lange³; Alexander A Makarov³; Lili Guo¹; Harvey Lieberman¹; Aharon Cohen¹; Alexei Belenky¹; Alexander R Ivanov²; ¹Sanofi, Waltham, MA; ²Northeastern University, Boston, MA; ³Thermo Fisher Scientific, Bremen, Germany
- ThP 089 **Peptide Identification Improvement on a Trapped-Ion-Mobility quadrupole-Time-Of-Flight Mass Spectrometer (TIMS-QTOF) by Optimized Parallel Accumulation Serial Fragmentation (PASEF) Acquisition;** Markus Lubeck¹; Jens Decker¹; Andreas Germanus¹; Michael Krause¹; Stephanie Kaspar-Schoenfeld¹; Victor Fursey²; Oliver Raether¹; ¹Bruker Daltonik GmbH, Bremen, Germany; ²Bruker Daltonics Inc., Billerica, MA
- ThP 090 **Mapping Protein Interactions Using Data-Dependent Acquisition without Dynamic Exclusion;** Shen Zhang¹; Brett Larsen²; Cassandra Wong²; Anne-Claude Gingras²; ¹Lunenfeld-Tanenbaum Research Institute, Sinai Health System, Toronto; ²Lunenfeld-Tanenbaum Research Institute, Sinai Health System, Toronto, ON
- ThP 091 **Development of Screening Method for Targeted and Undiscovered Per- and polyfluoroalkyl Substances in Surface Water on Q-TOF Mass Spectrometer;** Jun Xiang Lee¹; Jie Xing¹; Shiau Hang Tee²; Timothy Yan Ann Lim³; Zhaoqi Zhan¹; ¹Shimadzu Asia Pacific, Singapore, Singapore; ²School of Physical and Mathematical Sciences, Nanyang Technological University, 21 Nanyang Link SPMS-04-01, Singapore 627371, Singapore, Singapore; ³National University of Singapore, Singapore, Singapore
- ThP 092 **Mass Fractionation in the Survey Data Improve Protein Identification in Data Dependents Acquisition for Complex Proteome Samples;** Faraz Rashid¹; Dipankar Malakar¹; Nirpendra Singh²; Manoj Pillai¹; ¹SCIEX, Gurgaon, India; ²Advanced Technology Platform Centre, RCB, Faridabad, India

DATA-INDEPENDENT ACQUISITION

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- ThP 093 **Quantitative Proteomic and Phosphoproteomic Elucidation of Cancer Aneuploidy;** Alison M. Taylor¹; Wenxue Li²; Sejal Jain¹; Matthew Meyerson¹; Yansheng Liu^{2,3}; ¹Department of Medical Oncology, Dana-Farber Cancer Institute, Boston, MA; ²Yale Cancer Biology Institute, West Haven, CT; ³Department of Pharmacology, Yale University School of Medicine, New Haven, CT
- ThP 094 **Ultra-High Resolution 2D-FTMS for Truly DIA Analysis of Challenging Systems;** Christopher Andrew Wootton¹; Tomos E. Morgan¹; Bryan P. Marzullo¹; Yuko P. Y. Lam¹; Diana C. Palacio Lozano¹; Alina Theisen¹; Anisha Haris¹; Mark P. Barrow¹; Peter B. O'Connor¹; ¹University of Warwick, Coventry, United Kingdom
- ThP 095 **Low ppm Detection of Host Cell Proteins (HCPs) in Biopharmaceuticals with Optimised Orbitrap-Based UHPLC HRAM MS;** Amy J Claydon¹; Tom Buchanan¹; Philip J. Widdowson¹; Janusz Debski¹; Andrew Williamson²; Rowan Moore²; ¹Thermo Fisher Scientific, Runcorn, United Kingdom; ²Thermo Fisher Scientific, Hemel Hempstead, United Kingdom
- ThP 096 **Accelerating DIA Studies to Extend Workflow Utility, Using Ultra-Fast Microflow LC Gradients;** Christie Hunter¹; Nick Morrice²; Zuzana Demianova³; ¹SCIEX, Redwood City, CA; ²SCIEX, Warrington, United Kingdom; ³SCIEX, Darmstadt, Germany
- ThP 097 **SWATH-MS for Quantification of Mass Isotopologue Distribution of Cellular Metabolites and Fragments Labeled with Isotopic ¹³C Carbon in Cyanobacteria;** Damini Jaiswal¹; Charulata B Prasannan^{1,2,3}; John I Hendry¹; Pramod P Wangikar^{1,2,3}; ¹Department of Chemical Engineering, Indian Institute of Technology Bombay, Mumbai, India; ²DBT-Pan IIT Center for Bioenergy, Indian Institute of Technology Bombay, Mumbai, India; ³Wadhvani Research Center for Bioengineering, Indian Institute of Technology Bombay, Mumbai, India
- ThP 098 **Designing Data Independent Acquisition Methods for Orbitrap Instruments;** Léon Reubsæet^{1,2}; Michael Sweredoski²; Annie Moradian²; Spiros D Garbis²; ¹Department of Pharmaceutical Chemistry, School of Pharmacy, University of Oslo, Oslo, Norway; ²California Institute of Technology, Pasadena, CA
- ThP 099 **Rapid Proteome Analysis with Data-Independent Acquisition and Super-Resolution Orbitrap Mass Spectrometry;** Florian Meier¹; Arne Kreutzmann²; Daniel Mourad²; Konstantin Aizikov²; Dmitry Grinfeld²; André C Michaelis¹; Oliver Lange²; Alexander A Makarov²; Matthias Mann^{1,3}; ¹Max Planck Institute of Biochemistry, Martinsried, Germany; ²Thermo Fisher Scientific, Bremen, Germany; ³NNF Center for Protein Research University of Copenhagen, Copenhagen, Denmark
- ThP 100 **Assessment of Type 2 Diabetes Based upon Quantification of Plasma Proteomes;** Zhilong Lin^{1,2}; Guixue Hou^{1,2}; Siqi Li^{1,2}; Rongli Zhao^{1,2}; Huanzi Zhong^{1,2}; Fangming Yang^{1,2}; Huanming Yang^{1,3}; Siqi Liu^{1,2}; Yan Ren^{1,2}; ¹BGI-Shenzhen, Shenzhen, China; ²China National GeneBank, Shenzhen, China; ³James D. Watson Institute of Genome Sciences, Hangzhou, China
- ThP 101 **Identification and Quantification of Host Cell Proteins in Recombinant Therapeutic Proteins Using Data-Independent Acquisition Mass Spectrometry;** Hongbin Zhu¹; David Keire¹; Hongping Ye¹; ¹FDA, St. Louis, MO
- ThP 102 **Cysteine-DIA – the Use of Cysteine-Containing Peptides to Increase the Protein Coverage in DIA;** Muhammad Tahir¹; Arkadiusz Nawrocki¹; Martin Røssel Larsen¹; ¹Department of Biochemistry and Molecular Biology, University of Southern Denmark, Odense, Denmark



- ThP 103 **Effect of Aerobic Exercise on PBMC Protein Profile in Insulin Resistant (IR) and Insulin Sensitive (IS) Participants**; Kevin Paul Erazo Castillo¹; Sara Ahadi¹; Kevin Contrepois¹; Fredrik Edfors¹; Daniel Hornburg¹; Si Wu¹; Francois Haddad¹; Michael Snyder¹; ¹Stanford University, Stanford, CA
- ThP 104 **Characterization of the Insolubome in Aging and Age-related Diseases Using Mass Spectrometry with Data-Independent Acquisitions (DIA/SWATH)**; Xueshu Xie¹; Manish Chamoli¹; Dipa Bhaumik¹; Kathleen Dumas¹; Renuka Sivapatham¹; Suzanne Angeli¹; Anja Holtz¹; Julie Andersen¹; Birgit Schilling¹; Gordon J. Lithgow¹; ¹Buck Institute, Novato, CA
- ThP 105 **Elucidation of Organic Micropollutants Biodegradation Using Data-Independent Acquisition as Part of a Drinking Water Filter Process**; Morgan Solliec¹; Veronika Storck¹; Benoit Barbeau¹; ¹Polytechnique Montréal, Montréal, QC
- ThP 106 **Relative Quantitation of Aqueous Humor Proteins in a Juvenile Rabbit Model of Lensectomy Using Data Dependent and Data Independent Acquisition**; Theodore R. Keppel¹; Jonathon B. Young¹; Christine M.B. Skumatz¹; Alexander E. Salmon¹; Rebekah L. Gundry¹; Iris S. Kassem¹; ¹Medical College of Wisconsin, Milwaukee, WI
- ThP 107 **Employing Scanning SWATH to Support High Flow Proteomics Sample Acquisition**; Nic Bloomfield¹; Gordana Ivosev¹; Fras Wasim¹; Stephen Tate¹; Christoph B Messner²; Vadim Demichev²; Spyros Vernardis²; ¹SCIEX, Concord, ON; ²The Francis Crick Institute, London, United Kingdom
- ThP 108 **HLA-DO / H2-O Modulates the Diversity of the MHC class II Self Peptide Repertoire**; Padma P. Nanaware¹; Mollie M Jurewicz¹; John D Leszyk¹; Scott A Shaffer¹; Lawrence Stern¹; ¹University of Massachusetts Medical School, Worcester, MA
- ThP 109 **Targeted Detection of Enzyme Active-site Peptides via Data-Independent Selective Infrared Multiphoton Dissociation Liquid Chromatography/Mass Spectrometry**; Nicholas Borotto¹; Melanie Cheung-See-Kit¹; Chunyi Zhao²; Andrew H. Lowell¹; Jennifer Schmidt¹; Kinshuk Srivastava³; Brandon T. Ruotolo⁴; David H. Sherman¹; Brent R Martin⁴; Kristina Hakansson¹; ¹University of Michigan, Ann Arbor, MI; ²University of Michigan, Ann Arbor, Michigan; ³University of Michigan, Ann Arbor, MI; ⁴University of Michigan, Ann Arbor, MI
- ThP 110 **Use of DIA SWATH to Determine the Operational Envelope of a Synthetic Gene Circuit in Vibrio Natriegens**; Mary Ashley Rimmer¹; W Judson Hervey, Iv²; Dagmar H Leary²; Robert G Egbert³; Enoch Yeung⁴; Gary J Vora²; ¹NRC Post-doctoral Fellow, US Naval Research Laboratory, Washington, D.C.; ²Center for Bio/Molecular Science & Engineering, US Naval Research Laboratory, Washington, D.C.; ³Pacific Northwest National Laboratory, Richland, WA; ⁴University of Santa Barbara, Santa Barbara, CA
- ThP 111 **Fiber Supplements Induce Protein Variation on a Diverse Cohort: A Pilot Study**; Jennifer Quijada¹; Samuel M. Lancaster¹; Brittany Ann Lee¹; Daniel Hornburg¹; Sara Ahadi¹; Si Wu¹; Michael Snyder¹; ¹Stanford University School of Medicine, Stanford, CA, 94305
- ThP 112 **Capillary Electrophoresis-Mass Spectrometry-Based Identification of Unique Metabolic Profiles in Neurodegenerative Clinical Samples**; Kaylie I Kirkwood¹; Tharani Sabaretnam²; Gilles J Guillemain²; David C Muddiman¹; ¹North Carolina State University, Raleigh, NC; ²Macquarie University, Sydney, NSW, Australia
- ThP 113 **Identification of Candidate Biomarkers for Early Prediction of Prostate Cancer Progression Using Targeted Proteomics on Organ-confined Primary Tumors**; Yuqian Gao¹; Yi-Ting Wang¹; Hui Wang¹; Denise Young²; Yongmei Chen²; Yingjie Song²; Athena A. Schepmoes¹; Thomas L. Fillmore¹; Tujin Shi¹; Wei-Jun Qian¹; Richard D. Smith¹; Sudhir Srivastava³; Jacob Kagan³; Albert Dobi²; Inger L. Rosner²; Isabell A. Sesterhenn⁴; Shiv Srivastava²; Gyorgy Petrovics²; Karin D. Rodland¹; Jennifer Cullen²; Tao Liu¹; ¹Pacific Northwest National Laboratory, Richland, WA; ²Walter Reed National Military Medical Center, Bethesda, MD; ³National Cancer Institute, Bethesda, MD; ⁴Joint Pathology Center, Silver Spring, MD
- ThP 114 **Early Detection Hepatocellular carcinoma via MRM-MS with a Serum Protein-based Multi-marker panel: A Large-Scale Multicenter study**; Injoon Yeo¹; Hyunsoo Kim^{2,3,4}; Ji Hyeon Lee⁵; Young-Suk Lim^{6,7}; Youngsoo Kim^{2,5,8}; ¹Departments of Biomedical Engineering, Seoul National University College of Medicine, Seoul, South Korea; ²Departments of Biomedical Engineering, Seoul National University College of Medicine, Jongro-gu, South Korea; ³Department of Biomedical Sciences, Seoul National University College of Medicine, Seoul, South Korea; ⁴Institute of Medical and Biological Engineering, Medical Research Center, Seoul National University College of Medicine, Seoul, South Korea; ⁵Department of Biomedical Sciences, Seoul National University College of Medicine, Jongro-gu, South Korea; ⁶Department of Gastroenterology, University of Ulsan College of Medicine, Seoul, South Korea; ⁷Liver center, Asan Medical Center, Seoul, South Korea; ⁸Institute of Medical and Biological Engineering, Medical Research Center, Seoul National University College of Medicine, Jongro-gu, South Korea
- ThP 115 **LESA Sampling of Human Non-Alcoholic Fatty Liver Disease Tissue for the Profiling of Liver Fatty Acid Binding Protein**; James W Hughes¹; Iain B Styles¹; Patricia F Lalor¹; Helen J Cooper¹; ¹University of Birmingham, Birmingham, United Kingdom
- ThP 116 **Top-Down Mass Spectrometry of Appendix Derived Synuclein Proteoforms and Their Role in Parkinson Disease**; Bryan A Killinger¹; Zachary Madaj¹; Jacek W. Sikora²; Nolwen Rey^{1,3}; Alec J Haas¹; Yamini Vepa¹; Daniel Lindqvist^{4,5}; Honglei Chen⁶; Paul M Thomas²; Patrik Brudin¹; Lena Brudin¹; Neil L Kelleher²; Viviane Labrie^{1,7}; ¹Center for Neurodegenerative Science, Van Andel Research Institute, Grand Rapids, Michigan; ²Proteomics Center of Excellence, Northwestern University, Chicago, ILLINOIS; ³Paris-Saclay Institute of Neuroscience, Centre National de la Recherche Scientifique, Gif-sur-Yvette, France; ⁴Department of Clinical Sciences, Psychiatry, Faculty of Medicine, Lund University, Lund, Sweden; ⁵Psychiatric Clinic, Lund, Division of Psychiatry, Lund, Sweden; ⁶Department of Epidemiology and Biostatistics, College of Human Medicine, Michigan State University, East Lansing, Michigan; ⁷Centre for Addiction and Mental Health, Toronto, Ontario
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- ThP 196 **Rapid Evaporative Ionisation Mass Spectrometry for Detecting Compounds Related to Consumer Liking of Grilled Lamb**; Alastair Ross¹; Paul Middlewood¹; Stefan Clerens¹; Patricia L Johnson²; Patrick Silcock³; Graham T Eyres³; Carolina E Realini⁴; ¹*AgResearch Ltd, Lincoln, New Zealand*; ²*AgResearch Ltd, Invermay, New Zealand*; ³*University of Otago, Dunedin, New Zealand*; ⁴*AgResearch Ltd, Palmerston North, New Zealand*
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- ThP 199 **Combining Sensory and Chemical Analyses (GC-MS) to Evaluate Shelf Stability Related to Storage Condition for an American IPA Beer**; Joseph E Binkley¹; Elizabeth Humston-Fulmer²; Lorne Fell²; ¹*LECO Corporation, St. Joseph, MI*; ²*LECO Corporation, St. Joseph, MI*
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- Gutiérrez¹; Nikolas Kessler²; Heiko Neuweget²; Cory Lytle³; José María Olmo-Peinado⁴; Carsten Baessmann²; Alegría Carrasco-Pancorbo¹; ¹*Department of Analytical Chemistry, Faculty of Science, University of Granada, Granada, Spain*; ²*Bruker Daltonik GmbH, Bremen, Germany*; ³*Bruker Daltonics Inc., Billerica, MA*; ⁴*Acer Campestris S.L. Almendro, Jaén, Spain*
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- ThP 210 **Glycoproteomic Analysis of Cells Containing Unnatural Monosaccharides**; Yixuan (Axe) Xie¹; Ying Sheng¹; Qiongyu Li¹; Maurice Wong¹; Qingwen (Dave) Zhou¹; Carlito B. Lebrilla¹; ¹*University of California, Davis, Davis, CA*
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- ThP 213 **Confident and Efficient Characterization of Recombinant Human Follicle Stimulating Hormone with the Thermo Scientific Q Exactive HF-X BioPharma Platform**; Xiaoxi Zhang¹; Philip J. Widdowson²; Rowan Moore²; ¹*ThermoFisher Scientific, Shanghai, China*; ²*Thermo Fisher Scientific, Hemel Hempstead, UK, Hemel Hempstead, United Kingdom*
- ThP 214 **MS-Based Workflow for the Characterization of Glyco-Engineered Therapeutic Glycoproteins with Oligo/Poly-Sialic Acids in Bacteria**; Chia-wei Lin¹; Hanne L.P. Tytgat²; Timothy G. Keys²; Markus Aebi²; ¹*Functional Genomic Center Zürich, Zurich, Switzerland*; ²*Institute of Microbiology, ETHZ, Zurich, Switzerland*
- ThP 215 **Identification of N-Glycopeptides with MetaMorpheus**; Lei Lu¹; Michael R Shortreed¹; Robert J Millikin¹; Mark Scalf¹; Lloyd M Smith¹; ¹*University of Wisconsin-Madison, Madison, WI*
- ThP 216 **N-Glycan Sub-Type as a Pathogenic Factor in Influenza**; Lisa Parsons¹; John F. Cipollo¹; Yanming An¹; Li Qi²; Jeffery K. Taubenberger²; Kevan Hartshon³; Mitchell White³; ¹*FDA, Silver Spring, MD*; ²*NIH/NIAD, Bethesda, MD*; ³*Boston University School of Medicine, Boston, MA*
- ThP 217 **Construction of a Structure and Site Specific Glycopeptide Transition Library for Glycopeptide Quantitation by DIA/SWATH**; Miloslav Sanda¹; Nathan J Edwards²; Julius Benicky¹; Zuzana Brnakova Kenedy¹; Radoslav Goldman^{1,2}; ¹*Georgetown University, Lombardi Cancer Center, Washington, DC*; ²*Georgetown University, Department of Biochemistry and Molecular & Cellular Biology, Washington, DC*
- ThP 218 **High-Throughput and Site-Specific N-Glycosylation Analysis of Human Alpha-1-Acid Glycoprotein**; Toma Keser¹; Gordan Lauc^{1,2}; Mislav Novokmet²; ¹*Faculty of pharmacy and biochemistry, University of Zagreb, Zagreb, Croatia*; ²*Genos, Glycoscience Laboratory, Borongajska cesta 83h, Zagreb, Croatia*
- ThP 219 **Mass Spectrometric Elucidation of Global Glycosylation Profile on a Fungal Vaccine Adjuvant BL-ENG2**; Junfeng Huang¹; Lucas dos Santos Dias²; Marcel Wüthrich²; Lingjun Li^{1,3}; ¹*School of Pharmacy, University of Wisconsin-Madison, Madison, WI*; ²*Department of Pediatrics, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI*; ³*Department of Chemistry, University of Wisconsin-Madison, Madison, WI*
- ThP 220 **Effects of In-Source Supercharging and Subcharging for Glycopeptide Analysis in a Trapped Ion Mobility Quadrupole Time-of-Flight Mass Spectrometer**; Kristina Marx¹; Hans J.C.T. Wessels²; Pierre-Olivier Schmitz³; Alain J. Van Gool²; Dirk J. Lefeber²; ¹*Bruker Daltonik GmbH, Bremen, Germany*; ²*Translational Metabolic Laboratory, Department of Laboratory medicine, Radboudumc, Nijmegen, Netherlands*; ³*Bruker Daltonique S.A, Wissembourg, France*
- ThP 221 **Analysis of N- and O-Glycosylation on a Highly Glycosylated Protein Highlights Potential Sources of Error When Sequencing Intact Glycopeptide Spectra**; Gary Wilson¹; Miyoshi Haruta^{2,3}; Alexander Hebert¹; Michael S Westphall¹; Michael Sussman^{2,3}; Joshua Coon^{1,3,4,5}; ¹*Department of Chemistry, University of Wisconsin, Madison, WI*; ²*Department of Biochemistry, University of Wisconsin, Madison, WI*; ³*Genome Center of Wisconsin, Madison, WI*; ⁴*Morgridge Institute for Research, Madison, WI*; ⁵*Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI*
- ThP 222 **GlyProSILC: Glycan/Protein Stable Isotope Labeling in Cell Cultures Approach for Concurrent Glycomics/Proteomics/Glycoproteomics Analysis**; Wenjing Peng¹; Jingfu Zhao²; Mona Goli²; Yehia Mechref²; ¹*Texas Tech University, Lubbock, TX*; ²*Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, Texas*
- ThP 223 **LC-MS/MS Characterization of Isomeric Glycopeptides Using Extra-long C18 Column**; Aiyi Yu¹; Yifan Huang¹; Jingfu Zhao¹; Xue Dong¹; Yehia Mechref¹; ¹*Texas Tech University, Lubbock, TX*
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Lin¹; Rachel R. Ogorzalek Loo²; Joseph A Loo²; Robert P. Gunsalus²; Catherine E. Costello¹; ¹Boston University School of Medicine, Boston, MA; ²University of California LA, Los Angeles, CA

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- ThP 226 **DESI-IMS Revealed the Association of Linoleic Acid, Oleic Acid and Arachidonic Acid in the Rupture of Cerebral Aneurysm**; Ariful Islam¹; Ririko Takeda²; Tomohito Sato¹; Hiroki Kurita³; A s m Waliullah¹; Md. Al Mamun¹; Makoto Horikawa^{1,4}; Mitsutoshi Setou^{1,4}; ¹Department of Cellular and Molecular Anatomy, Hamamatsu University School of Medicine, Hamamatsu, Japan; ²Department of Neurosurgery, Mizonokuchi Hospital, Teikyo University School of Medicine, Kanagawa, Japan, Kawasaki, Japan; ³Department of Cerebrovascular Surgery, Saitama Medical University International Medical Center, Hidaka, Saitama, Japan, Hidaka, Japan; ⁴International Mass Imaging Center, Hamamatsu University School of Medicine, Hamamatsu, Japan
- ThP 227 **Multimodal MALDI IMS to Visualize Staphylococcal Molecular Adaptation within the Infectious Microenvironment**; William J Perry^{1,2,3}; Jeffrey M. Spraggins^{1,2,4}; Caroline M. Grunenwald^{3,5}; Jessica R Sheldon^{3,5}; Eric P. Skaar^{3,5}; Richard M. Caprioli^{1,2,4,6,7}; ¹Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; ²Department of Chemistry, Vanderbilt University, Nashville, TN; ³Vanderbilt Institute for Infection, Immunology, and Inflammation, Vanderbilt University Medical Center, Nashville, TN; ⁴Department of Biochemistry, Vanderbilt University, Nashville, TN; ⁵Department of Pathology, Microbiology and Immunology, Vanderbilt University School of Medicine, Nashville, TN; ⁶Department of Pharmacology, Vanderbilt University, Nashville, TN; ⁷Department of Medicine, Vanderbilt University, Nashville, TN
- ThP 228 **MALDI Imaging to Characterise the Lipid Signature of Clinical Prostate Tumours**; Shadrack M Mutuku^{1,2}; Paul J Trim³; Xander Spotbeen^{2,4}; Johan O R Gustafsson⁵; Jessica M Logan⁶; Alexandra Sorvina⁶; Margaret M Centenera^{1,2}; Johannes V Swinnen⁴; Marten F Snel⁵; Lisa M Butler^{1,2}; ¹Adelaide Medical School, The University of Adelaide, Adelaide, Australia; ²Prostate Cancer Research Group, South Australian Health and Medical Research Institute (SAHMRI), Adelaide, Australia; ³Mass Spectrometry Core Facility, South Australian Health and Medical Research Institute (SAHMRI), Adelaide, Australia; ⁴Laboratory of Lipid Metabolism and Cancer, Department of Oncology, LKI-Leuven Cancer Institute, KU Leuven – University of Leuven, Leuven, Belgium; ⁵ARC CoE in Convergent Bio-Nano Science & Technology, Future Industries Institute, University of South Australia, Adelaide, Australia; ⁶Mechanisms in Cell Biology and Disease Research Group, Cancer Research Institute, University of South Australia, Adelaide, Australia
- ThP 229 **Classification and Identification of Lipid Biomarkers for the Prediction of Melanoma**; Jone Garate¹; Roberto Fernandez²; Lucia Martin-Saiz²; Arantza Perez-Valle²; Sergio Lage²; Veronica Velasco³; Aintzane Asumendi^{2,3}; Jesus Gardeazabal³; Juan Luis Artola³; Ignacio Zabalza⁴; Rosa Marti-Laborda⁵; Begoña Ochoa²; Maria Dolores Boyano^{2,3}; Jose Andres Fernandez²; ¹University of Basque Country, Leioa, Spain; ²University of Basque Country, Leioa, Spain; ³Cruces University Hospital, Leioa, Spain; ⁴Galdakao-Usansolo Hospital, Galdakao, Spain; ⁵Hospital Universitari Arnau de Vilanova, Lleida, Spain
- ThP 230 **Mass Spectrometry Imaging Identifies Altered Lipid Metabolites in the Mouse Testis in Mice Lacking Liver-X Receptors**; Sheba Jarvis¹; Mark Towers²; Charlotte Bevan¹; Emmanuelle Claude²; ¹Imperial College London, Hammersmith Hospital, London, United Kingdom; ²Waters Corporation, Wilmslow, United Kingdom
- ThP 231 **Tissue Mass Spectrometry Imaging: Profiling of Secondary Human Lymphoid Organs**; Constantinos Petrovas¹; Cristina Silvescu²; Shannon Cornett²; Giulia Fabozzi¹; Frank Arnold³; Paula Lei³; ¹Tissue Analysis Core, VRC, NIAID, NIH, Bethesda, MD; ²Bruker Daltonics Inc., Billerica, MA; ³Vaccine Production Program, VRC, NIAID, NIH, Gaithersburg, MD
- ThP 232 **Identification of Therapeutic Targets of Multiple Sclerosis through MALDI - Imaging Mass Spectrometry of Experimental Autoimmune Encephalomyelitis (EAE) Mouse Model**; Nami Tanaka¹; Hiroki Yamashita¹; Takashi Nirasawa²; Ryo Kajita²; Katsutoshi Taguchi³; Masaki Tanaka³; Takayuki Kondo⁴; Yudai Tsuji¹; Nobuto Kakuda¹; Masaya Ikegawa¹; ¹Doshisha University, Kyoto, Japan; ²Bruker Japan K.K., Yokohama, Japan; ³Department of Anatomy and Neurobiology, Graduate School of Medical Science, Kyoto Prefectural University of Medicine, Kyoto-city, Japan; ⁴Kansai Medical University Medical Center, Hirakata, Japan
- ThP 233 **Nanomanipulation-Coupled MALDI Imaging Mass Spectrometry for Single Organelle Analysis to Measure Metabolic Changes responding to Oxidative Stress in Neuroblastoma Cells**; Imesha W. De Silva¹; R. Scott Duncan²; Peter Koulen²; Guido F. Verbeck¹; ¹University of North Texas, Denton, TX; ²Vision Research Center, Department of Ophthalmology, School of Medicine, University of Missouri-Kansas City, Kansas City, MO
- ThP 234 **Analysis of Liver Transplant Biopsies for Biomarkers of Transplant Rejection**; Michelle Reyzer¹; Audra M. Judd¹; Jennifer L. Harvey¹; Bryna E. Burell²; Drew Lesniak²; Anthony Demetrius²; Richard M. Caprioli¹; ¹Vanderbilt University, Nashville, TN; ²Immune Tolerance Network, Seattle, WA
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- ThP 236 **MALDI-MSI Approaches for Visualizing Lipid Markers of Alzheimer's Disease**; Matthias Holzlechner¹; Daniela D'Amico¹; Maribel Donoso Rivera¹; Eliseo Eugenin¹; Brendan Prideaux¹; ¹University of Texas Medical Branch, Galveston, TX
- ThP 237 **Identification of Novel Aldosterone Derivatives on Adrenal Sections of Primary Aldosteronism Patients**; Yuki Sugiura; Keio University, Tokyo, Japan
- ThP 238 **Dissecting Pathogenesis of Dilated Cardiomyopathy (DCM) on J2N-k Hamster Model Using MALDI-Imaging Mass Spectrometry in Combination with Shotgun Proteomics**; Inori Shintani¹; Takashi Tsuji²; Mizuki Ishida³; Takashi Nirasawa⁴; Ryo Kajita⁴; Hatsue Ishibashi-Ueda⁵; Hidetoshi Masumoto²; Kenji Minatoya²; Masaya Ikegawa³; ¹Doshisha university, Kyotanabe City, Japan; ²Kyoto University, Kyoto, Japan; ³Doshisha University, Kyotanabe city, Kyoto, Japan; ⁴Bruker Japan K. K., Yokohama, Japan; ⁵National Cerebral and Cardiovascular Center Research Institute, Suita, Japan
- ThP 239 **Comprehensive Quantitative Lipidomic Analysis of Mouse Hearts Using AP-SMALDI Mass Spectrometry Imaging and LC-MS/MS**; Vannuruswamy Garikapati^{1,2}; Claudia Colasante²; Eveline Baumgart-Vogt²; Bernhard



- Spengler¹; ¹*Institute of Inorganic and Analytical Chemistry, Justus Liebig University Giessen, Giessen, Germany*; ²*Institute for Anatomy and Cell Biology II, Division of Medical Cell Biology, Justus Liebig University Giessen, Giessen, Germany*
- ThP 240 **3D-Surface AP-SMALDI MS Imaging Reveals Tegument-Specific Lipid Compositions in Human Pathogen *Schistosoma mansoni***; Patrik Kadesch¹; Thomas Quack²; Stefanie Gerbig¹; Christoph G. Grevelding²; Bernhard Spengler¹; ¹*Institute of Inorganic and Analytical Chemistry, Justus Liebig University Giessen, Giessen, Germany*; ²*Institute of Parasitology, Giessen, Germany*
- ThP 241 **Analysis of Malaria-causing Plasmodia Infected Hepatocytes in Mouse Liver via Spatially Targeted Imaging Mass Spectrometry**; Michael D. Tuck¹; Michelle L. Reyzer¹; Nathan Heath Patterson¹; David M. Anderson¹; Elizabeth Glennon²; Adam Lewis²; Alexis Kaushansky²; Richard M. Caprioli¹; ¹*Vanderbilt Mass Spectrometry Research Center and Department of Biochemistry, Nashville, TN*; ²*Center for Infectious Disease Research, Seattle, Washington*
- ThP 242 **Multi-Modal Imaging Visualizes HIV-Mediated Cardiac Damage**; Matthias Holzlechner¹; Eliseo Eugenin¹; Brendan Prideaux¹; ¹*The University of Texas Medical Branch (UTMB), Galveston, TX*
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- ThP 244 **Non-destructive Tissue Lipids Profiling and Imaging Using Tip-Contact Sampling/Ionization Mass Spectrometry**; Xiaoming Chen¹; Jianmin Wu¹; ¹*Zhejiang University, Hangzhou, China*
- ThP 245 **Combining MALDI Imaging and Liquid Extraction Surface Analysis for Spatial Metabolomics**; Jeremy Wolff¹; Alain Creissen²; Matt Orcutt²; Jan H. Kobarg³; Shannon Cornett¹; ¹*Bruker Daltonics Inc., Billerica, MA*; ²*HTX Technologies, Chapel Hill, NC*; ³*Bruker Daltonik GmbH, Bremen, Germany*
- ThP 246 **Impact of the DIUTHAME for Distribution Analysis of Metabolites on Biological Tissues by DESI-MSI**; Daisuke Saigusa¹; Masahiro Kotani²; Takayuki Ohmura²; ¹*Tohoku University, Sendai, Japan*; ²*Hamamatsu Photonics, Iwata, Japan*
- ThP 247 **Automated Mass Spectrometry Imaging of over 2,000 Proteins from Tissue Sections at 100- μ m Spatial Resolution**; Paul D. Piehowski¹; Ying Zhu¹; Lisa M. Bramer¹; Kelly G. Stratton¹; Rui Zhao¹; Daniel J. Orton¹; Ronald J. Moore¹; Jia Yuan²; Hugh D. Mitchell¹; Yuqian Gao¹; Bobbie-jo M. Webb-robertson¹; Sudhansu K. Dey²; Ryan T. Kelly^{1,3}; Richard D. Smith¹; ¹*Kristin E Burnum-Johnson*; ¹*Pacific Northwest National Laboratory, Richland, WA*; ²*Cincinnati Children's Hospital, Cincinnati, OH*; ³*Brigham Young University, Provo, UT*
- ThP 248 **Dual Polarity IMS of Phospholipids from Whole-body *Drosophila* Tissue Sections**; Ethan Yang¹; Chiara Gamberi²; Pierre Chaurand¹; ¹*University of Montreal, Montreal, QC*; ²*Concordia University, Montreal, Qc*
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- ThP 250 **MALDI Mass Spectrometry Imaging Reveals Distinct Spatio-Molecular Lipid Distributions in Mouse Lungs**; Caitlin M. Tressler¹; Cristina Silvescu²; Shannon Cornett²; Kanchan Sonkar¹; Ruoqing Cai¹; Vinay Ayyappan¹; Oluwatobi Adelaja¹; Kristine Glunde¹; ¹*Johns Hopkins University School of Medicine, Baltimore, MD*; ²*Bruker Daltonics Inc., Billerica, MA*
- ThP 251 **Desorption Electrospray Ionization (DESI) and Dielectric Barrier Discharge (DBD) Ionization Mass Spectrometry Imaging of Lipid Metabolism in Alzheimer's Disease**; Isabella James¹; John C Price¹; Paul B Farnsworth¹; Mercedes N Erickson¹; ¹*Brigham Young University, Provo, UT*
- ThP 252 **MALDI Imaging of Eucalyptus Leaves from Rust Resistant and Susceptible Genotypes**; Thais Regiani Cataldi¹; Ilara Gabriela Frasson Budzinski²; Andressa Peres Bini²; Mônica Teresa Veneziano Labate²; Carlos Alberto Labate²; ¹*ESALQ, Piracicaba, Brazil*; ²*ESALQ, Piracicaba, Brazil*
- ThP 253 **Single-Filament Imaging Mass Spectrometry-based Lipidomics in *Arthrospira platensis***; Lieve M. Laurens¹; Peter V. Shanta¹; Steven M Rowland¹; ¹*National Renewable Energy Laboratory, Golden, CO*
- ThP 254 **DESI-MS Imaging and the World of Extractables and Leachables on Glass Screens: Looking for Residue that Shouldn't Even Be There**; Samuel Merenbloom¹; Wanda J Walczak²; ¹*Corning Incorporated, Painted Post, 14870*; ²*Corning Incorporated, Painted Post, New York*
- ThP 255 **Novel Tissue Washing Procedure for the Removal of Cation Adducts Prior to Selective Cation Formation for DESI and MALDI Imaging**; Mark Towers¹; Lisa Reid¹; Emmanuelle Claude¹; ¹*Waters Corporation, Wilmslow, United Kingdom*
- ThP 256 **A Multimodal Approach Using DESI-MSI and Laser Capture Microdissection for Single Tissue Section Analysis**; Emine Kazanc¹; Evdokia Karali²; Vincen Wu¹; James Mckenzie¹; Olof Isberg¹; Andreas Dannhorn¹; Paolo Inglese¹; Sadaf Ghaem-Maghmi³; George Poulgiannis²; Zoltan Takats¹; ¹*Imperial College London, Department of Surgery and Cancer, United Kingdom*; ²*Institute of Cancer Research, Division of Cancer Biology, United Kingdom*; ³*Imperial College London, Hammersmith Hospital, London, United Kingdom*
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- ThP 258 **Three-Dimensional (3D) Imaging with Infrared Matrix-Assisted Laser Desorption Electrospray Ionization (IR-MALDESI) Mass Spectrometry**; Hongxia Bai¹; Sitora Khodjanizayova¹; Therese M. Robinson¹; Kenneth P. Garrard^{1,2}; David C Muddiman^{1,3}; ¹*North Carolina State University, Raleigh, NC*; ²*Precision Engineering Consortium, North Carolina State University, Raleigh, NC*; ³*Molecular Education, Technology, and Research Innovation Center (METRIC), North Carolina State University, Raleigh, NC*
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ThP 422 **On-Target Recrystallization of 2,5-Dihydroxybenzoic Acid Using Acetonitrile Droplet as an Enhancement of Surface Homogeneity for MALDI-MS Dried-Droplet Sample Preparation**; Huu-Quang Nguyen¹; Dabin Lee¹; Yeoseon Kim¹; Min Sun Kim²; Kyoung-Soon Jang³; Jeongkwon Kim¹; ¹Chungnam National University, Daejeon, South Korea; ²Scientific Instruments Reliability Assessment Center, Korea Basic Science Institute, Daejeon, South Korea; ³Biomedical Omics Center, Korea Basic Science Institute, Daejeon, South Korea
 ThP 423 **High-Speed Characterization of Candle Waxes Using Surface-Assisted Laser Desorption/Ionization Mass Spectrometry (SALDI-MS) with Etched Silver Foil as Substrates**; Andreas Schnapp¹; Ann-Christin Niehoff¹; ¹Shimadzu Europa GmbH, Duisburg, Germany
 ThP 424 **Nanodiamond Assisted MALDI-MS Analysis of High Mass Proteins in the Nanomolar Concentration Range**; Avinash Adhikrao Patil¹; Mhikee Janella N. Descanzo¹; Chen-Hao Wen¹; Wen-Ping Peng¹; ¹National Dong Hwa University, Shoufeng, Taiwan
 ThP 425 **Serial Detachment of Amino Acids from Microwave-Assisted Weak Acid Protein Hydrolysis**; Jihyun Paek¹; Jeongkwon Kim¹; ¹Chungnam National University, Daejeon, South Korea
 ThP 426 **Assessing the Effects of Tissue Fixation, Freezing, Embedding, and Washing on the Global Lipidome Utilizing MALDI FT-ICR IMS**; Marissa A. Jones^{1,2}; Jeffrey M. Spraggins^{1,2,3}; Nathan Heath Patterson^{1,4}; William J. Perry^{1,2}; Richard M. Caprioli^{1,2,4,5,6}; ¹Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; ²Department of Chemistry, Vanderbilt University, Nashville, TN; ³Department of Biochemistry, Vanderbilt University, Nashville, Tennessee; ⁴Department of Biochemistry, Vanderbilt University, Nashville, TN; ⁵Department of Pharmacology, Vanderbilt University, Nashville, TN; ⁶Department of Medicine, Vanderbilt University, Nashville, TN

ThP 427 **N-glycan MALDI Fingerprinting and All-In-One Reducing-End Derivation Matrix Optimization**; Nicolas Eskenazi¹; Ophelia Djimatey¹; Chiara Giangrande¹; Joëlle Vinh¹; ¹SMBP, ESPCI, PSL University, PARIS, France
 ThP 428 **Simple Surface Modification for Enhancing Carbohydrate Ion Sensitivity in Matrix-Assisted Laser Desorption/Ionization Time-Of-Flight Mass Spectrometry**; Chia-Hsin Chi¹; Yu-Meng Ou^{1,2}; Yi-Sheng Wang¹; ¹Genomics Research Center, Academia Sinica, Taipei, Taiwan; ²Department of Chemistry, National Taiwan University, Taipei, Taiwan
 ThP 429 **Toward Seamless Incorporation of Paternò-Büchi Carbon-Carbon Double Bond Localization in Common MALDI-MSI Workflow**; Andrew E Paulson¹; Young-Jin Lee¹; ¹Iowa State University, Ames, IA
 ThP 430 **Rapid Isolation of Peptides and Proteins from Biological Fluids for Proteomic Analysis by MALDI-TOF Mass Spectrometry**; Ryan Walsh¹; Matt Texter²; Robert English³; Eric Weaver⁴; ¹Shimadzu Scientific Instruments Corp., Columbia, MD; ²Shimadzu Scientific Instruments, Inc., Columbia, MD; ³Shimadzu Scientific Instruments, Inc., Columbia, Maryland; ⁴University of Texas, Arlington, Arlington, TX

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ThP 431 **Utilizing Microfluidic Devices to Evaluate Cellular Metabolism of Therapeutics with Online Mass Spectrometric Detection**; Campbell B Mousseau¹; Chengpeng Chen²; R. Scott Martin²; Amanda B. Hummon¹; ¹The Ohio State University, Columbus, OH; ²Saint Louis University, St. Louis, MO
 ThP 432 **Integrated Workflow with Quality Control for Large Cohort and Clinical Metabolomics Research Using Robust Hardware and Signal Correction**; Sebastian Goetz¹; Ulrike Schweiger-Hufnagel¹; Matthias Szesny¹; Aiko Barsch¹; Sven W. Meyer¹; Matthew R. Lewis²; Nikolas Kessler¹; ¹Bruker Daltonics, Bremen, Germany; ²Imperial College London, London, United Kingdom
 ThP 433 **Dynamic Assessment of the Human Saliva Structural Lipidome using MS/MSALL Shotgun Lipidomics for Population Health Applications**; Valerie Bussberg¹; Hannah Rockwell¹; Gramoz Kondakci¹; Emily Y. Chen¹; Fei Gao¹; Niven R. Narain¹; Michael A. Kiebish¹; ¹BERG, LLC, Framingham, MA
 ThP 434 **Development of a Functional Neurometabolomics Platform to Enable MOA and Functional Studies in Drug Development and Precision Medicine**; Bennett Greenwood¹; Collin Hill¹; Vladimir Tolstikov¹; Reinhard Roessler¹; Christine Denny²; Josephine McGowan²; Vivek Vishnudas¹; Rangaprasad Sarangarajan¹; Niven R. Narain¹; Michael A. Kiebish¹; ¹BERG, LLC, Framingham, MA; ²Columbia University, New York, NY
 ThP 435 **Metabolomics Analysis of Adults-Onset Still's Disease by SWATH-MS**; Chien-Chen Lai¹; Hsuan-Jen Chen¹; ¹National Chung Hsing University, Taichung, Taiwan
 ThP 436 **Influenza Viral Infection Detection in Seconds Using LDTD-MS and Machine Learning**; Pier-Luc Plante^{1,2}; Éliana Francovic-Fontaine^{1,2}; Francis Brière^{1,2}; Nancy Boucher²; Julie Carbonneau²; Marie-Ève Hamelin²; Guy Boivin²; Jacques Corbeil^{1,2}; ¹Université Laval, Québec, Québec; ²Infectiology Research Centre, CHU de Québec, Laval University, Québec, QC
 ThP 437 **Multiomics Analysis of The Metabolome and Intestinal Microbiome of Antibiotics versus Pathogen-Specific Monoclonal Antibodies**; Omari Jones-Nelson¹; Matthew Glover¹; Andrey Tovchigrechko¹; Taylor Cohen¹; Fiona Fernandes²; Udaya Rangaswamy²; Liu Hui²; David Tabor²; Paul Warrener¹; Jose Martinez¹; Wen Yu¹; Gina Dangelo¹; Sonja Hess³; Bret Sellman¹; ¹MedImmune, Gaithersburg,



- MD; ²Medimmune, South San Francisco, California; ³MedImmune, Gaithersburg
- ThP 438 **A Novel Derivatization LC-MS/MS-Based Method for Quantifying Metanephrines from Dried Blood Spots for the Diagnosis of Pheochromocytomas and Paragangliomas (PPCs/PPGLs);** Vincent R. Richard¹; Rene Zahedi¹; Shaun Eintracht²; Christoph H. Borchers^{1,3,4,5}; ¹Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; ²Department of Diagnostic Medicine, Jewish General Hospital, McGill University, Montreal, QC; ³University of Victoria-Genome BC Proteomics Centre, Victoria, BC; ⁴Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC; ⁵Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC
- ThP 439 **High Resolution Mass Spectrometry Newborn Screening Applications for Quantitative Analysis of Amino Acids and Acylcarnitines from Dried Blood Spots;** C. Austin A Pickens¹; Konstantinos Petritis¹; ¹Centers for Disease Control and Prevention, Chamblee, GA
- ThP 440 **Development of a New Vitamin D Assay and Its Application to Profile Vitamin D Metabolites in a Pediatric Population;** Brian C DeFelice¹; Theresa L Pedersen¹; Hanan Shorosh²; Randi K. Johnson²; Jennifer A Seifert²; Jill M. Norris²; Oliver Fiehn³; ¹University of California, Davis, Davis, CA; ²University of Colorado, Denver - Anschutz, Aurora, CO; ³University of California Davis, Davis, CA
- ThP 441 **Metabolomic Studies in Newborn Exposed to Zika Virus;** Danielle Zildeana Souza Furtado¹; Luiz André Zanluqui¹; Cleber N. Barretos¹; Fabiana A. Marques²; Regina V. Oliveira³; Nilson Antonio Assuncao¹; ¹Universidade Federal de São Paulo (UNIFESP), São Paulo, Brazil; ²Instituto Federal de Educação, Ciência e Tecnologia Goiano, Campus Ceres., Ceres, Brazil; ³Universidade Federal de São Carlos, São Carlos, Brazil
- ThP 442 **New Secondary Electrospray Ionization Configuration with Improved Background Levels and Repeatability for Online Analysis of Relevant Metabolites in Breath;** Pedro A. Barreiro¹; Miriam Macia¹; Kapil D. Singh²; Pablo Sinues²; Guillermo Vidal-De-Miguel¹; ¹Fossil Ion Technology, Madrid, Spain; ²University of Basel, Basel, Switzerland
- ThP 443 **Metabolic Profile of Saliva and Biofilm of 30 Patients during Hospitalization in ICU;** Monira Samaan Kallas Kallas¹; Meriellen Dias²; Isaac Castro¹; Maria Anita Mendes²; Luciano Cesar Pontes Azevedo¹; ¹Sirio Libanes Hospital, São Paulo, Brazil; ²Dempster MS Lab- Poli-USP, Sao Paulo, Brazil
- ThP 444 **Metabolic Assessment of Multi-Risk Factors of Alzheimer's Disease Based on Integrative Metabolomic Analysis;** Soo Jin Park¹; Eosu Kim²; Soo ah Jang²; Do Yup Lee¹; ¹kookmin university, Seoul, South Korea; ²Yonsei University College of Medicine, Seoul, South Korea
- ThP 445 **MALDI-FTMS and NMR Serum Analysis for Biomarker Based Determination of Diabetes During Pregnancy;** Franklin E. Leach III¹; Jacquelyn Walejko¹; Maureen Keller-Wood²; Arthur S. Edison¹; ¹University of Georgia, Athens, GA; ²University of Florida, Gainesville, FL
- ThP 446 **Biomarker Discovery and Validation for Delirium Syndrome Using Mass Spectrometry-Based Metabolomics Analysis of Serum Samples;** Don E. Davis, Jr.^{1,2,3,4}; Simona G. Codreanu^{1,2,3,4}; Stacy D. Sherrod^{1,2,3,4}; Jennifer Colby⁵; Jin H. Han⁶; John A. McLean^{1,2,3,4}; ¹Vanderbilt University Department of Chemistry, Nashville, TN; ²Vanderbilt Institute of Chemical Biology, Nashville, TN; ³Center for Innovative Technology, Nashville, TN; ⁴Vanderbilt Institute for Integrative Biosystems Research and Education, Nashville, TN; ⁵Vanderbilt University Medical Center Department of Pathology, Microbiology and Immunology, Nashville, TN; ⁶Vanderbilt University Medical Center
- Department of Emergency Medicine, Nashville, TN
- ThP 447 **Metabolic Preference Assay for Rapid Diagnosis of Bloodstream Infections;** Thomas Ryzak¹; Ryan A Groves¹; Heather Semeniuk²; Rajnigandha Pushpker¹; Ruichuan Zhang¹; Daniel Gregson²; Deirdre Church²; Ian A Lewis¹; ¹University of Calgary, Calgary, AB; ²Calgary Laboratory Services, Alberta Health Services, Calgary, AB
- ThP 448 **Investigating the Complex Interaction between Host Prostate Cancer Cells and Common Microbes Using LC-IM-QTOF-MS Based Platform;** Sumankalaj Ramachandran¹; Minas Sakellakis¹; Gary Gallick¹; Christopher Logothetis^{1,2}; Mark Titus¹; ¹Department of Genitourinary Medical Oncology, The University of Texas MD Anderson Cancer Center, Houston, TX, Houston, TX; ²Department of Clinical Therapeutics, University of Athens, Athens, Greece
- ThP 449 **UPLC-MS Based Plasma Metabolomics Reveal Aromatic Amino Acids Metabolites are Associated with Nonalcoholic Steatohepatitis;** Nisreen Nimer^{1,2}; Zeneng Wang²; Ina Nemet²; Valentin Gogonea^{1,2}; Stanley L Hazen^{1,2}; ¹Cleveland State University, Cleveland, OH; ²Cleveland Clinic, Cleveland, OH
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- ThP 450 **Novel Metabolite Interactions between Branched Amino Acid Aminotransferase 2 (BCAT2), Phenyl Compounds, and Biocytin;** Carol Nilsson¹; Kevin G. Hicks²; Jared Rutter²; ¹Lund University, Lund, Sweden; ²University of Utah School of Medicine, Salt Lake City, UT
- ThP 451 **Metabolomics Analysis of IL-2 and IL-15 Expanded γδ2 T Cells Co-Cultivated with Cancer Cell Lines;** Thomas P. Wyche¹; Rurun Wang¹; Kalya Schriefer¹; Samantha O'Hara¹; Jason Killough¹; Dario Gutierrez¹; Theodore Sana¹; ¹Merck & Co., Inc., Cambridge, MA
- ThP 452 **Where Does Tcrz1 Hide? A Mass Spectrometric Study of T. cruzi Infection in Mouse Models.;** Ekram Hossain¹; Sharon Lostracco-Johnson²; Diane Thomas²; Laura-Isobel McCall¹; ¹University of Oklahoma, Norman, OK; ²UCSD, San Diego, CA
- ThP 453 **Development of Chemical Isotope Labeling Nanoflow LC-MS for Profiling Hydroxyl Submetabolome of Small Numbers of Cells;** Xian Luo¹; Liang Li¹; ¹University of Alberta, Edmonton, AB
- ThP 454 **Rapid Quantification of Extremely Polar Metabolites in Biological Fluids Using Negative Electrospray HILIC-Mass Spectrometry;** Xiaoding Wang¹; Liangqiao Bian²; Maciej Kukula²; Zhao Wang¹; ¹Division of Cardiology, Department of Internal Medicine, University of Texas Southwestern Medical Center, Dallas, Texas; ²Shimadzu Center for Advanced Analytical Chemistry, University of Texas at Arlington, Arlington, TX
- ThP 455 **Metabolic Profiling Shows that Glutathione Depletion is Rescued Along with Growth Rate in Yeast Methionine Auxotrophs;** Matthew A. Kukurugya¹; Bernd J. Wranik¹; Tina Mahatdejkul-Meadows¹; R. Scott McIsaac¹; Bryson D. Bennett¹; ¹Calico Life Sciences, South San Francisco, CA
- ThP 456 **Analysis of Single Liver Cells to Study Drug Uptake, Metabolism and Effects on Endogenous Metabolome at the Single Cell Level;** Lilitiana Pedro¹; Patrick Rudewicz¹; ¹Novartis Institutes for Biomedical Research, Emeryville, CA
- ThP 457 **Evaluation of Inter-protocol Quality Control Samples Used for Metabolomic Analyses;** Bethanne M. Warrack¹; Michael D. Reily¹; Petia Shipkova¹; Joelle Onorato¹; ¹Bristol-Myers Squibb, Princeton, NJ
- ThP 458 **Development and Validation of a High Throughput Metal Ion Panel of 23 Elements for Analysis of Bio Fluids;** Matthew T Doyle¹; Richard Robinson¹; Afton Starling¹; Brent Overcash¹; Lori Wright¹; Fred Hubbard¹; Anne Evans¹; Luke Miller¹; ¹Metabolon, Inc., Durham, NC



- ThP 459 **Modelling Cancer Lipogenesis Using LA-REIMS Metabolic Flux analysis in Breast Cancer Cell Lines;** Seyma Turkseven¹; Nikolaos Koundouros²; Simon Cameron³; Alvaro Perdones-Montero³; Renata Soares³; Luisa Doria³; George Pouligiannis²; Zoltan Takats³; ¹Imperial College London, London, United Kingdom; ²Institute of Cancer Research, London, United Kingdom; ³Imperial College, London, United Kingdom
- ThP 460 **Ion-Pair Selection Method for Pseudotargeted Metabolomics Based on SWATH MS Acquisition and Its Application in Type 2 Diabetes study;** Xinjie Zhao^{1,2}; Lichao wang^{1,2}; Benzhe Su³; Zhongda Zeng¹; Chao Li³; Wangjie Lv^{1,2}; Qihui Xuan^{1,2}; Lina Zhou^{1,2}; Xin Lu^{1,2}; Xiaohui Lin^{1,2}; Guowang Xu^{1,2}; ¹CAS Key Laboratory of Separation Science for Analytical Chemistry, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China; ²University of Chinese Academy of Sciences, Beijing, China; ³School of Computer Science & Technology, Dalian University of Technology, Dalian, China
- ThP 461 **A Comprehensive Heart Metabolome Enabled by Ultra-High Resolution Fourier-Transform Ion Cyclotron Resonance Mass Spectrometry (FTICR-MS);** Benjamin Wancewicz¹; Yutong Jin¹; Yanlong Zhu¹; Ying Ge¹; ¹UW Madison, Madison, WI
- ThP 462 **Large-Scale Metabolomic Analysis of Hydrophilic Metabolites Using Hydrophilic Interaction Liquid Chromatography Tandem Mass Spectrometry with a Novel Polymer-Based Amino Column;** Kohta Nakatani¹; Yoshihiro Izumi¹; Masatomo Takahashi¹; Keita Sakurai²; Michio Butsugan²; Takeshi Bamba¹; ¹Medical Institute of Bioregulation, Kyushu University, Fukuoka, Japan; ²Hitachi Chemical Techno Service Co., Ltd., Ibaraki, Japan
- ThP 463 **Identification of a Malate-Aspartate Shuttle Mediated Mechanism Supporting Drug Resistance in Lung Cancer Cells Triggered by Reduced GLUL Expression;** Anders Nordstrom¹; Magesh Muthu¹; ¹Umeå University, Umeå, Sweden
- ThP 464 **Next Generation Metabolomics Approach for Isolation and Higher Throughput Annotations of Metabolites from *Medicago truncatula* Using UHPLC-MS2-SPE-NMR;** Anil Bhatia^{1,2}; Feng Qiu^{1,3}; Dennis Fine⁴; Daniel Wherritt^{4,5}; Zhentian Lei^{1,2}; Lloyd W. Sumner^{1,2}; ¹Biochemistry Department, University of Missouri, Columbia, MO; ²MU Metabolomics Center, University of Missouri, Columbia, MO; ³International Flavors & Fragrances, Union Beach, NJ; ⁴The Samuel Roberts Noble Foundation, Ardmore, OK; ⁵University of Texas at San Antonio, San Antonio, TX
- ThP 465 **Mass Spectrometric Analysis of Metabolic Profile Alterations in Cataractous Lenses Due to Point Mutations in Two Alpha Crystallins;** Cheryl Frankfater¹; Stephanie Bozeman²; Paul Hamilton²; Fong-Fu Hsu¹; Usha Andley²; ¹NIH/NIGMS Biomedical Mass Spectrometry Resource, Washington University School of Medicine, St. Louis, MO; ²Department of Ophthalmology and Visual Sciences, Washington University School of Medicine, St. Louis, MO
- ThP 466 **Untargeted and Targeted Metabolomics Approach for Characterizing the Hypoxia-Induced Metabolic Alterations in Primary and Metastatic Colorectal Cancer;** Sujatha Chilakala¹; Colin Flinders¹; Ah Young Yoon¹; Mario M Alba¹; Shannon M Mumenthaler¹; Jonathan E Katz¹; ¹Lawrence J. Ellison Institute for Transformative Medicine of USC, Los Angeles, CA
- ThP 467 **Quatitaon of Glycine Using LC-MS to Investigate Its Role in Sex-Specific Association with Coronary Heart Diseases *in vivo* Studies;** Ah Young Yoon¹; Nicholas C. Woodward²; Janet Gukasyan²; Sujatha Chilakala¹; Hooman Allayee²; Jonathan E Katz¹; ¹Lawrence J. Ellison Institute for Transformative Medicine of USC, Los Angeles, California; ²University of Southern California, Los Angeles, California
- ThP 468 **Integrating LC/MS-Based Metabolomics and Solid-State NMR for Total Accounting of Carbon;** Miriam Sindelar^{1,2}; Xiangfeng Niu^{1,2}; Jacob Schaefer¹; Brian N Finck²; Gary J Patti^{1,2}; ¹Washington University in St. Louis, St. Louis; ²Washington University School of Medicine in St. Louis, St. Louis, MO
- ThP 469 **Metabolic Phylogeny: Evidence for Speciation through Metabolic Selection in the Evolution of *Borrelia*, the Causative Agent of Lyme Disease;** Ryan A Groves¹; Thomas Rydzak¹; Mildred Castellanos²; Peter Kraiczky³; George Chaconas²; Ian A Lewis¹; ¹Lewis Research Group, Department of Biological Sciences, University of Calgary, Calgary, AB; ²Department of Biochemistry and Molecular Biology, University of Calgary, Calgary, AB; ³Institute of Medical Microbiology and Infection Control, University Hospital of Frankfurt, Frankfurt Am Main, Germany
- ThP 470 **Cancer Metabolome Dictates Susceptibility to Oncolytic Viral Therapy;** Barry Kennedy¹; Patrick Murphy¹; Michael Giacomantonio¹; Prathyusha Konda²; Derek R Clements¹; Namit Holay¹; Shashi Gujar^{1,2}; ¹Department of Pathology, Dalhousie University, Halifax, NS, Canada, Halifax, NS; ²Department of Microbiology and Immunology, Dalhousie University, Halifax, NS, Canada, Halifax, NS, Canada, Halifax, NS
- ThP 471 **HPLC-MS as a Detection Method for Pigments, Phenolics, and Co-Regulation in a Hybrid Wine Grape Family to Optimize Plant Breeding;** Abigail L Diering¹; David Tork¹; Dana Freund¹; Matthew Clark¹; Adrian Hegeman¹; Anna Underhill¹; ¹University of Minnesota, St. Paul, MN
- ThP 472 **Cancer Cell Metabolism in KRAS Mice Revealed by Direct Sample Analysis with MALDI-TOF and High Resolution Mass Spectrometry;** Bo Wei¹; Lin Tan¹; Robyn Rhea¹; Peiyong Yang¹; ¹M D Anderson Cancer Center, Houston, TX
- ThP 473 **Characterization of Future Urine Reference Materials for the NIST Metabolomics Quality Assurance and Quality Control Program;** Abraham Kuri Cruz¹; David A. Sheen¹; Werickson F. C. Rocha²; Christina M. Jones¹; ¹National Institute of Standards and Technology, Gaithersburg, MD; ²INMETRO, Duque De Caxias, Brazil
- ThP 474 **Database Assisted Globally Optimized Targeted Mass Spectrometry (dGOT-MS): Reliable Metabolomics Analysis with Broad Coverage;** Xiaojian Shi¹; Haiwei Gu¹; Paniz Jasbi¹; ¹Arizona State University, Scottsdale, AZ
- ThP 475 **How the Isotope Exchange Mass Spectrometry can Help Tandem Mass Spectrometry for Identification of Unknowns?;** Yury kostyukevich¹; Alexander Zherebker¹; Alexey orlov¹; Eugene (evgeny) Nikolaev²; ¹Skolkovo Institute of Science and Technology, Skolkovo, Russian Federation; ²Skolkovo institute of science and technology, Moscow Region, Russian Federation
- ThP 476 **LC-HRMS Analysis of Small Molecules Formed in Cigarette Smoke-Exposed 3D Cellular Models Derived from Smokers and Non-Smokers;** Yuichiro Takanami¹; Nobumasa Kitamura¹; Shigeaki Ito¹; ¹Japan Tobacco Inc., Yokohama, Kanagawa, Japan
- ThP 477 **Rock Varnish as a Source of Biosignatures for Mars Extant Life;** Hiro Teshima¹; Chris M Yeager¹; Nina L Lanza¹; Ricardo Marti-Arbona¹; ¹Los Alamos National Lab., Los Alamos, NM
- ThP 478 **An Integrated Ultra-High Resolution FTICR-MS based Platform for Metabolomics;** Yanlong Zhu¹; Benjamin Wancewicz¹; Kent Wenger¹; Yutong Jin¹; Heino M. Heyman²; Christopher J. Thompson²; Aiko Barsch²; Allan Brasier¹; Ying Ge¹; ¹University of Wisconsin - Madison, madison; ²Bruker Daltonics Inc., Billerica, MA


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- ThP 479 **Metabolomics Links Doxycycline, Used Widely in Inducible Gene Silencing Experiments, with Metabolic Dysregulation in Breast Cancer Cells;** Ashish Vaswani; Oregon State University, Corvallis, OR
- ThP 480 **Optimization of *C. elegans* Homogenization and Extraction Methods for LC-MS Untargeted Metabolomics;** Brianna M Garcia¹; Bennett Fox^{2,3}; Goncalo Gouveia⁴; Franklin E. Leach III⁵; Facundo M. Fernandez⁶; Frank Schroeder^{2,3}; Arthur S. Edison⁴; I. Jonathan Amster¹; ¹Department of Chemistry, University of Georgia, Athens, GA; ²Department of Chemistry and Chemical Biology, Cornell University, Ithaca, NY; ³Boyce Thompson Institute, Ithaca, NY; ⁴Department of Biochemistry, University of Georgia, Athens, Georgia; ⁵Department of Environmental Health Science, University of Georgia, Athens, GA; ⁶School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA
- ThP 481 **On-Surface Derivatization Reactions for the High-Throughput Analysis of the Poultry Gut Microbiome using MALDI-MS;** Trevor T Forsman¹; Torey Looft²; Young-Jin Lee¹; ¹Iowa State University, Ames, IA; ²US Department of Agriculture, National Animal Disease Center, Ames, IA
- ThP 482 **Optimizing Methods to Extract Metabolites from Zebrafish Tissue;** Michaela Schwaiger-Haber¹; Fuad J Naser¹; Miriam Sindelar¹; Jonathan L Spalding¹; Gary J Patti¹; ¹Washington University, St. Louis, MO
- ThP 490 **Multi-Feature Based Data Processing of Data Independent Acquisition (DIA) Metabolomics Data without Retention Time Information;** Pradeep Narayanaswamy¹; Adam Iau²; Lyle Burton²; Stephen Tate²; ¹Industry, Singapore, Singapore; ²SCIEX, Concord, ON
- ThP 491 **Reacomics for LC-MS Based Untargeted Analysis;** Miao Yu^{1,2}; Sofia Lendor³; Mariola Olkowicz³; Leslie Bragg³; Anna Roszkowska^{3,4}; Mark Servos³; Janusz Pawliszyn³; ¹University of Waterloo, Waterloo; ²Icahn School of Medicine at Mount Sinai, New York, NY; ³University of Waterloo, Waterloo, ON; ⁴Medical University of Gdańsk, Gdańsk, Poland
- ThP 492 **Effect of a Mediterranean Based Diet on Plasma Metabolites;** Francis Briere¹; Nancy Boucher²; Pier-Luc Plante¹; Didier Brassard¹; Simone Lemieux^{1,3}; Benoit Lamarche^{1,3}; Jacques Corbeil^{1,2}; ¹Université Laval, Québec, QC; ²Infectiology Research Centre, CHU de Québec, Laval University, Québec, QC; ³Institute of nutrition and functional foods, Université Laval, Québec, QC
- ThP 493 **Comprehensive Cell Culture Profiling of iPS Cell Using LC-QTOFMS: Simultaneous Analysis of SIM and Scan Mode in a Single Run;** Takanari Hattori¹; Toshiya Matsubara¹; Tsuyoshi Nakanishi¹; Jun Watanabe¹; ¹Shimadzu Corporation, Kyoto, Japan
- ThP 494 **Multi-Omic Analysis of Macrophage and Macrophage Derived Exosomes with *Leishmania donovani* Infection;** Andrew P Kurland¹; Vanessa Rubio¹; Anna Gioseffi¹; Peter Kima¹; Timothy Garrett¹; ¹University of Florida, Gainesville, FL

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- ThP 483 **Interlaboratory Reproducibility of an Untargeted Metabolomics GC-MS Assay for Analysis of Human Plasma;** Yan-Ping Lin¹; Ying Li¹; Wen-sheng Lang¹; John Masucci¹; Gary W. Caldwell¹; ¹Janssen Research and Development, Spring House, PA
- ThP 484 **Establishing a Shareable Spectral MSMS Library and Accurate Mass Retention Time (AMRT) Database for Pediatric Metabolomics Analysis;** Chiara Lavarello¹; Sebastiano Barco¹; Anas Kamleh²; Igor Fochi³; Martina Bartolucci¹; Gino Tripodi¹; Giuliana Cangemi¹; Andrea Petretto¹; ¹IRCCS Istituto Giannina Gaslini, Genova, Italy; ²Thermo Fisher Scientific Europe, Hågersten, Sweden; ³Thermo Fisher Scientific, Milano, Italy
- ThP 485 **Metabolic Characterization of Cell Clones in *X. laevis* Embryos by HPLC-MS;** Jie Li¹; Peter Nemes¹; ¹Department of Chemistry and Biochemistry, University of Maryland, College Park, MD
- ThP 486 **A Comprehensive N-Glycan Profiling Analysis of Bevacizumab Biosimilar by UHPLC with Fluorescence Detection and Q-TOF Mass Spectrometry;** Yonghai Lu¹; Jie Xing¹; Zhaoqi Zhan¹; ¹Shimadzu Asia Pacific, Singapore, Singapore
- ThP 487 **Discovery of Metabolite Biomarkers of Transition Period Diseases in Dairy Cows Using Chemical Isotope Labeling LC-MS;** Minglei Zhu¹; Elda Dervishi²; Graham Plastow²; Marcos Colazo³; Liang Li¹; ¹University of Alberta, Edmonton, AB; ²University of Alberta, Edmonton, Alberta; ³Alberta and Agriculture Forestry, Edmonton, Alberta
- ThP 488 **Comprehensive Studies of Drug-induced Stemness of Cancer Cells at Single-cell Level;** Mei Sun¹; Xingxiu Chen¹; Zhibo Yang¹; ¹University of Oklahoma, Norman, OK
- ThP 489 **Comprehensive Untargeted Metabolite Identification with Kinetex F5 Microflow Liquid Chromatography and Variable Window Data Independent Acquisition;** Khatereh Motamedchaboki¹; Remco van Soest¹; Robert Proost²; Jason Anspach³; ¹Sciex, Redwood City, CA; ²Sciex, Framingham, MA; ³Phenomenex, Torrance, CA
- ThP 495 **Metabolomic Approach to Investigate Alteration in Metabolites Associated with 25-Hydroxyvitamin D in Healthy Korean Adults;** Mi-ri Gwon¹; Bo Kyung Kim¹; Seungil Cho¹; Sook Jin Seong¹; Young-ran Yoon¹; ¹Kyungpook National University, Daegu, South Korea
- ThP 496 **Investigation of Combined Tolcapone Metabolism and Brain Biochemistry Using an Integrated Human Multi-organ Microphysiological System;** Xin Wang¹; Murat Cirit¹; John Wishnok¹; Linda Griffith¹; Steven Tannenbaum¹; ¹Massachusetts Institute of Technology, Cambridge, MA
- ThP 497 **Beyond Aflatoxins: Untargeted Metabolic Profiling and Time Aligned Parallel fragmentation approach to Determine Gene Function in *A. flavus*;** José Diana Di Mavungu¹; Perng-Kuang Chang²; Leslie L. Scharfenstein²; Natalia Arroyo-Manzanares³; Valdet Uka¹; Sarah De Saeger¹; ¹Ghent University, Ghent, Belgium; ²US Department of Agriculture, Southern Regional Research Center, New Orleans, LA; ³University of Murcia, Murcia, Spain
- ThP 498 **Application of Metabolite Derivatization for Simplification of Metabolomics Analysis by LC-MS;** Taylor F. Berryhill¹; Landon S. Wilson¹; Stephen Barnes¹; ¹University of Alabama at Birmingham, Birmingham, AL
- ThP 499 **Comparison and Evaluation of CCS Values Obtained via Direct Infusion IM-MS and LC-IM-MS for the Characterization of Rat Urine Metabolites;** Leanne Nye¹; Jonathan P Williams²; Nyasha C Munjoma²; Marine PM Letertre¹; Hernando J Olivios³; Muireann Coen¹; Robbin Bouwmeester⁴; Lennart Martens⁴; Jeremy Nicholson⁵; Robert S Plumb⁶; Mike McCullagh²; Lee A Gethings²; Steven Lai³; James I Langridge²; Johannes PC Vissers⁷; Ian D Wilson¹; ¹Imperial College, London, United Kingdom; ²Waters Corporation, Wilmslow, United Kingdom; ³Waters Corporation, Beverly, MA; ⁴Ghent University, Ghent, Belgium; ⁵Murdoch University, Perth, Australia; ⁶Waters Corporation, Milford, MA; ⁷Waters Corporation, Wilmslow, United Kingdom
- ThP 500 **Intelligent Acquisition for Comprehensive Metabolome Coverage in Plants, Mammals, and Bacteria;** Tatjana D Talamantes¹; Sven Hackbusch²; Ioanna Ntai²; Amanda



- Souza²; ¹Thermo Fisher Scientific, West Palm Beach, FL; ²Thermo Fisher Scientific, San Jose, CA
- ThP 501 **Exploring Nematocidal Metabolites of Nematode-Trapping Fungi with LC-MS/MS-Based Untargeted Metabolomics**; Hsin-Yuan Chang¹; Ting-Hao Kuo¹; Ching-Ting Yang²; Yen-Ping Hsueh²; Cheng-Chih Hsu¹; ¹Department of Chemistry, National Taiwan University, Taipei, Taiwan; ²Institute of Molecular Biology, Academia Sinica, Taipei, Taiwan
- ThP 502 **High-Throughput and Sensitive Data Independent Acquisition Workflow Differentiating Pre-Classified Healthy from Prediabetic and Diabetes Samples**; Khatereh Motamedchaboki¹; Robert Proos²; Sara Ahadi³; Raghav Seghal⁴; Hemen Boro⁴; Abhishek Jha⁴; Latha Palaniappan³; ¹Sciex, Redwood City, CA; ²Sciex, Framingham, MA; ³Stanford University, Palo Alto, CA; ⁴Elucidata, Cambridge, MA
- ThP 503 **Using Quality Control Samples for Evaluating Quantification Reproducibility in Untargeted Metabolomics Based on Label-free and Chemical Isotope Labeling LC-MS**; Wei Han¹; Shuang Zhao¹; Liang Li¹; ¹University of Alberta, Edmonton, AB
- ThP 504 **Untargeted Metabolomic Analysis of Brain Sections Tissues from Mice with Low-Tryptophan Diet Using UHPLC-HRMS**; Frederico Garcia Pinto¹; Vanessa Y. Rubio²; Gary P Wang²; Timothy J. Garrett¹; ¹Universidade Federal de Viçosa, Rio Paranaíba, Brazil; ²University of Florida, Gainesville, FL
- ThP 505 **Rapid Detection of Drugs and Metabolites in Urine by Flow Injection Analysis Coupled to Magnetic Resonance Mass Spectrometry**; Matthias Witt¹; Markus Godejohann²; Heino M. Heyman³; Aiko Barsch¹; ¹Bruker Daltonik GmbH, Bremen, Germany; ²Bruker Biospin GmbH, Rheinstetten, Germany; ³Bruker Daltonics Inc., Billerica, MA
- ThP 506 **Metabolomics as a Discovery Tool for Bioprospecting and Detection of Defense Compounds During Fungal Infection of Spruce Wood**; Marit ALmvik¹; Nina Elisabeth Nagy¹; Hans Ragnar Norli¹; Ari Hietala¹; Sven-Roar Odenmarck¹; Monica Fongen¹; Anas M Kamleh²; ¹Norwegian Institute of Bioeconomy Research (NIBIO), Oslo, Norway; ²Thermo Fisher Scientific Europe, Hagersten, Sweden
- ThP 507 **Biological Signal Averaging and PLSDA Variable Statistics in a High-Yield Drought-Tolerant Maize Transgene vs. Wildtype High-Throughput GC-MS Plant Metabolomics Experiment**; Brian M. Ruddy¹; Teresa K. Harp¹; Layton A. Peddicord¹; Shai J. Lawit¹; Jingrui Wu¹; Jeffrey E. Habben¹; Jan P. Hazebroek¹; ¹Corteva Agriscience, Johnston, IA
- ThP 508 **Assessing the Bioactivity of Environmental Surface Waters by Metabolomics Using Multiple Cell Lines**; Yang Yue¹; Jonathan Mosley¹; Paul Bradley²; Jenna Cavallin³; Daniel Villeneuve³; Gerald Ankle³; Drew Ekman¹; Timothy Collette¹; Quincy Teng¹; ¹U.S. Environmental Protection Agency, Athens, GA; ²U.S. Geological Survey, Columbia, SC; ³U.S. Environmental Protection Agency, Duluth, MN
- ThP 509 **Challenges of Data Acquisition for Large Set of Untargeted Metabolomics Studies**; Linxing Yao¹; Tove Fall²; Erik Ingelsson³; Lars Lind⁴; Jessica E. Prenni⁵; Amy M Sheflin⁵; Corey D. Broeckling¹; ¹Proteomics & Metabolomics Facility, Colorado State University, Fort Collins, CO; ²Department of Medical Sciences, Molecular Epidemiology and Science for Life Laboratory, Uppsala University, Uppsala, Sweden; ³School of Medicine, Stanford University, Stanford, CA; ⁴Department of Medical Sciences, Cardiovascular Epidemiology, Uppsala University, Uppsala, Sweden; ⁵Department of Horticulture and Landscape Architecture, Colorado State University, Fort Collins, CO
- ThP 510 **Using Metabolomics to Assess Physiological Changes Accompanying Cyanide Metabolism in Pseudomonas**

- fluorescens NCIMB 11764**; Prajita Pandey¹; Lauren Jones¹; Daniel A. Kunz¹; Vladimir Shulaev¹; ¹University of North Texas, Denton, TX
- ThP 511 **GC-MS Profiling of Soy-Induced Correlated Changes in the Fecal Metabolome and Gut Microbiome of Ovariectomized Female Rats**; Saurav J. Sarma^{1,2}; Victoria J Vieira-Potter³; Tzu-Wen L Cross⁴; Kelly S Swanson^{5,6}; Zhentian Lei^{1,2,7}; Lloyd W Sumner^{1,2,7}; Cheryl S Rosenfeld^{8,9,10}; ¹Metabolomics Center, University of Missouri, Columbia, MO; ²Bond Life Sciences Center, University of Missouri, Columbia, MO; ³Department of Nutrition and Exercise Physiology, University of Missouri, Columbia, MO; ⁴Department of Bacteriology, University of Wisconsin-Madison, WI, Madison, WI; ⁵Division of Nutritional Sciences, University of Illinois at Urbana-Champaign, Urbana, IL; ⁶Department of Animal Sciences, University of Illinois at Urbana-Champaign, Urbana, IL; ⁷Department of Biochemistry, University of Missouri, Columbia, MO; ⁸Biomedical Sciences, University of Missouri, Columbia, MO; ⁹Thompson Center for Autism and Neurobehavioral Disorders, University of Missouri, Columbia, MO; ¹⁰Genetics Area Program, University of Missouri, Columbia, Columbia, MO
- ThP 512 **Quantitative Evaluation of Untargeted Metabolomic Methods for Zebrafish Blood**; Fuad J Naser¹; Ronald Fowle-Grider¹; Kevin Cho¹; Jonathan L Spalding¹; Gary J Patti¹; ¹Washington University in St. Louis, St. Louis, MO

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- ThP 513 **Typing of emm1 Group A Hemolytic Streptococci Using MALDI-TOF MS**; Megumi Sakuma¹; Keisuke Shima²; Shinji Funatsu²; Koretsugu Ogata²; Miyuki Morozumi¹; Satoshi Iwata¹; ¹Keio University School of Medicine, Shinjuku-ku, Japan; ²SHIMADZU, Kyoto, Japan
- ThP 514 **MALDI-MS Proteotyping of Cutibacterium acnes**; Kanae Teramoto¹; Tatsuki Okubo¹; Yoshihiro Yamada¹; Sadanori Sekiya¹; Shinichi Iwamoto¹; Koichi Tanaka¹; ¹Shimadzu Corporation, Kyoto, Japan
- ThP 515 **Epigenetic “Memory” During Bacterial Adaptation to Environmental Changes**; Alena Calm¹; Gabrielle Rizzo²; Trevor Glaros¹; Henry S Gibbons¹; ¹ECBC, Aberdeen Proving Ground, Maryland; ²ECBC, Excet Contractor, Aberdeen Proving Ground, Maryland
- ThP 516 **Improved MALDI-MS method in stability and reproducibility of peak detection of the biomarkers for proteotyping of Salmonella serotypes**; Yuko Fukuyama¹; Teruyo Ojima-Kato²; Satomi Nagai²; Keisuke Shima²; Shinji Funatsu¹; Yoshihiro Yamada¹; Hiroto Tamura²; Shizuo Nomura¹; Koretsugu Ogata¹; Sadanori Sekiya¹; Shinichi Iwamoto¹; Koichi Tanaka¹; ¹Shimadzu Corporation, Kyoto, Japan; ²Meijyo University, Nagoya, Japan
- ThP 517 **Chemical Changes On, and through, the Bacterial Envelope in E. coli Mutants Exhibiting Impaired Plasmid Transfer Identified Using ToF-SIMS**; Kelly Dimovska Nilsson¹; John Fletcher¹; ¹University of Gothenburg, Gothenburg, Sweden
- ThP 518 **Electroporation and LESA-MS: A New Paradigm for Top-Down Analysis of Proteins Direct from Living Yeast Colonies**; Klaudia I Kocurek^{1,2}; Robin C May¹; Helen J Cooper¹; ¹University of Birmingham, Birmingham, United Kingdom; ²Texas A&M University, College Station, TX
- ThP 519 **Keeping it Clean: Metaproteomic Characterization of a Microbiome Capable of Degrading Personal Care Product and Pharmaceutical Contaminants found in Water**; Kitty J. Brown¹; Karen E. Rossmassler²; Lisa M Wolfe¹; Parker J. Muck¹; Jean F. Challacombe³; Jessica E. Prenni⁴; Susan K. De Long⁵; Corey D. Broeckling¹; ¹Proteomics & Metabolomics Facility, Colorado State



- University, Fort Collins, CO; ²Pulmonary Section, Denver Veterans Affairs Medical Center; Division of Pulmonary Sciences & Critical Care Medicine, University of Colorado Denver, Denver, CO; ³College of Agricultural Sciences, Colorado State University, Fort Collins, CO; ⁴Department of Horticulture & Landscape Architecture, Colorado State University, Fort Collins, CO; ⁵Department of Civil & Environmental Engineering, Colorado State University, Fort Collins, CO
- ThP 520 **Model Based Spectral Library for Bacterial Identification via Membrane Glycolipids**; So Young Ryu¹; George A. Wendt^{1,2}; Robert K. Ernst³; David R. Goodlett³; ¹University of Nevada, Reno, NV; ²University of California, Berkeley, CA; ³University of Maryland, Baltimore, MD
- ThP 521 **The *Trichomonas vaginalis* Cytoskeletal Proteome**; Katherine Muratore¹; Patricia Johnson¹; ¹University of California Los Angeles, Los Angeles, CA
- ThP 522 **HAMA: High-Throughput Automated Muropeptide Analysis Framework for Revealing Composition of Bacterial Peptidoglycan**; Pin-Rui Su^{1,2}; Ya-Chen Hsu¹; Hsin-Hsiang Chung¹; Yun Lin¹; Tsuey-Ching Yang³; Cheng-Chih Hsu¹; ¹National Taiwan University, Taipei, Taiwan; ²Erasmus MC, Rotterdam, Netherlands; ³National Yang-Ming University, Taipei, Taiwan
- ThP 523 **Typing Environmental Microorganisms To Genomic Databases Using MALDI Mass Spectrometry**; Kenneth C. Parker; SimulTOF/ VIC Instruments, Marlborough, MA
- ThP 524 **Characterization of Lysine Acetylation in Human Gut Microbiome**; Xu Zhang¹; Zhibin Ning¹; Janice Mayne¹; Shelley Deeke¹; Krystal Walker¹; David Mack²; Alain Stintzi¹; Daniel Figeys¹; ¹University of Ottawa, Ottawa, ON; ²Children's Hospital of Eastern Ontario, Ottawa, ON
- ThP 525 **Top Down Protein Identification of ESKAPE Pathogens from *in vitro* Skin Models and *ex vivo* Human Skin by LESA MS**; Jana Havlikova^{1,2}; Robin C. May^{2,3}; Iain B. Styles⁴; Helen J. Cooper²; ¹EPSRC Centre for Doctoral Training in Physical Sciences for Health, University of Birmingham, Birmingham, United Kingdom; ²School of Biosciences, University of Birmingham, Birmingham, United Kingdom; ³Institute of Microbiology and Infection, University of Birmingham, Birmingham, United Kingdom; ⁴School of Computer Science, University of Birmingham, Birmingham, United Kingdom
- ThP 526 **Cell-Free Identification of *S. cerevisiae* Strains Used in Beer Production using LC-MS**; Cathy Muste¹; Kevin Owens¹; ¹Drexel University, Philadelphia, PA
- ThP 527 **Integrated, Multi-Omics Strategy to Study the Gut Microbiota Response to Salmonella enterica Typhimurium Infection in Humanized Mice**; Pingli Wei¹; Caitlin Keller¹; Jennifer R. Bratburd²; Rui Liu³; Eugenio Vivas²; Erin Gemperline¹; Federico E. Rey²; Cameron R. Currie²; Lingjun Li^{1,4}; ¹Department of Chemistry, University of Wisconsin-Madison, Madison, WI; ²Department of Bacteriology, University of Wisconsin-Madison, WI, Madison, WI; ³School of Pharmacy, Nanjing University of Chinese Medicine, Nanjing, China; ⁴School of Pharmacy, University of Wisconsin-Madison, Madison, WI
- ThP 528 **Characterization of Novel Assembly Mechanisms of a Large Viral Icosahedral Capsid**; Erin Reilly¹; Zein Haidar¹; Ru-ching Hsia²; Sammy Pardo³; Dana Molleur³; Susan T. Weintraub³; Julie A. Thomas¹; ¹Rochester Institute of Technology, Rochester, NY; ²University of Maryland School of Dentistry, Baltimore, MD; ³University of Texas Health Science Center at San Antonio, San Antonio, TX
- ThP 529 **Molecular Networking Guided Profiling of Metabolic Pathways in Engineered Microorganisms for Industrial Production of Chemical Intermediates**; Alexey V. Melnik¹; Bryan Fonslow¹; Ali Khodayari¹; Julia Khandurina¹; Pieter C. Dorrestein²; ¹Genomatica Inc., San Diego, CA; ²UCSD, La Jolla, CA
- ThP 530 **Examining the Discrimination Power of MAI, vMAI, and SAI for Identification of Microorganisms**; Darrell D. Marshall^{1,2}; Santosh Karki^{1,2}; Khoa Hoang^{1,3}; Milan Pophristic^{1,3}; Chuping Lee²; Ellen Inutan^{1,4}; Samantha Leach⁵; Charles N McEwen^{1,3}; Sarah Trimpin^{1,2}; ¹MSTM, LLC, Newark, DE; ²Wayne State University, Detroit, MI; ³University of the Sciences, Philadelphia, PA; ⁴MSU-Iligan Institute of Technology, Iligan City, Philippines; ⁵Department of Forensic Sciences, Washington, DC
- ThP 531 **Time-Dependent Analysis of *Paenarthrobacter nicotinovorans* pAO1 Nicotine-Related Proteome**; Marius Mihan¹; Cornelia Babii¹; Devika Channaveerappa²; Roshanak Aslebagh²; Emmalyn Dupree²; Costel C Darie²; ¹Alexandru Ioan Cuza University of Iasi, Iasi, Romania; ²Clarkson University, Potsdam
- ThP 532 **Real-time, Automated Characterization of Algal Lipidome and Metabolome Using Laser-Assisted Rapid Evaporative Ionization Mass Spectrometry**; Julia Balog^{1,2}; Richard Schäffer¹; Milan Szabo^{3,4}; Unnikrishnan Kuzhiumparambil³; Steven D Pringle⁵; Peter Ralph³; Zoltan Takats²; ¹Waters Research Center, Budapest, Hungary; ²Imperial College, London, United Kingdom; ³University of Technology Sydney, Sydney, Australia; ⁴Biological Research Centre of the Hungarian Academy of Sciences, Szeged, Hungary; ⁵Waters Corporation, Wilmslow, United Kingdom
- ThP 533 **MS-Based Metaproteomics Can Be Integrated with Metagenome Assembled Genomes to Provide Genome Specific Protein Identification in Gut Microbiomes**; Jose Alfredo Blakeley-Ruiz¹; Carlee S McClintock²; Richard J. Giannone³; Helen A Baghdoyan¹; Ralph Lydic¹; Mircea Podar³; Robert L. Hettich³; ¹University of Tennessee, Knoxville, TN; ²Pain Consultants of East Tennessee, Knoxville, Tennessee; ³Oak Ridge National Laboratory, Oak Ridge, TN
- ThP 534 **Characterization of Microorganisms by Proteins and Lipids MALDI-TOF Fingerprints: Case Studies**; Vincent Guérineau¹; Morgane Barthélemy¹; Marceau Levasseur¹; Téó Hébra¹; Véronique Eparvier¹; David Touboul¹; ¹CNRS-ICSN, Gif Sur Yvette, France
- ThP 535 **Distinguishing Bacteria from Near Neighbors by Paper Spray Mass Spectrometry**; Daniel Carmany¹; Ethan M McBride²; Phillip Mach²; Elizabeth S Dhummakupt²; Paul S Demond¹; Gabrielle Rizzo¹; Nicholas E Manicke³; Trevor Glaros²; ¹Excet, Inc., Springfield, VA; ²ECBC, Aberdeen Proving Ground, Maryland; ³IUPUI Department of Chemistry & Chemical Biology, Indianapolis, IN
- ThP 536 **Typing/Subtyping Shiga Toxin from Pathogenic *Escherichia coli* Using MALDI-TOF-TOF Tandem Mass Spectrometry and Top-Down Proteomic Analysis**; Clifton K. Fagerquist¹; William J. Zaragoza¹; Michelle Q. Carter¹; ¹USDA/ARS, Albany, CA
- ThP 537 **Developing Sample Preparation Conditions to Analyze a Remarkably Resilient Protein Assembly, the Methanosaeta concilii Sheath**; John Muroski¹; Farzaneh Sedighian¹; Robert P. Gunsalus¹; Joe A Loo¹; Rachel R Orgazalek Loo¹; ¹UCLA, Los Angeles, CA
- ThP 538 **Influence of Phage SPN3US Infection on the Salmonella Host Proteome**; Caleb Emmons¹; Julie A. Thomas²; Susan Ludwigsen¹; Jimar Miller¹; Sammy Pardo³; Dana Molleur³; Susan T. Weintraub³; ¹Proteome Software, Portland, OR; ²Rochester Institute of Technology, Rochester, NY; ³University of Texas Health Science Center at San Antonio, San Antonio, TX
- ThP 539 **Microbial Synthesis of a Novel Vitamin B9 Derivative and its Immunomodulatory Impact**; Abby J. Chiang¹; Daniel Röth¹; Anne E. Hall²; Gabriel B Gugiu¹; James Versalovic^{2,3}; Markus Kalkum¹; ¹City of Hope, Duarte, CA; ²Baylor College of Medicine, Houston, Texas; ³Texas Children's Hospital, Houston, Texas



ThP 540 **Evidence of Sodium Substitution for Hydrogen in Negative Ion Lipid A Tandem Mass Spectra of *Burkholderia thailandensis***; Sung Hwan Yoon^{1,2}; Courtney E. Chandler¹; Inga V. Leus³; Aleksandra Nitalazar²; Helen I. Zgurskaya³; David R. Goodlett¹; Robert K. Ernst¹; ¹University of Maryland, Baltimore, MD; ²NIH/NIAD, Bethesda, Maryland; ³University of Oklahoma, Norman, OK

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- ThP 542 **Rapid Determination of Progestogens by Solid-Phase Extraction with Functionalized Metal-Organic Frameworks Coupled to Direct Analysis in Real Time Mass Spectrometry**; Linnan Li¹; Yuangui Yang¹; Mei Tian¹; Ruirong Zheng¹; Li Yang^{1,2}; Zhengtao Wang^{1,2}; ¹Shanghai University of Traditional Chinese Medicine, Shanghai, China; ²Shanghai R&D Center for Standardization of Chinese Medicines, Shanghai, China
- ThP 543 **Preparation of Gas Phase Naked Silver Cluster Cations Outside a Mass Spectrometer from Ligand Protected Clusters in Solution**; Madhuri Jash¹; Arthur C. Reber²; Atanu Ghosh¹; Depanjan Sarkar¹; Mohammad Bodiuzzaman¹; Pallab Basuri¹; Ananya Bakshi¹; Shiv N. Khanna²; Thalappil Pradeep¹; ¹Indian Institute of Technology, Madras, Chennai, India; ²Virginia Commonwealth University, Richmond, VA
- ThP 544 **Top-Down Phosphoproteomics Enabled by Novel Nanoproteomics Platform**; David S Roberts¹; Bifan Chen¹; Timothy N. Tiambeng¹; Zhijie Wu¹; Ying Ge^{1,2,3}; Song Jin¹; ¹Department of Chemistry, University of Wisconsin-Madison, Madison, WI; ²Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI; ³Human Proteomics Program, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI
- ThP 545 **Determination of Molecular and Topographical Organization on Cicada Wings: Mass Spectrometry's Impact on Material Characterization and Design**; Jessica K Román^{1,2}; Jacob B Hoffman²; Julian H Reed²; Nenad Miljkovic³; Donald M Cropek²; Marianne Alleyne³; ¹Sandia National Laboratories, Albuquerque, NM; ²US Army Corps of Engineers, Champaign, IL; ³University of Illinois at Urbana Champaign, Urbana, IL
- ThP 546 **Neutrophil Extracellular Trap Formation in the Lung as Response to Magnetic Cobalt Ferrite Nanoparticles**; Anja M Billing¹; Kristina B Knudsen²; Håkan Wallin³; Selina VY Tang⁴; Iseult Lynch⁵; Ulla Vogel^{3,6}; Frank Kjeldsen¹; ¹Department of Biochemistry and Molecular Biology, University of Southern Denmark, Odense, Denmark; ²National Research Centre for the Working Environment, Copenhagen, Denmark; ³National Research Centre for the Working Environment, Copenhagen, Denmark; ⁴Promethean Particles, Nottingham, United Kingdom; ⁵School of Chemistry and Chemical Biology, University College Dublin, Dublin, Ireland; ⁶Department of Micro- and Nanotechnology, Technical University of Denmark, Lyngby, Denmark
- ThP 547 **Pre-Adsorption of Antibodies on Nanocarriers: Retaining Targeting Properties in a Complex Protein Environment**; Johanna Simon¹; Manuel Tonigold²; Katharina Landfester¹; Volker Mailänder^{1,2}; ¹Max Planck Institute for Polymer Research, Mainz, Germany; ²University of Mainz, Mainz, Germany
- ThP 548 **Complementary Molecular Profiling of Neuropeptides and Lipids from *Lymnaea stagnalis* by LDI-Mass**

Spectrometry on Matrix-Assisted and Silicon Nanopost Array Platforms; Ellen A Wood¹; Sylwia A Stopka¹; Akos Vertes¹; ¹The George Washington University, Washington, DC

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- ThP 550 **The Dynamic Sampling Platform (DSP) for ESI-MS Monitoring of Bioreactors for Therapeutic Cell Manufacturing**; Mason A Chilmonczyk¹; Gian C Rivera²; Peter A Kottke¹; Robert E Guldborg³; Andrei G Fedorov¹; ¹Georgia Institute of Technology, Atlanta, GA; ²University of Puerto Rico - Mayagüez, Mayagüez, PR; ³University of Oregon, Eugene, OR
- ThP 551 **Deep and Sensitive Proteomics Using Capillary Electrophoresis-Mass Spectrometry with the Identification of 7000 Proteins from nanograms of MCF7 Proteome Digests**; Zhichang Yang¹; Xiaojing Shen¹; Daoyang Yang¹; Liangliang Sun¹; ¹Michigan State University, East Lansing
- ThP 552 **Extending the Lower Limits of Quantification of a Therapeutic Oligonucleotide through Microflow LC-MS/MS**; Daniel Warren¹; Sean McCarthy²; Lei Xiong³; Anthony Romanello²; ¹AB SCIEX, Framingham; ²Sciex, Framingham, MA; ³Sciex, Redwood City, CA
- ThP 553 **Water and Temperature-Assisted Trap Focusing for Ultra-Large Volume Injection in Reversed-Phase Nano-Liquid Chromatography Mass-Spectrometry**; Veronica Termopoli¹; Pierangela Palma¹; Giorgio Famigliini¹; Gian Luca Morini²; Pamela Vocale³; Mansoor Saeed⁴; Simon Perry⁴; Achille Cappiello¹; ¹University of Urbino, Urbino, Italy; ²University of Bologna, Bologna, Italy; ³University of Parma, Parma, Italy; ⁴Syngenta Jealott's Hill International Research Centre, Bracknell, United Kingdom
- ThP 554 **ESI-MS Intracellular Metabolite Profiling for Therapeutic Cell Manufacturing via Microfabricated Mass Exchanger**; Austin L Culberson¹; Mason A Chilmonczyk¹; Peter A Kottke¹; Andrei G Fedorov¹; ¹Georgia Institute of Technology, Atlanta, GA
- ThP 555 **Rapid Characterization of Recombinant Protein Processing Using Microchip-Based Capillary Electrophoresis-ESI-MS**; David McCaskill¹; Vimbai Chikwana¹; Jeffrey Gilbert¹; ¹Corteva Agriscience, Indianapolis, IN
- ThP 556 **High-Sensitivity Glycomic and Proteomic Profiling of Limited Biological Samples Using Capillary Zone Electrophoresis-Mass Spectrometry**; Anne-Lise Marie¹; Kendall Johnson¹; Marcia Santos²; Somak Ray¹; Antonius Koller¹; David Frank³; Helen Gandler³; Shulin Lu³; John Tigges³; Ionita Ghiran³; Alexander R Ivanov¹; ¹Northeastern University, Boston, MA; ²Sciex, Brea, CA; ³Harvard Medical School, Boston, MA
- ThP 557 **Microchip Capillary Electrophoresis-Negative Electropray Ionization-Mass Spectrometry for High Sensitivity Anion Detection**; Yury Desyaterik¹; Jean Pierre Alarie¹; J. Michael Ramsey¹; ¹UNC, Chapel Hill, NC
- ThP 558 **Monitoring Amino Acid Composition of Cell Culture Media using Microfluidic CE-MS**; Erin Redman¹; Kathryn Elliot²; Cameron Schnabel²; Sarah Harcum²; J. Scott Mellors¹; Glenn Harris³; ¹908 Devices, Inc., Carrboro, NC; ²Department of Bioengineering, Clemson University, Clemson, SC; ³908 Devices, Boston, MA
- ThP 559 **Multilevel Characterization and Identification of Trastuzumab Posttranslational Modifications by Imaged cIEF-MS**; Erik Gentalen¹; Steve Lacy¹; Jennifer Ji¹; Lena Wu¹; Scott Mack¹; ¹Intabio, Inc., Newark, CA



- ThP 560 **High-Sensitivity Analysis of Drugs in Ultra-Small Volumes Plasma Samples using Micro-Flow LC-MS/MS;** Daive Vecchiotti¹; Mikaël Levi¹; Hidetoshi Terada¹; Jonathan Edwardsen²; Keiko Matsumoto¹; Kyoko Watanabe¹; Masami Tomita¹; ¹Shimadzu Corporation, Kyoto, Japan; ²Shimadzu Scientific Instruments, Inc., Columbia, Maryland
- ThP 561 **Integrating Nanofluidic/Microfluidic Interface Concentrators/Microreactor with ESI-MS for Proteome Analysis;** Dayi Chen¹; Kantaphon Suddhapas¹; Timothy J Fogliatti¹; Aaron T Timperman¹; ¹University of Illinois Urbana-Champaign, Urbana, IL
- ThP 562 **In-syringe Electrokinetic Clean-up of Weakly Acidic Drugs in Biological Samples for Direct Injection Electrospray Ionization Mass Spectrometry;** Ibraam E. Mikhail^{1,2,3}; Masoomah Tehranirokh^{1,4}; Andrew A Gooley^{1,4}; Rosanne M Guijt^{1,5}; Michael C Breadmore^{1,2}; ¹ARC Training Centre for Portable Analytical Separation Technologies (ASTech), Hobart, Australia; ²Australian Centre for Research on Separation Science (ACROSS), School of Physical Sciences (Chemistry), University of Tasmania, Hobart, Australia; ³Department of Analytical Chemistry, Faculty of Pharmacy, Mansoura University, Mansoura, Egypt; ⁴Trajan Scientific and Medical, Ringwood, Australia; ⁵Centre for Regional and Rural Futures, Deakin University, Geelong, Australia
- ThP 563 **High-Throughput Proteome Analysis Using 50 cm Long Micro Pillar Array Columns (µPACTM);** Jeff Op. De Beeck¹; Geert Van Raemdonck¹; Paul Jacobs¹; Gert Desmet²; Wim De Malsche²; Francis Impens³; Kris Gevaert³; ¹PharmaFluidics, Ghent, Belgium; ²Vrije Universiteit Brussel, Brussels, Belgium; ³VIB-UGent Center for Medical Biotechnology, Ghent, Belgium
- ThP 564 **Microchip Integration of Imaged cIEF with Mass Spectrometry Accelerates the Identification of Charge Variants in Intact Monoclonal Antibodies;** Scott Mack¹; Steve Lacy¹; Jennifer Ji¹; Guillaume Tremintin²; Lena Wu¹; Erik Gentalen¹; ¹Intabio, Inc., Newark, CA; ²Bruker Daltonics Inc., Billerica, MA
- ThP 565 **Analysis of Peptides Using Nano LC with Micro Pillar Array Columns (µPAC™) and Microsaic Real-Time 4500 MID® Mass Spectrometer;** Victoria Ordsmith¹; Bin Chen¹; Chris Harris¹; ¹Microsaic Systems, Woking, United Kingdom
- ThP 566 **Ultra-Sensitive Deep LC-MS Proteomic Profiling Using Ultra-Low Flow Monolithic and Porous-Layer Open Tubular Capillary Columns;** Michal Gregus¹; Antonius Koller¹; Alexander R Ivanov¹; ¹Northeastern University, Boston, MA
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- ThP 567 **Cytochrome P450 Inhibition by Licorice Glycyrrhiza uralensis Fisch. ex DC.;** Luying Chen^{1,2}; Laura Tyler²; Dejan Nikolic²; Guido F. Pauli²; Richard B. van Breemen^{1,2}; ¹Linus Pauling Institute, College of Pharmacy, Oregon State University, Corvallis, OR; ²UIC/NIH Center for Botanical Dietary Supplements Research, Chicago, IL
- ThP 568 **Unequivocal identification of alkylpyrazines by Gas Chromatography-Mass Spectrometry (GC-MS);** Sihang Xu¹; Athula Attygalle¹; Ramu Errabelli²; ¹Stevens Institute of Technology, Hoboken, NJ; ²SGS New Jersey laboratory, Fairfield, NJ
- ThP 569 **Automation and Application of Magnetic Based Affinity Selection Screening for Targets of Retinoid X Receptor alpha (RXRα);** Ruth N Muchiri¹; Jaewoo Choi¹; Katherine A Carter¹; Brett M Tyler¹; Richard B. van Breemen¹; ¹Oregon State University, Corvallis, OR
- ThP 570 **PepSAVI-MS Reveals a Novel Antimicrobial Peptide from Amaranth;** Lilian R. Heil¹; Tessa E. Bartges¹; Christine L. Kirkpatrick¹; Nicole C. Parsley¹; Dennis Goldfarb²; Leslie M Hicks¹; ¹Department of Chemistry, University of North Carolina at Chapel Hill, Chapel Hill, NC; ²Department of Cell Biology and Physiology, Lineberger Comprehensive Cancer Center, University of North Carolina at Chapel Hill, Chapel Hill, NC
- ThP 571 **Finding Alkaloids in Plant Extracts by LC-QToF Mass Spectrometry in Combination with Mass Defect Analysis;** Armando Alcazar Magana^{1,2}; Bayissi Bading-Taika³; Jaewoo Choi¹; Cristobal L. Miranda¹; Claudia S. Maier²; Jan F. Stevens¹; ¹Linus Pauling Institute, College of Pharmacy, Oregon State University, Corvallis, OR; ²Department of Chemistry, Oregon State University, Corvallis, Oregon; ³Department of Clinical and Pharmaceutical Sciences, School of Life and Medical Sciences, University of Hertfordshire, Hertfordshire, United Kingdom
- ThP 572 **LC-MS-Based Analysis of Antimicrobial Compounds Produced by Streptomyces coelicolor Harboring Metagenome-Derived Biosynthetic Gene Clusters ;** Angela I Calderon¹; Megan Sandoval-Powers¹; Yilue Zhang¹; Hannah Kim¹; Alinne Santana-Pereira¹; Mark Liles¹; David Mead²; ¹Auburn University, Auburn, Alabama; ²Varigen Biosciences Corporation, Madison, WI
- ThP 573 **Ozone-Induced Dissociation Mass Spectrometry as a New Tool to Determine the C=C Double Bond Locations in Natural Products;** Ngoc Vu¹; Sonja Knowles¹; Nicholas Oberlies¹; Qibin Zhang^{1,2}; ¹UNC Greensboro, Greensboro, NC; ²Center for Translational Biomedical Research, Kannapolis, NC
- ThP 574 **LC-MS-Based Chemical Characterization of Constituents of Açai Methanol Extract and Metabolites Obtained from an in vitro Intestinal First-Pass Metabolism Study;** Yilue Zhang¹; Turner Shirley¹; Tyler Wietlake¹; Richard A. Hansen²; Jingjing Qian²; Angela I. Calderon¹; ¹Department of Drug Discovery and Development, Auburn University, Auburn, AL; ²Department of Health Outcomes Research and Policy, Auburn University, Auburn, AL
- ThP 575 **LC-HRMS followed by Enhanced Product Ion Scanning for Flavonoids Profiling of Primula boveana;** Ehab Mahran^{1,2}; Michael Keusgen¹; ¹Institute of Pharmacy, Philipps-Universität Marburg, Marburg, Germany; ²Faculty of Pharmacy, Al-Azhar University, Nasr city, Egypt
- ThP 576 **Identification of Biofilm-Stimulating Peptides from Bacillus cereus with PepSAVI-MS;** Tessa E. Bartges¹; Steven R. Fleming¹; Sarah A. Barr¹; Elizabeth A. Shank¹; Albert A. Bowers¹; Leslie M. Hicks¹; ¹University of North Carolina, Chapel Hill, NC
- ThP 577 **Determination and Visualization of Components from a Medical Fungus Using High-Performance Liquid Chromatography Mass Spectrometry and Imaging Mass Spectrometry;** Jing Dong¹; Satoshi Yamaki¹; Xiaodong Li¹; Naoki Hamada¹; ¹SHIMADZU CHINA MS CENTER, Beijing, China
- ThP 578 **Using Ozone Induced Dissociation Mass Spectrometry (OzID-MS) for Natural Product Analysis: Pure Compound, Complex Extract, and in situ;** Sonja L. Knowles¹; Ngoc Vu¹; Daniel A. Todd¹; Huzefa A. Raja¹; Antonis Rokas²; Qibin Zhang^{1,3}; Nicholas H. Oberlies¹; ¹University of North Carolina at Greensboro, Greensboro, NC; ²Vanderbilt University, Nashville, TN; ³Center for Translational Biomedical Research, Kannapolis, NC
- ThP 579 **Isolation and Identification of Naphthomycins Production by Actinomycetes as Antifungal Compounds against Colletotrichum acutatum;** Fernando L.S. Fugita¹; Nicolas L. M. Freiria¹; Luiz A.B. Moraes¹; ¹Faculty of Philosophy, Sciences and Letters at Ribeirao Preto (USP), Ribeirão Preto, Brazil
- ThP 580 **Bacteria Fight Club: Mapping Microbial Interactions for Drug Discovery;** Berkley Ellis¹; Caleb N Fischer¹; Brian



- O Bachmann¹; John A. McLean¹; ¹Vanderbilt University, Nashville, TN
- ThP 581 **Analysis of Diterpenoids in *Tripterygium wilfordii* by Supercritical Fluid Chromatography Coupling Tandem Mass Spectrometry**; Lingna Ke¹; Ming Yuan²; Qing Fu¹; Zhengwei Jia²; Yu Jin¹; ¹East China University of Science and Technology, Shanghai, China; ²Waters Technologies (Shanghai) Co., Ltd, Shanghai, China
- ThP 582 **Modulation of the Secondary Metabolites Production in *Streptomyces Caat 8-25* under Metal Stress by LC-MS/MS**; Talita C. T. Medeiros¹; Bruna B. Loiola¹; Luiz A.B. Moraes¹; ¹Faculty of Philosophy, Sciences and Letters at Ribeirão Preto (USP), Ribeirão Preto, Brazil
- ThP 583 **Determination of Artemisinin and Its Precursors in *Artemisia annua* L using LC/MS/MS**; Huihua Ji¹; Lowell Bush¹; Neil Fannin¹; ¹University of Kentucky, Lexington, KY
- ThP 584 **Putative Identification of Phenolic Compounds and Evaluation of Antioxidant, Anti-Inflammatory and Neuroprotective Activities of Extracts of 3 Endemic Colombian Fruits**; Daniel Esteban Arias; Professor, Bogota, Colombia
- ThP 585 **Using Dereplication for Targeted and Untargeted Re-Isolation of Fungal Secondary Metabolites**; Allison J. Wright¹; Sonja L. Knowles¹; Huzefa A. Raja¹; Nicholas H. Oberlies¹; ¹University of North Carolina at Greensboro, Greensboro, NC
- ThP 586 **Screening of a Natural Product Library for Antimicrobial Activity Targeting Metal Homeostasis**; Charles Veltri¹; Maria Lozoya¹; Jennifer Foster²; Pete Manchen²; Cynthia Reck³; Genna Gallas³; Andrew Salywon⁴; Jose Hernandez³; ¹Midwestern University College of Pharmacy-Glendale, Glendale, AZ; ²Midwestern University Arizona College of Osteopathic Medicine, Glendale, AZ; ³Midwestern University College of Graduate Studies-Glendale, Glendale, AZ; ⁴Desert Botanical Garden, Phoenix, AZ
- ThP 587 **Uptake and Health Effects of Phytochemicals in Honey Bees and Their Larvae Investigated by LC-QTRAP-MS Quantitation and GC-TOF-MS Metabolomics**; Nanna H. Vidkjær¹; Per Kryger¹; Inge S. Fomsgaard¹; ¹Aarhus University, Slagelse, Denmark
- ThP 588 **Enhancing Confidence in Screening and Quantitation of Phytochemicals in Herbal Extracts by Nominal Mass LC-MS/MS**; Prasanth Joseph¹; Saikat Banerjee¹; Samir Vyas¹; ¹Agilent Technologies, Whitefield, Bengaluru, India
- ThP 589 **Rapid Characterization of *Valeriana jatamansi* Jones Using Online Supercritical Fluid Extraction-High Performance Liquid Chromatography Combined with High Resolution Mass Spectrometry**; Jing Dong¹; Shizhong Chen²; Naoki Hamada¹; Xiaodong Li¹; Satoshi Yamaki¹; ¹SHIMADZU CHINA MS CENTER, Beijing, China; ²Peking University, Beijing, China
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- ThP 590 **Determination of Length and Composition of polyA Tails in Phosphate-Modified *in vitro* Transcribed mRNAs using LC-MS/MS**; Dominika Strzelecka¹; Mirosław Smietanski²; Marcin Warminski¹; Paweł Jan Sikorski²; Joanna Kowalska¹; Jacek Jemielity²; ¹Faculty of Physics, University of Warsaw, Warsaw, Poland; ²Centre of New Technologies, University of Warsaw, Warsaw, Poland
- ThP 591 **The Effect of G-Quadruplexes on the Stability of Adjacent DNA Domains Studied by Temperature-Controlled nanoESI-MS**; Adam Pruška¹; Adrien Marchand¹; Renato Zenobi¹; ¹ETH Zurich, Zurich, Switzerland
- ThP 592 **Rapid Detection of Ribonucleoside Modifications by Liquid Chromatography Higher-Energy Collisional Dissociation Mass Spectrometry and Spectral Matching**; Manasses Jora¹; Peter A. Lobue¹; Robert L. Ross¹; Balasubrahmanyam Addepalli¹; Patrick A. Limbach¹; ¹Department of Chemistry, University of Cincinnati, Cincinnati, OH
- ThP 593 **Gas Phase Fractionation to Increase Sensitivity of a Data Dependent-Constant Neutral Loss-MS3(DDA-CNL/MS3) DNA Adductomic Analysis**; Valeria Guidolin¹; Peter W. Villalta²; Foster Jacobs²; Silvia Balbo^{1,2}; ¹School of Public Health, University of Minnesota, Minneapolis, MN; ²Masonic Cancer Center, Minneapolis, Minnesota
- ThP 594 **High Performance Oligonucleotide Analysis by HILIC-MS: Ion-Pairing Reagents Not Required**; Peter A. Lobue¹; Manasses Jora¹; Balasubrahmanyam Addepalli¹; Patrick A. Limbach¹; ¹Department of Chemistry, University of Cincinnati, Cincinnati, OH
- ThP 595 **Construction of A New Porous Covalent Organic Polymer via Schiff-base Reaction and Its Application in Desalination of Oligonucleotides**; Li-Juan Wang^{1,2}; Qian-Yu Zhou¹; Yu-Fang Ma¹; Yue Yu¹; Ying-Lin Zhou¹; Xin-Xiang Zhang¹; ¹Peking University, Beijing, China; ²Hebei University, Baoding, China
- ThP 596 **LC-MS Detection of UV-Induced Oxidative Damage to Ribosomal RNA**; Mariana Bonafim Piveta¹; Manasses Jora¹; Patrick A. Limbach¹; Balasubrahmanyam Addepalli¹; ¹University of Cincinnati, Cincinnati, OH
- ThP 597 **Enzymatic Labeling of Oligonucleotides for Multiplexed LC-MS/MS**; Scott Abernathy¹; Kayla M. Borland²; Peter A. Lobue¹; Patrick A. Limbach¹; ¹University of Cincinnati, Cincinnati, OH; ²Ludwig-Maximilians-University Munich, Munich, Germany
- ThP 598 **Improving Transfer RNA Isolation for more Accurate LC-MS/MS Characterization of Modified Nucleosides**; Ruoxia Zhao¹; Robert L. Ross¹; Andrew Wood¹; Manasses Jora¹; Patrick A. Limbach¹; ¹University of Cincinnati, Cincinnati, OH
- ThP 599 **Development of High-Sensitive and High-Throughput Quantitative Analysis Method of Modified Nucleosides Using UHPLC-UniSpray /MS/MS**; Takahiro Kogaki¹; Ikumi Oshio¹; Souta Iyama¹; Hiroaki Hase¹; Kentaro Jingushi²; Yuko Ueda¹; Zenzaburo Tozuka¹; Daisuke Saigusa³; Kazutake Tsujikawa¹; ¹Mol. Cell. Physiol., Grad. Sch. Pharm. Sci., Osaka University, Suita, Japan; ²Department of Urological Immuno-oncology, Graduate School of Medicine, Osaka University, Suita, Japan; ³Department of Integrative Genomics, Tohoku Medical Megabank Organization, Tohoku University, Sendai, Japan
- ThP 600 **Accurate Mass Determination of Long DNA Fragments Prepared for Structural Biology Study of Epigenetic DNA Methylation**; Hiroshi Ushijima¹; Rena Maekawa¹; Eri Igarashi¹; Satoko Akashi¹; ¹Yokohama City University, Yokohama, Japan
- ThP 601 **A Software Platform for the Quality Control of Synthetic Oligonucleotides**; Detlev Suckau¹; Sam Kyritsoglou²; Yue Ju³; Guillaume Tremintin³; Anjali Alving⁴; Michael Greig³; Robert Kane³; ¹Bruker Daltonics, Bremen, Germany; ²Kaneka Eurogentec SA, Liège, Belgium; ³Bruker Scientific, San Jose, CA; ⁴Bruker Daltonics Inc., Billerica, MA
- ThP 602 **Investigation of Matrix Conditions for Nucleic Acid Analysis in Positive Ion Detection Using a Linear Benchtop MALDI-TOFMS**; Shuichi Nakaya¹; Akihiro Kunisawa²; Zenzaburo Tozuka²; Yuzo Yamazaki¹; ¹Shimadzu Corporation, Kyoto, Japan; ²Shimadzu Analytical Innovation Research Laboratory, Osaka University, Suita, Japan
- ThP 603 **Pythas: Software to Analyze and Map RNA Post-Transcriptional Modifications with Tandem MS and Stable Isotope Labelling**; Luigi D'Ascenzo, Ph.D.¹; Anna Popova, Ph.D.¹; James R. Williamson, Ph.D.¹; ¹The Scripps Research Institute, La Jolla, CA
- ThP 604 **Leveraging Ion-tagged Oligonucleotides and Mass Spectrometry for the Detection of RNA Modifications**; Kevin D. Clark¹; Colin Lee²; Jonathan V. Sweedler^{1,2}



- ¹Beckman Institute, Urbana, IL; ²University of Illinois at Urbana-Champaign, Urbana, IL
- ThP 605 **Mass Spectrometry-Based Identification of Mono-Methylated RNA Nucleoside Positional Isomers: Application for Structural Analysis of RNA Modifications in the Leishmania ribosome;** Hiroshi Nakayama¹; Yoshio Yamauchi²; Yuko Nobe²; Masami Koike¹; Nobuhiro Takahashi³; Moran Shalev-Benami⁴; Toshiaki Isobe²; Masato Taoka²; ¹RIKEN Center for Sustainable Resource Science, Wako, Japan; ²Tokyo Metropolitan University, Hachioji, Japan; ³Tokyo University of Agriculture and Technology, Fuchu, Japan; ⁴Weizmann Institute of Science, Rehovot, Israel
- ThP 606 **High-throughput Oligonucleotide Analysis using RapidFire/TOF MS and OligoSearch Software;** Peter Rye¹; Jim Lau²; Tony Brand³; ¹Agilent Technologies, Lexington, MA; ²Agilent Technologies, Wilmington, DE; ³Agilent Technologies, Raleigh-Durham, NC
- ThP 607 **Simultaneous Quantification of dA-Ap and dG-Ap Interstrand Cross-Links in Cellular and Tissue DNA;** Su Guo¹; Jiapeng Leng¹; Yinsheng Wang¹; ¹UC Riverside, Riverside
- ThP 608 **Multiplex Quantification of RNA Methylation by Targeted Mass Spectrometry;** Jerome Vialaret¹; Aurore Attina¹; Helene Guillorit²; Amandine Bastide²; Sebastien Relier²; Jean Jacques Vasseur³; Françoise Debart³; Sylvain Lehmann¹; Alexandre David²; Christophe Hirtz¹; ¹Montpellier University - LBPC/PPC, Montpellier, France; ²Institut de Génomique Fonctionnelle, Montpellier, France; ³Institut des Biomolécules Max Mousseron, Montpellier, France
- ThP 609 **Ultraviolet Photodissociation of Silver Nanocluster/DNA Complexes;** Ines C Santos¹; Molly S Blevins¹; John Armstrong¹; Christopher M Crittenden¹; Jennifer S Brodbelt²; ¹University of Texas at Austin, Department of Chemistry, Austin, TX; ²The University of Texas, Austin, TX
- ThP 610 **MALDI MS Study of Activity of DNA Specific Enzymes in the Vicinity of G-Quadruplex Structures;** Alexandra V. Sekridova¹; Galina E. Pozmogova²; Igor P. Smirnov²; ¹Institute of agricultural biotechnology, Moscow, Russia; ²Research and Clinical Center for Physical-Chemical Medicine, Moscow, Russia
- ThP 611 **Collision-Induced Dissociation Studies of protonated ions of Alkylated Thymidine and 2'-deoxyguanosine;** Yuxiang Cui¹; Jun Yuan¹; Pengcheng Wang¹; Jun Wu¹; Yang Yu¹; Yinsheng Wang¹; ¹University of California, Riverside, Riverside, CA
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- ThP 612 **Metal Cationization of Immunopeptides for Improved Dissociation and Measurement by Differential Ion Mobility-Mass Spectrometry;** James E. Keating¹; Chris Chung¹; Shengjie Chai²; Benjamin G. Vincent³; Sally A. Hunsucker³; Paul M. Armistead³; Gary L. Glish¹; ¹Department of Chemistry, University of North Carolina at Chapel Hill, Chapel Hill, NC; ²Curriculum in Genetics & Molecular Biology, University of North Carolina at Chapel Hill, Chapel Hill, NC; ³Lineberger Comprehensive Cancer Center, University of North Carolina at Chapel Hill, Chapel Hill, NC
- ThP 613 **Investigation of CID and HCD Tandem Mass Spectra of Double Derivatized Histone (H3) Model Peptide Using High-Resolution Hybrid Mass Spectrometer;** Leila Afjehi-Sadat¹; Benjamin A Garcia¹; ¹University of Pennsylvania, Philadelphia, PA
- ThP 614 **Comparative Study of Average Probabilities of Fragment Ion Formation in Peptides with Different Aspartate Isoforms;** Daniil Ivanov¹; Stanislav Pekov^{1,2}; Maria Indeykina^{1,3}; Anna Bugrova³; Alexey Kononikhin^{1,2,3}; Igor Popov^{1,2}; Eugene (evgeny) Nikolaev⁴; ¹Moscow Institute of Physics and Technology (State University), Dolgoprudny, Russia; ²Institute for Energy Problems of Chemical Physics RAS, Moscow, Russia; ³Institute of Biochemical Physics RAS, Moscow, Russia; ⁴Skolkovo institute of science and technology, Moscow Region, Russian Federation
- ThP 615 **Combined Density Functional and Statistical Analyses of Doubly Protonated Tryptic Peptide Series;** Shanshan Guan¹; Benjamin J Bythell¹; ¹University of Missouri, St. Louis, St. Louis, MO
- ThP 616 **Fast and Accurate MS² Peak Intensity Prediction for Multiple Fragmentation Methods, Instruments and Labeling Techniques;** Ralf Gabriels^{1,2}; Lennart Martens^{1,2}; Sven Degroeve^{1,2}; ¹VIB-Ugent Center for Medical Biotechnology, Ghent, Belgium; ²Department of Biomolecular Medicine, Ghent University, Ghent, Belgium
- ThP 617 **Optimizing Parallel HCD and ETD with supplemental HCD Data Acquisition using the Tribrid Orbitrap Lumos;** Lauren R. DeVine¹; Robert N. Cole¹; ¹Johns Hopkins University School of Medicine, Baltimore, MD
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- ThP 618 **Nanoscale Ion Emitters in Native Mass Spectrometry for Measuring Ligand-Protein Binding Affinities;** Giang Nguyen¹; Thanh N. Tran²; Matthew N. Podgorski³; Stephen G. Bell³; Claudiu T. Supuran⁴; William A. Donald¹; ¹School of Chemistry, University of New South Wales, Sydney, NSW, Australia; ²School of Electrical Engineering and Telecommunications, University of New South Wales, Sydney, NSW, Australia; ³Department of Chemistry, University of Adelaide, Adelaide, Australia; ⁴University of Florence, Department of Neuroscience, Psychology, Drug Research and Child's Health, Section of Pharmaceutical and Nutraceutical Sciences, Via Ugo Schiff 6, Sesto Fiorentino, Italy
- ThP 619 **Investigating the Interactions of the First 17 Residues of Huntingtin with Lipid Vesicles Using ESI-MS Experiments and MD Simulations.;** Ahmad Kiani Karanjii¹; Maryssa Beasley¹; Ali Ranjbaran²; Justin Legleiter¹; Stephen Valentine¹; ¹West Virginia University, C. Eugene Bennett Department of Chemistry, Morgantown, WV; ²West Virginia University, Morgantown, WV
- ThP 620 **Intact Transition Epitope Mapping – Targeted High-Energy Rupture of Extracted Epitopes (ITEM - THREE);** Bright D. Danquah¹; Claudia Röwer¹; Kwabena F.M. Opuni²; Reham A. El-Kased³; Harald Illges⁴; Cornelia Koy¹; Michael O. Glocker¹; ¹Proteome Center Rostock, Rostock, Germany; ²School of Pharmacy, University of Ghana, Legon, Ghana; ³Microbiology and Immunology Faculty of Pharmacy, The British University in Egypt, Cairo, Egypt; ⁴University of Applied Sciences Bonn-Rhein-Sieg, Bonn, Germany
- ThP 621 **The Application of Direct MS for the Investigation of Complex Biological Systems;** Gili Ben-Nissan¹; Jelena Cvetichanin¹; Ravit Netzer¹; Sarel J Fleishman¹; Michal Sharon¹; ¹Weizmann Institute of Science, Rehovot, Israel
- ThP 622 **Uniting Microchip Capillary Electrophoresis-MS and Ultraviolet Photodissociation Technologies for On-line Separation and Characterization of Native Protein Complexes;** M. Rachel Mehaffey¹; Ashley Bell²; J. Scott Mellors²; Michael B. Lanzillotti¹; Jennifer S. Brodbelt¹; ¹The University of Texas at Austin, Austin, TX; ²908 Devices, Boston, MA
- ThP 623 **Native Ion-Mobility Mass Spectrometry of Staph. Aureus Alpha-Hemolysin Membrane Pore Complexes;** Jesse W. Wilson¹; Amber D Rolland¹; Grant M Klausen¹; Alexander S Skochko¹; James S Prell¹; ¹University of Oregon Department of Chemistry and Biochemistry, Eugene, OR
- ThP 624 **Determination of Protein-Brain Ganglioside Interactions by Chip-Based Nano-electrospray Quadrupole-Time-of-**



- ThP 625 **Flight Tandem Mass Spectrometry**; Laurentiu Popescu¹; Mirela Sarbu¹; Raluca Ica¹; Alina Petrut¹; Alina D. Zamfir²; ¹National Institute for Research and Development in Electrochemistry and Condensed Matter, Timisoara, Romania; ²Nat'l Inst, Electrochemistry & Condensed Matter, Timisoara, Romania
- ThP 626 **High Resolution - Mass Spectrometry Cellular Thermal Shift Assay (HR-MS-CETSA)- Impact of Phosphorylation on Thermal Protein Stability**; Yan Ting Lim¹; Tianyun Zhao²; Wint Wint Phoo¹; Lingyun Dai²; Loo Chien Wang¹; Liyan Chen¹; Par Nordlund^{1,2,3}; Radoslaw Sobota¹; ¹Institute of Molecular and Cell Biology Agency for Science, Technology and Research (A*STAR), Singapore, Singapore; ²School of Biological Sciences, Nanyang Technological University, Singapore, Singapore, Singapore; ³Karolinska Institutet, Department of Oncology-Pathology, Stockholm, Sweden
- ThP 627 **Data-Driven Detection of Functional Proteoforms in SEC-SWATH-MS Data**; Isabell Bludau¹; Max Frank^{1,2}; Moritz Heusel¹; Yujia Cai²; George Rosenberger³; Yansheng Liu⁴; Ashok Venkitaraman⁵; Vihandha Wickramasinghe⁶; Ben C Collins¹; Hannes Roest²; Ruedi Aebersold^{1,7}; ¹ETH Zurich, Zurich, Switzerland; ²Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, ON; ³Columbia University, New York, NY; ⁴Yale University, New Haven; ⁵Medical Research Council Cancer Unit, University of Cambridge, Cambridge, United Kingdom; ⁶Peter MacCallum Cancer Centre, Melbourne, Australia; ⁷University of Zurich, Zurich, Switzerland
- ThP 628 **Real-Time Enzymatic Catalysis by Variable-Temperature Nano-Electrospray Ionization Ion Mobility Spectrometry-Mass Spectrometry**; Brooke A. Brown¹; Christopher R. Conant¹; Tarick J. El-Baba¹; Daniel W. Woodall¹; David E. Clemmer¹; ¹Indiana University, Bloomington, IN
- ThP 629 **UVPD-MS of Protein-Ligand Complexes Governed by Different Binding Modes and Affinities**; Ines C Santos¹; Jennifer S Brodbelt¹; ¹University of Texas at Austin, Austin, TX
- ThP 630 **Identifying Protein Complexes of Endocrine Disrupting Organotin Compounds Using Mild LC-MS Techniques**; Jonas M. Will¹; Michael Sperling^{1,2}; Uwe Karst¹; ¹University of Muenster, Institute of Inorganic and Analytical Chemistry, Muenster, Germany; ²European Virtual Institute for Speciation Analysis (EVISA), Muenster, Germany
- ThP 631 **Investigation of Charge Partitioning from Gas-phase Dissociation of Dimeric Proteins**; Mengxuan Jia¹; Chen Du¹; Yang Song¹; Zibo Chen²; David Baker²; Vicki H. Wysocki^{1,3}; ¹Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH; ²Department of Biochemistry, University of Washington, Seattle, WA; ³Resource for Native Mass Spectrometry Guided Structural Biology, Columbus, OH
- ThP 632 **Identification of Smyd1's Chromatin Binding Partners via CHIP-MS**; Anna Bakhtina¹; Aman Makaju²; Sarah Franklin³; ¹University of Utah, Salt Lake City, UT; ²University of Utah School of Medicine, Department of Biochemistry, Salt Lake City, Utah; ³University of Utah School of Medicine, Salt Lake City, UT
- ThP 633 **High Resolution Structural Footprinting for 15-PGDH Inhibitor Binding Site Assessment**; Janna Kiselar¹; Joseph Ready²; Yuan Yiyuan¹; Mark R Chance¹; Sanford Markowitz¹; ¹Case Western Reserve Univ, Cleveland, OH; ²UT Southwestern, Dallas, TX
- ThP 634 **Integrated Structural Proteomics and Dynamics of a Solid-Body Organism by Combined XLMS, Solvent Accessible Surface Modification and QconCAT**; Yeve Mirzakhanyan¹; Paul Gershon¹; ¹UC-Irvine, Irvine, CA
- ThP 635 **Analysis of Human Nuclear Protein Complexes by Quantitative Mass Spectrometry Profiling**; Katelyn E. Connelly¹; Victoria Hedrick²; Tiago J. P. Sobreira²; Emily C. Dykhuizen¹; Uma K. Aryal²; ¹Department of Medicinal Chemistry and Molecular Pharmacology Purdue University, West Lafayette, IN; ²Purdue Proteomics Facility, Bindley Bioscience Center, West Lafayette, IN
- ThP 636 **Characterization of Protein-Ligand Binding Interactions of Polyphenol Inhibitors of FabI by Molecular Docking Simulations and Native MS**; P. Matthew Joyner¹; Denise P. Tran²; Joseph A. Loo²; ¹Pepperdine University, Malibu, CA; ²UCLA, Los Angeles, CA
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- ThP 637 **Native Mass Spectrometry Analysis of Protein and Protein Complexes Formed from Non-volatile Salt Buffers through use of Gábor Transformation**; Sean P. Cleary¹; Jesse W Wilson¹; James S Prell¹; ¹University of Oregon, Eugene
- ThP 638 **Integrated Structural Biology Study of Roundabout1 Interaction with Fondaparinux**; Robert Williams¹; Jeong Yeh Yang¹; Yunyun Gao²; Arwen Pearson²; Kelley Moremen¹; James H. Prestegard¹; I. Jonathan Amster¹; ¹University of Georgia, Athens, GA; ²University of Hamburg, Hamburg, Germany
- ThP 639 **Unexpected Asp-isomerization Behavior in Monoclonal Antibodies: Connecting Primary Sequence with High Order Structure and Molecular Dynamics**; Andrew D. Mahan¹; Dorina Saro²; Jeffrey Brelford¹; Weiping Shen¹; Sandeep Somani¹; Hirsh Nanda¹; ¹Janssen R&D, Spring House, PA
- ThP 640 **Structural Characterization of Ternary Complexes for Selective Protein Degradation by Hydrogen-Deuterium Exchange Mass Spectrometry**; Jing Li¹; Aaron Balog¹; Louis Lombardo¹; John Newitt¹; Mark Witmer¹; Guodong Chen¹; ¹Bristol-Myers Squibb, Princeton, NJ
- ThP 641 **Native Ion Mobility Mass Spectrometry as a Powerful Tool to Dissect α -Synuclein Conformational Space - Small Molecules, Metal Ions, PTMs**; Rani Moons¹; Albert Konijnenberg¹; Anne-Marie Lambeir²; Frank Sobott^{1,3,4}; ¹Biomolecular and Analytical Mass Spectrometry group, University of Antwerp, Belgium; ²Laboratory of Medical Biochemistry, University of Antwerp, Belgium; ³Astbury Centre for Structural Molecular Biology, University of Leeds, United Kingdom; ⁴School of Molecular and Cellular Biology, University of Leeds, United Kingdom
- ThP 642 **Cytochrome c / Cardiolipin Interactions in Apoptosis: The Roles of Protein Auto-Oxidation and *in situ* Covalent Modifications**; Victor Yin¹; Lars Konermann²; ¹University of Western Ontario, London, ON; ²University of Western Ontario, London, ON
- ThP 643 **Coupling FPOP with IM-MS for Detailed Structural Characterization of the Native Ensemble of cytochrome c**; Emily E Chea¹; Daniel Deredge¹; Lisa M Jones¹; ¹University of Maryland, Baltimore- School of Pharmacy, Baltimore, MD
- ThP 644 **Deep Profiling of Proteome Structural Changes by TMT-Mass Spectrometry**; Kaiwen Yu¹; Junmin Peng¹; ¹St Jude Children's Research Hospital, Memphis, TN
- ThP 645 **Investigation of Gas-Phase Unfolding Transitions of Protein Ions Using Ion Mobility-Mass Spectrometry**; Micah T. Donor¹; Samantha O Shepherd¹; James S Prell¹; ¹University of Oregon Department of Chemistry and Biochemistry, Eugene, OR
- ThP 646 **Metal-Induced Oxidation of Transthyretin Studied via Ion Mobility-Orbitrap Mass Spectrometry and Surface-Induced Dissociation**; Mehdi Shirzadeh¹; Michael L Poltash¹; Jacob W McCabe¹; Klaudia I Kocurek¹; zahra Moghadamchargari¹; Arthur Laganowsky¹; David H. Russell¹; ¹Texas A&M University, College Station, TX



- ThP 646 **Structural Analysis of Gas-Phase Phosphoproteins;** Carter Lantz¹; Rachel R. Ogorzalek Loo¹; Joseph A. Loo¹; ¹University of California Los Angeles, Los Angeles, CA
- ThP 647 **Protein Structural Accessibility Differences in Cerebrospinal Fluid by Limited Proteolysis-Mass Spectrometry;** Danielle A Faivre¹; Eric L Huang¹; Michael J MacCoss¹; ¹University of Washington, Seattle, WA
- ThP 648 **Assessing the Comparability of Ion Mobility Mass Spectrometry to Measure Collision Cross Section Distributions for Protein Standards;** Aidan P France¹; Lukasz Migas²; Bruno Bellina²; Eleanor Sinclair²; Perdita E. Barran²; ¹University of Manchester, Manchester, United Kingdom; ²Manchester Institute of Biotechnology, University of Manchester, United Kingdom
- ThP 649 **Distinguishing Subtle Conformational Differences in Protein Complexes using Ion Mobility Mass Spectrometry and Collision Induced Unfolding;** Stacey Nash¹; Tyler Marcinko¹; Richard W. Vachet¹; ¹University of Massachusetts at Amherst, Amherst, MA
- ThP 650 **MALDI Analysis for Protein Footprinting;** Jerry Jiang¹; Michael L Gross¹; Nicole D Wagner¹; ¹Washington University in St. Louis, St. Louis
- ThP 651 **Characterization and Biochemical Analysis of a Low-Molecular Weight Cysteine-Rich Protein in Black Widow Dragline Silk;** Mikayla Shanafelt¹; Jared Deyarmin¹; Ryan Hekman²; Taylor Rabara¹; Camille Larracas³; Liang Xue¹; Craig Vierra¹; ¹University of the Pacific, Stockton, CA; ²Boston University, Boston, MA; ³University of the Pacific, San Francisco, CA
- ThP 652 **Characterization of Co-Existing Enfvirtide Conformational States by Ion Mobility Mass Spectrometry and Hydrogen/Deuterium Exchange;** Bradley Stocks¹; Gregory H. Bird²; Loren D. Walensky²; Jeremy E. Melanson¹; ¹National Research Council Canada, Ottawa, ON; ²Dana-Farber Cancer Institute, Boston, MA
- ThP 653 **Microcontoller Timing, OPO and FPOP for T-Jump Measurement of Protein Conformational Kinetics;** Don L Rempel¹; Roger (Xiaoran) Liu²; Michael L Gross²; ¹Washington University, St Louis, MO; ²Washington University, St.Louis, MO
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- ThP 654 **Better Investigation of Integrin Expression in Cancer Cell Lines by Comparison of Different Membrane Protein Enrichment Methods;** Mona Goli¹; Jair Montford¹; Katya Y Torres-Ulloa¹; Wenjing Peng¹; Ahmed Hussien^{1,2}; Yehia Mechref¹; ¹Texas Tech University, Lubbock, TX; ²University of Alexandria, Alexandria, Egypt
- ThP 655 **Co-Localization of CD147 with Oncogenic Proteins Confers Drug-Resistant Phenotype in Breast Cancer Stem Cells;** Sohyun Kim¹; Yuri Seo¹; Hyeryeon Jung¹; Jieun Jung²; Yeojin Jung²; Kristine M Kim²; Eugene C Yi¹; ¹Department of Molecular Medicine and Biopharmaceutical Sciences, Graduate School of Convergence Science and Technology, Seoul National University, Seoul, South Korea; ²College of Biomedical Science, Kangwon National University, Seoul, South Korea
- ThP 656 **Novel Strategies for Top-down Proteomics of Endogenous Membrane Protein Complexes;** Kyle Brown¹; Bifan Chen¹; Ziqing Lin¹; Tania Guardado¹; Song Jin¹; Ying Ge¹; ¹University of Wisconsin-Madison, Madison, WI
- ThP 657 **Comparative Proteomic Profiling of Five 2D and 3D Grown Cancer Cell Lines Using HRAM LC-MS.;** Josip Blonder¹; Jan A Kaczmarczyk¹; Rhonda R Roberts¹; Gordon R Whiteley¹; Robin A Felder²; Richard G Saul¹; ¹Frederick Nat'l Lab for Cancer Research, Frederick, MD; ²Department of Pathology, University of Virginia School of Medicine, Charlottesville, VA
- ThP 658 **Evaluation of Six Different Sample Preparation Strategies for Enhanced In-Depth Proteomic Analysis of Milk Fat Globule Membrane;** Yongxin Yang¹; Ruchika Bhowal²; Elizabeth T. Anderson²; Sheng Zhang²; ¹Anhui Academy of Agricultural Sciences, Hefei Shi, China; ²Cornell University, Ithaca, NY
- ThP 659 **Selective Binding of a Toxin and Phosphatidylinositides to a Mammalian Potassium Channel;** Yang Liu¹; Michael L Poltash²; Wen Liu¹; David H. Russell²; Arthur Laganowsky²; ¹TAMU Health Science Center, Houston, TX; ²Texas A&M University, College Station, TX
- ThP 660 **Quantification of Mitochondrial Membrane Proteins in Dried Blood Spots for the Detection of Blood Doping Practices in Sport;** Holly Cox¹; Abhilasha Manandhar¹; Daniel Eichner¹; ¹Sports Medicine Research and Testing Laboratory, Salt Lake City, UT
- ThP 661 **Native MS and Surface Induced Dissociation Provide Insight into Eye Lens Aquaporins;** Sophie R Harvey^{1,2}; Wendy L White³; Zachary L VanAernum^{1,2}; Erin M Panczyk^{1,2}; Kevin L Schey³; Vicki H Wysocki^{1,2}; ¹Department of Chemistry and Biochemistry, The Ohio State University, Columbus, Ohio; ²Resource for Native Mass Spectrometry Guided Structural Biology, The Ohio State University, Columbus, Ohio; ³Department of Biochemistry, Vanderbilt University, Nashville, Tennessee
- ThP 662 **Detergents' Supercharging Effects on Soluble Proteins and Membrane Proteins;** Wonhyeuk Jung¹; Frederik Lermyte²; Carter Lantz¹; Rachel Loo¹; Joseph A. Loo¹; ¹UCLA, Los Angeles, CA; ²University Of Antwerp, Antwerp, Belgium
- ThP 663 **Intact and Subunit Mass Analysis Using Native Ion Exchange Chromatography Coupled to an Orbitrap Mass Spectrometer;** Qian Liu¹; Stephane Houel¹; Hao Zhang¹; Alla Polozova¹; ¹Amgen Inc., Cambridge, MA
- ThP 664 **Proteomic Analysis of Cell Surface Proteins with Improved Specificity of Enrichment;** Betsy Benton¹; Sergei Snovidia¹; Katherine Herting¹; Hongbin Zhu¹; John C. Rogers¹; Barbara Kaboord¹; ¹Thermo Fisher Scientific, Rockford, IL
- ThP 665 **Probing Adhesion GPCR-G Protein Interaction by Chemical Cross-Linking and Mass Spectrometry;** Bill Huang¹; Hee-Yong Kim¹; ¹NIAAA/NIH, Rockville, MD
- ThP 666 **Applying a Quantitative, Cell Surface Glycoproteomic Approach to Understanding Phenotypic Changes Induced by Extended Culturing of Explanted Human Cardiac Fibroblasts;** Linda Berg Luecke¹; Amanda Rae Buchberger^{1,2}; Matthew Waas¹; Rebekah L. Gundry^{1,2}; ¹Medical College of Wisconsin, Milwaukee, WI; ²Center for Biomedical Mass Spectrometry Research, Medical College of Wisconsin, Milwaukee, WI
- ThP 667 **Ion Mobility-Mass Spectrometry Reveals α -Synuclein Conformational Changes within Lipid Bicelles;** Denise P Tran¹; Joseph A Loo¹; ¹UCLA, Los Angeles, CA
- ThP 668 **Application of the CellSurfer Platform Enables Generation of a Chamber-Resolved Map of Surface N-Glycoproteins on Primary Human Cardiomyocytes;** Rachel A. Jones Lipinski¹; Ranjuna Weerasekera¹; Linda Berg Luecke¹; Amanda Rae Buchberger¹; Matthew Waas¹; Rebekah L. Gundry¹; ¹Medical College of Wisconsin, Milwaukee, WI
- ThP 669 **Comparison of Reverse Phase and Ion Exchange Fractionation Strategies for 2D-LC-MS/MS Based Liver Proteomics;** Maxime Sansoucy¹; Felix Friedrich¹; Lekha Sleno¹; ¹UQAM, Montreal, QC
- ThP 670 **Characterization of the Intact Proteins of Influenza Primary Liquid Standards;** Lidoshka Marc¹; John R Barr¹; Tracie Williams¹; ¹Centers for Disease Control and Prevention, Atlanta, Georgia
- ThP 671 **Bioinformatic Analysis of MS Data to Assess G-Protein Coupled Receptor Targets for Transactivation of**



ThP 672 **Proliferative Pathways in Cancer Cells; Arba Karcini¹; Iulia M. Lazar¹; ¹Virginia Tech, Blacksburg, VA**
Therapeutic Utility of LIFR Inhibitor EC359 in Treating HDAC Inhibitor Resistance in Ovarian Cancer; Suryavathi Viswanadhapalli¹; Susan T. Weintraub¹; Mengxing Li¹; Hareesh B. Nair²; Klaus J. Nickisch²; Sammy Pardo¹; Dana Molleur¹; Ratna K. Vadlamudi¹; ¹University of Texas Health Science Center at San Antonio, San Antonio, TX; ²Evestra, San Antonio, TX

ThP 673 **LC-MS Characterization of Polysorbate 80 Raw Materials from Multi-Use Containers; Rashmi Menon¹; Erin Laskowich¹; Linda Yi¹; ¹Biogen, Morrisville, NC**

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ThP 674 **Developing Novel Enrichment Strategies to Facilitate Proteomic Analysis of NR5A2in Triple Negative Breast Cancer; Valentine V Courouble¹; Yuanjun He¹; Ruben Garcia-Ordonez¹; Patrick R. Griffin¹; ¹Scripps Research, Jupiter, FL**

ThP 675 **Surface Glycoproteomic Analysis Reveals that Both Unique and Differential Expression of Surface Glycoproteins Determine the Cell Type; Suttipong Suttapitugsakul¹; Lindsey D. Ulmer¹; Chendi Jiang¹; Fangxu Sun¹; Ronghu Wu¹; ¹Georgia Institute of Technology, Atlanta, GA**

ThP 676 **Proteomic Differences and Protein Acetylation by Sirtuins in Response to Cell Aging; Liting Deng¹; Mehdi Mirzaei¹; Paul Andrew Haynes¹; ¹Macquarie University, Sydney, Australia**

ThP 677 **PPPome Profiling Using Quantitative Proteomics Reveals the Role of PP2Ac phosphorylation in Regulating PP2A-B55 Mediated Dephosphorylation of Mitotic Substrates; Isha Nasa^{1,2}; Lauren Cressey¹; Thomas Kruse³; Emil PT Hertz³; Jakob Nilsson³; Arminja N Kettenbach^{1,2}; ¹Department of Biochemistry and Cell Biology, Dartmouth College, Hanover, NH; ²Norris Cotton Cancer Center, Lebanon, NH; ³Novo Nordisk A/S, Måløv, Denmark**

ThP 678 **Improving Confidence and Productivity for N-Linked Glycan Analysis in Biotherapeutics Development Using an Integrated and Compact LC-FLR-HRMS System; Ximo Zhang¹; Corey Reed¹; Henry Shion¹; Robert Birdsall¹; Ying Qing Yu¹; ¹Waters Corporation, Milford, MA**

ThP 679 **Phosphonate-Modified Core-Shell Structured Fe₃O₄-SiO₂ Nanoparticles: Synthesis, Characterization and Application to the Enrichment of Phosphopeptides; Qingshi Meng¹; Xiaohui Feng¹; Xiangfang Tang¹; Hongfu Zhang¹; ¹Institute of Animal Sciences, CAAS, Beijing, China**

ThP 680 **The Acetylation of Lysine-376 of G3BP1 Regulates RNA Binding and Stress Granule Dynamics; Jing Chen¹; Jozsef Gal²; Duck-Young Na²; Laura Tichacek²; Kelly R Barnett²; Haining Zhu^{2,3}; ¹University of Kentucky, Lexington, KY; ²University of Kentucky, Lexington, Kentucky; ³Lexington VA Medical Center, Research & Development, Lexington, Kentucky**

ThP 681 **Ischemic Stress to Kidneys from SIRT5 Mice is mitigated by Succinylation Response; Kevin Peasley¹; Anja N Holtz²; Nathan Basisty²; Takuto Chiba¹; Birgit Schilling²; Sunder Sims-Lucas¹; Eric Goetzman¹; ¹University of Pittsburgh, Pittsburgh, PA; ²Buck Institute, Novato, CA**

ThP 682 **Middle-Down Characterization of Poly-Ubiquitin by 193 nm UVPD and EThcd; Aarti Bashyal¹; Jennifer S Brodbelt¹; ¹University of Texas - Austin, Austin, TX**

ThP 683 **LC-MS Analysis of Bound Sulfane Sulfur in Hypoxic Endothelial Cells; Xinggui Shen¹; Christopher B. Pattillo B. Pattillo¹; Hyung W. Nam¹; Christopher G. Kevil¹; ¹LSU Health-shreveport, Shreveport, LA**

ThP 684 **Ion-Exchange Chromatography On-Line Hyphenated to Mass Spectrometry for the Native Intact In-Depth**

Characterisation of Cationic and Anionic Proteins; Florian Fuessl¹; Angela Criscuolo²; Ken Cook³; Jonathan Bones¹; ¹Nibr, Dublin, Ireland; ²Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, Leipzig, Germany; ³Thermo Fisher Scientific, Hemel Hempstead, UK, Hemel Hempstead, United Kingdom

ThP 685 **Proteome-Wide Detection of Cysteine Nitrosylation Targets and Motifs Using Bioorthogonal Cleavable-Linker-Based Enrichment and Switch Technique (Cys-BOOST); Ruzanna Mnatsakanyan¹; Stavroula Markoutsai¹; Steven H.L. Verhelst^{1,2}; René Zahedi³; ¹Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Dortmund, Germany; ²Laboratory of Chemical Biology, Department of Cellular and Molecular Medicine, KU Leuven - University of Leuven, Leuven, Belgium; ³Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC**

ThP 686 **Quantitative Middle Down Proteomics of Histone H3 Variant-Specific Proteoforms; Tao Wang¹; Matthew V. Holt¹; Nicolas L. Young¹; ¹Baylor College of Medicine, Houston, TX**

ThP 687 **Analysis of the Human Brain Ubiquitylation Pattern Associated with Alzheimer's Disease Using Quantitative Proteomics; Measho Abreha¹; Eric B. Dammer^{1,2}; Lingyan Ping^{1,2}; Tian Zhang¹; Duc M Duong^{1,3}; Marla Gearing¹; James J. Lah¹; Allan I. Levey¹; Nicholas T. Seyfried^{1,2}; ¹Emory University - Center of Neurodegenerative Diseases, Atlanta, GA; ²Emory University-Biochemistry, Atlanta, GA; ³Emory Integrated Proteomics Core, Emory University, Atlanta, GA**

ThP 688 **System-Wide Temporal Characterization of the Phosphoproteome of esophageal squamous Cell Carcinoma Cells; Jun Adachi; National Institutes of Biomedical Innovation, Health and Nutrition, Ibaraki, Japan**

ThP 689 **Scop3P: The Bridge between Human Phosphosites, Protein Structure and Proteomics Data; Pathmanaban Ramasamy^{1,2,3,4}; Demet Turan^{1,2}; Elien Vandermarliere^{1,2}; Lennart Martens^{1,2}; Wim Vranken^{3,4}; ¹VIB-UGent Center for Medical Biotechnology, Ghent, Belgium, Ghent, Belgium; ²Department of Biochemistry, Faculty of Health Sciences, Ghent University, Ghent, Belgium, Ghent, Belgium; ³Interuniversity Institute of Bioinformatics in Brussels, ULB-VUB, Brussels, Belgium; ⁴Structural Biology Brussels, Vrije Universiteit Brussel, Brussels, Belgium**

ThP 690 **Sequence Liability and Developability Assessment of mAb-A; Samuel Korman¹; Mingyan Cao²; Dengfeng Liu²; Sri Hari Raju Mulagapati²; ¹MedImmune, Gaithersburg, MD; ²MedImmune, Gaithersburg, MD**

ThP 691 **Cross-talk between Crucial Protein Post-Translational Modifications (PTMs): O-GlcNAcylation, Phosphorylation, and lys-acetylation; Junfeng Ma; Georgetown Univ., Washington, DC**

ThP 692 **Ubiquitinome Dynamics Upon Proteasome Modulation; Jeroen Demmers; Erasmus University Medical Center, Rotterdam, Netherlands**

ThP 693 **Exploring the Open Proteome: Proteomics Open Search Analysis with PTM-Shepherd; Daniel J Geiszler¹; Andy T. Kong¹; Dmitry M Avtonomov¹; Felipe Da Veiga Leprevost¹; Hui-Yin Chang¹; Alexey I. Nesvizhskii¹; ¹University of Michigan, Ann Arbor, MI**

ThP 694 **Investigation of KRAS 4B C-terminal peptides; James Wilkins; UCSF, San Francisco, CA**

ThP 695 **Impact of Oxidants on Anastellin - a Mediator of Fibronectin Assembly; Per Häggglund¹; Jianfei He²; Huan Cai²; Eva Ramos Becares²; Pontus Gourdon²; Michael J Davies²; ¹University of Copenhagen, Copenhagen N, Denmark; ²University of Copenhagen, Copenhagen, Denmark**

ThP 696 **Identification and Functional Characterizations of Novel Proteins Promoting α-N-demethylation; David Bade¹;**



Lin Li¹; Xiaoxia Dai¹; Yinsheng Wang¹; ¹UC Riverside, Riverside, CA

- ThP 697 **Streamlined Workflows for N-Glycan Analysis of Biotherapeutics Using InstantPC and 2-AB with LC-FLD-MS**; John Yan¹; Andres Guerrero¹; Ace G Galermo¹; Ted Haxo¹; Sergey Vlasenko¹; Justin Hyche¹; Tom Rice¹; Aled Jones¹; ¹ProZyme, A part of Agilent, Hayward, CA

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- ThP 698 **Treasure Hunt for Peptides with Undefined Chemical Modifications: Revealing Differential Albumin Adducts of 2-Nitroimidazole-Indocyanine Green in Hypoxic Tumors**; Lei Wang¹; Christopher Dietz¹; Feifei Zhou²; Mohsen Erfanzadeh²; Quing Zhu^{2,3}; Michael Smith¹; Xudong Yao¹; ¹Department of Chemistry, University of Connecticut, Storrs, CT; ²Department of Electrical and Computer Engineering, University of Connecticut, Storrs, CT; ³Department of Biomedical Engineering, Washington University, St. Louis, MO
- ThP 699 **A Proline/Alanine-Specific Protease for Bottom-up Mass Spectrometry Workflows**; Chris Hosfield¹; Michael Rosenblatt¹; Marjeta Urh¹; ¹Promega, Madison, WI
- ThP 700 **Cysteine-Selective Middle-Down Proteomics with Ultraviolet Photodissociation Analysis**; Sean D. Dunham¹; Jennifer S Brodbelt¹; ¹University of Texas at Austin, Austin, TX
- ThP 701 **Carrier-Assisted Single-Tube Processing Approach for Targeted Proteomics Analysis of Low Numbers of Mammalian Cells**; Pengfei Zhang¹; Matthew J. Gaffrey¹; Ying Zhu¹; William B. Chrisler¹; Thomas L. Fillmore¹; Carrie D. Nicora¹; Wei-Jun Qian¹; Richard D. Smith¹; Tao Liu¹; Tujin Shi¹; ¹PNNL, Richland, WA
- ThP 702 **Enhancing Middle-Down Proteomics by Limited Carbamylation of Intact Proteins and Lys-C Digestion**; Michael B Lanzillotti¹; Jennifer S Brodbelt¹; ¹University of Texas at Austin, Austin, TX
- ThP 703 **An MS Approach based on Randomized Phosphopeptide Libraries to Study the Sequence Preference of Protein Phosphatases 1 and 2A**; Bernhard Hoermann^{1,2}; Dominic Helm³; Thomas Kokot¹; Jeremy Chojnacki¹; Mikhail Savitski^{2,3}; Maja Koehn^{1,2}; ¹BIOSS Centre for Biological Signaling, Freiburg University, Freiburg, Germany; ²Genome Biology Unit, EMBL, Heidelberg, Germany; ³Proteomics Core Facility, EMBL, Heidelberg, Germany
- ThP 704 **A Novel Automated LC-MS Data Processing Platform for Immuno Reactivity Assessment of Antibodies Developed against Host Cell Proteins**; Yu Zhou¹; Meghna Patel¹; Riccardo Staccini¹; Geuncheol Gil¹; Sushmita Mimi Roy¹; ¹BioMarin, Novato, CA
- ThP 705 **Systematic Identification of Direct Substrates of Src Homology 2 Containing Protein Tyrosine Phosphatase 2**; Peipei Zhu¹; Ruoyu Zhang²; Chuan-Chih Hsu³; Zhong-Yin Zhang²; Weiguo Andy Tao²; ¹Purdue University, West Lafayette, IN; ²Purdue University, West Lafayette, IN; ³Stanford University, Stanford, CA
- ThP 706 **Assessing Protein Sequence Database Suitability Using de novo Sequencing**; Richard S. Johnson¹; Brook L. Nunn¹; Brian C Searle^{2,3}; Molly Phillips^{1,4}; Chris T. Amemiya⁴; Michelle Heck⁵; Micheal J MacCoss¹; ¹University of Washington, Seattle, WA; ²Institute for Systems Biology, Seattle, WA; ³Proteome Software, Portland, OR; ⁴University of California, Merced, Merced, CA; ⁵USDA ARS, Ithaca, NY
- ThP 707 **QCforLife (QC4L) Harmonization Study: A Core Facility Alliance to Improve Proteomics Quality Control and Instruments Performance**; Cristina Chiva^{1,2}; Roger Olivella^{1,2}; Amanda Solé^{1,2}; Daniel Mancera^{1,2}; Dominic Helm³; Mikhail Savitski³; Teresa Mendes Maia^{4,5}; Evy Timmerman^{4,5}; Francis Impens^{4,5}; Damarys Loew⁶; Christian Panse⁷; Tobias Kockmann⁷; Laura Kunz⁷; Paolo Nanni⁷; Henrik Thomas⁸; Andrea Schuhmann⁸; Anna Shevchenko⁸; Thibault Douche⁹; Mariette Matondo⁹; Karl Mechtler¹⁰; Eduard Sabido^{1,2}; ¹Centre de Regulació Genòmica, Barcelona, Spain; ²Universitat Pompeu Fabra, Barcelona, Spain; ³EMBL, Heidelberg, Heidelberg, Germany; ⁴VIB, Gent, Belgium; ⁵Ghent University, Gent, Belgium; ⁶Institute Curie, Paris, France; ⁷Functional Genomic Center Zürich, Zurich, Switzerland; ⁸Max Planck Institute for Molecular Cell Biology and Genetics, Dresden, Germany; ⁹Institut Pasteur, Paris, France; ¹⁰Institute of Molecular Pathology, Vienna, Austria
- ThP 708 **Application of Human and Mouse Immunodepletion Reagents to Mouse Plasma with Proteomic Depth/Coverage Comparison Utilizing a Data-Independent Acquisition Workflow**; Daryl Bulloch¹; Matthew Rardin¹; Bradford W Gibson¹; ¹Amgen, South San Francisco, CA
- ThP 709 **Application of Logic Programming to Large-Scale Phosphoproteomics Data Reveals New Biological Insight**; George A Elder¹; Conrad Bessant¹; Pedro Cutillas¹; ¹Queen Mary University of London, London, United Kingdom
- ThP 710 **High-Resolution Proteolipidome Analysis of Hippocampal Tissue in an Alzheimer's Disease Mouse Model**; Whitaker Cohn¹; Lucy Wanrong Gao¹; Annie Tagvoryan¹; Jesus Campagna¹; Kym Faull¹; Varghese John¹; Julian Whitelegge¹; ¹University of California Los Angeles, Los Angeles, CA
- ThP 711 **Filter Aided, Single Tip Based (FAST) Method for High Throughput, Ultrasensitive Proteomics Analysis**; Zhenbin Zhang¹; Norman Dovichi¹; ¹University of Notre Dame, Notre Dame, IN
- ThP 712 **Five-Minute Proteome: An MS/MS-Free Approach to Protein Identification and Quantification**; Mark V Ivanov¹; Julia A Bubis^{1,2}; Vladimir Gorshkov³; Irina A Tarasova¹; Elizaveta M Solovyeva^{1,2}; Lev I Levitsky¹; Anna A Lobas¹; Marina L Pridatchenko¹; Frank Kjeldsen³; Mikhail V Gorshkov^{1,2}; ¹Institute for Energy Problems of Chemical Physics RAS, Moscow, Russia; ²Moscow Institute of Physics and Technology (State University), Dolgoprudny, Russia; ³University of Southern Denmark, Odense, Denmark
- ThP 713 **Next Generation StageTip for Capturing Extremely Hydrophilic Peptides**; Kosuke Ogata¹; Chia-Feng Tsai²; Naoyuki Sugiyama¹; Yasushi Ishihama¹; ¹Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, Japan; ²Pacific Northwest National Laboratory, Richland, WA
- ThP 714 **Chemical Modification of Proteins to Mimic LysC Proteolysis: Application of 1,2-dicarbonyl Compounds for Arginine Modification**; Boomathi Pandeswari Pandi¹; Varatharajan Sabareesh¹; A.s. Kamalanathan¹; Sripathi Prabhakar²; ¹Advanced Centre for Bio Separation Technology (CBST), Vellore Institute of Technology (VIT), Vellore, India; ²Centre for Mass Spectrometry, Analytical Department, CSIR – Indian Institute of Chemical Technology (IICT), Hyderabad, India
- ThP 715 **Deep Proteome Profiling of Human Hair Shafts**; Evelyne Maes¹; Jolon M Dyer^{1,2,3,4}; Stefan Clerens^{1,2,3}; ¹AgResearch Ltd., Christchurch, New Zealand; ²Biomolecular Interaction Centre, Christchurch, New Zealand; ³Riddet Institute, Massey University, Christchurch, New Zealand; ⁴Wine, Food and Molecular Biosciences, Lincoln, New Zealand
- ThP 716 **Proteome Profiling of 1–10 Circulating Tumor Cells Isolated from Whole Blood**; Yiran Liang¹; Jennifer Podolak²; Yongzheng Cong¹; George V. Thomas²; Ying Zhu³; Ryan T. Kelly^{1,3}; ¹Brigham Young University, Provo, UT; ²Oregon Health and Science University, Portland, OR; ³Pacific Northwest National Laboratory, Richland, WA



- ThP 717 **Comparative Analysis of Lectin Based Glycoproteins among Elderly Non-Cancer Yoga Groups;** Min-gyu Youn¹; Junghoon Kang¹; Youngwon Jung²; Wonryeon Cho¹; ¹Wonkwang University, Iksan, South Korea; ²Yonsei University, Seoul, South Korea
- ThP 718 **Fast-track MyHC Profiling Reveals Fiber Type-Specific Protein Changes in Myostatin-Deficient Skeletal Muscle Tissue;** Sebastian Kallabis¹; Hendrik Nolte²; Lena Abraham¹; Clara Tuerk³; Janica Wiederstein³; Thomas Braun⁴; Marcus Krueger³; ¹CECAD Research Center / University of Cologne, Cologne, Germany; ²Max Planck Institute for Biology of Ageing, Cologne, Germany; ³CECAD Research Center / University of Cologne, Cologne, Germany; ⁴Max Planck Institute for Heart and Lung Research, Bad Nauheim, Germany
- ThP 719 **Comparison of Peptide Separation Methods to Maximize the Mutational Landscape in a Cell Line Model System Used for Neoantigen Discovery;** Sachin Kote¹; Jakob Faktor²; Goran Mitulovic³; Georges Bedran¹; Javier Alfaro¹; Satya Saxena^{1,4}; David Goodlett^{1,5}; Borek Vojtesek²; Theodore Hupp^{1,2,6}; ¹International Centre for Cancer Vaccine Science, University of Gdansk, Gdansk, Poland; ²RECAMO, Brno, Czech Republic; ³Medical University of Vienna, Vienna, Austria; ⁴Deurion LLC, Seattle, WA; ⁵University of Maryland, Baltimore, MD; ⁶CRUK, University of Edinburgh, Edinburgh, United Kingdom
- ThP 720 **Wheat Pan-Proteomics: Unifying Data-Independent LC-MS Proteome Measurements across Diverse Genetic Backgrounds for Trait Screening and Classification;** James A Broadbent¹; Sally Stockwell¹; Keren Byrne¹; Utpal Bose¹; Shannon Dillon²; Kerrie Ramm²; Ben Trevasakis²; Michelle Colgrave¹; ¹CSIRO, St Lucia, Australia; ²CSIRO, Canberra, Australia
- ThP 721 **Improved Data Acquisition Settings on a Q Exactive HF-XTM Mass Spectrometer for Proteomic Analysis of Limited Samples;** Antonius Koller¹; Michal Gregus¹; Alexander Ivanov¹; ¹Northeastern University, Boston, MA
- ThP 722 **High-Throughput Single-Cell Proteomics Enabled by a Simplified Method for Automated Sample Preparation;** Harrison Specht¹; Guillaume Harmange¹; David H. Perlman^{1,2}; Edward Emmott¹; Zachary Niziolek³; Bogdan Budnik³; Nikolai Slavov¹; ¹Northeastern University, Boston, MA; ²Merck Exploratory Sciences Center, Cambridge, MA; ³Harvard University, Cambridge, MA
- ThP 723 **Optimizing Peptide Fractionation to Maximize Content in Cancer Proteomics;** Victoria Izumi¹; Bin Fang¹; Paula Oliveira¹; Mark Meads¹; Kenneth Shain¹; John Koomen¹; ¹Moffitt Cancer Center & Research Institute, Tampa, FL
- ThP 724 **Detection of Aberrant Proteoforms from Alternative Splicing Events in Tandem Mass Tagged Proteomic Datasets;** Daniel Roeth¹; Meiling Jin¹; Yiming Wu¹; Lili Wang¹; Markus Kalkum¹; ¹City of Hope, Duarte, CA
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- ThP 725 **Quantitation of Specific Membrane Proteins Allows Distinguishing between Microparticles and Exosomes;** Linwen Zhang^{1,2}; Illarion V. Turko^{1,2}; ¹Institute for Bioscience and Biotechnology Research, Rockville, MD; ²National Institute of Standards and Technology, Gaithersburg, MD
- ThP 726 **Efficient Reduction of Oxidized Methionine Residues for Quantitative Proteomics;** Siyu Wang¹; Clementina Mesaros¹; Ian A. Blair¹; ¹University of Pennsylvania, Philadelphia, PA
- ThP 727 **Quantitative Proteomics of Lethal Thrombosis Model Mice and Vascular Endothelial Cells by SWATH Analysis;** Hinano Tasaki¹; Mina Kawamura¹; Seiya Kawahara¹; Fumihiko Nagano¹; Ayaka Goto¹; Kei-ichiro Iwaki¹; Mai Sakai¹; Fumitaka Tani¹; Mie Shimizu¹; Tomohiro Mizuno¹; Ken-ichi Harada¹; Susumu Y. Imanishi¹; ¹Meijo University, Nagoya, Japan
- ThP 728 **Evaluation of Thermal Proteome Profiling with an Extended Temperature Range and Different Mass Spectrometry Data Acquisition Methods;** Yingrong (Mary) Xu¹; Graham M. West¹; Robert A. Everley¹; ¹Pfizer Inc., Groton, CT
- ThP 729 **Advances in Single Cell Proteomics through Profiling of Cardiac Micro Tissue;** Claudia Ctordecka¹; Johannes Stadlmann²; Pablo Hofbauer²; Katherina Tavernini²; Sasha Mendjan²; Karl Mechtler^{1,2,3}; ¹Research Institute of Molecular Pathology, Vienna, Austria; ²Institute of Molecular Biotechnology, Vienna, Austria; ³Gregor Mendel Institute of Molecular Plant Biology, Vienna, Austria
- ThP 730 **Proteomics of Red-sided Garter Snake (Thamnophis Sirtalis Parietalis).— Identification and Quantification of Putative Pheromone Binding Proteins in Harderian Gland;** Liping Yang¹; Ehren Bentz²; Robert T. Mason²; Claudia S. Maier^{1,3}; ¹Department of Chemistry, Oregon State University, Corvallis, Oregon; ²Department of Integrative Biology, Oregon State University, Corvallis, OR; ³Linus Pauling Institute, Oregon State University, Corvallis, OR
- ThP 731 **Identification of Dynamic Heme-Binding Proteins by Quantitative Mass Spectrometry;** Hyojung Kim¹; David A. Hanna¹; Amit R. Reddi¹; Matthew P. Torres¹; ¹Georgia Institute of Technology, Atlanta, GA
- ThP 732 **The Mechanistic Understanding of Apc Mutation and p16 Epimutation in Intestinal Tumorigenesis;** Jong Min Choi¹; Jin Feng¹; Antrix Jain¹; Hamssika Chandrasekaran¹; Yue Chen¹; Matthew V. Holt¹; Li Yang¹; Anusha Mandala¹; Lanjing Zhang²; Sayantani Goswami¹; Nan Gao²; Yi Wang¹; Anna Malovannaya¹; Lanlan Shen¹; Sung Yun Jung¹; ¹Baylor College of Medicine, Houston, TX; ²Rutgers University, Newark, NJ
- ThP 733 **Cellular Responses of Breast Cancer Cell Line to Anti-Cancer Medicinal Compounds from Ginger Root;** Parvin Mirzaei¹; Luke Brown²; Jaicee Tudman²; Adam Reinhart²; Masoud Zabet Moghaddam¹; ¹Texas Tech University, Lubbock, TX; ²Wayland Baptist University, Plainview, TX
- ThP 734 **Development of Targeted Mass Spectrometry-Based Approaches for Quantitation of Proteins Enriched in the Post Synaptic Density (PSD);** Rashaun Wilson¹; Navin Rauniyar²; Tukiet T. Lam¹; Kenneth R. Williams¹; Angus C. Nairn¹; ¹Yale University, New Haven, CT; ²Tanvex BioPharma Inc., San Diego, CA
- ThP 735 **KIT QUANTA - Standardization Kit for Absolute Protein Quantitation: Monitoring of Methionine Oxidation Induced by Chromatography Separation;** France Baumans¹; Dominique Baiwir^{1,2}; Maria Colombo³; Camille Allain⁴; Vincent Tavernier⁴; Baptiste Leroy⁴; Ruddy Wattiez⁴; Edwin De Pauw¹; Gauthier Eppe¹; Gabriel Mazzucchelli^{1,2}; ¹University of Liege, Mass Spectrometry Laboratory, MolSys Research Unit, Liege, Belgium; ²University of Liège, GIGA Proteomics Facility, Liege, Belgium; ³Kaneka Eurogentec S.A., Seraing, Belgium; ⁴University of Mons, Proteomics and Microbiology Laboratory, Mons, Belgium
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