Welcome to the 71st ASMS Conference on Mass Spectrometry and Allied Topics. Conference program activities and exhibit booths are in the George R. Brown Convention Center. Corporate Hospitality Suites are at the Hilton Americas.

Sponsors
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BADGE PRINTING is open 10:00 am - 8:00 pm on Sunday and 7:30 am - 5:00 pm Monday - Thursday.

ATTENTION

UNDERGRADUATE STUDENTS AND FIRST TIME (at ASMS)

GRADUATE STUDENTS

4:00 - 4:45 pm, Sunday, Hall B3

Plan Your Strategy: What to See and Do at ASMS

SUNDAY TUTORIAL SESSION I, Hall B3
5:00 – 5:45 pm
Mass Spectrometry and Medicine
Livia Eberlin
Baylor College of Medicine

SUNDAY TUTORIAL SESSION II, Ballroom A
5:00 – 5:45 pm
Mass Spectrometry and Anti-Doping Research
Mario Thevis
Institute of Biochemistry, Center for Preventive Doping Research, German Sport University Cologne

SUNDAY SPECIAL KEYNOTE SESSION 5:45 - 6:30 pm, Hall B3
Jeremy Edwards
Chair, Houston LGBTQ Advisory Committee
Activism in Houston - Boots on the Ground: Progress & Challenges

SUNDAY CONFERENCE OPENING 6:45 - 7:45 pm, Hall B3
Welcome
Joseph A. Loo
University of California, Los Angeles
ASMS Vice President for Programs

From Human Genome Project to Precision Medicine - A Journey in Chemistry and Technology
Richard A. Gibbs
Baylor College of Medicine

SUNDAY WELCOME RECEPTION 7:45 - 9:00 pm
Posters-Exhibits Hall (Level One). Conference name badge is required.

Monday Award Lecture 4:45 - 5:30 PM, Hall B3
John B. Fenn Award for a Distinguished Contribution in Mass Spectrometry
Carol V. Robinson
University of Oxford

Tuesday Award Lecture 4:45 - 5:30 PM, Hall B3
Biemann Medal
Brandon Ruotolo
University of Michigan

Wednesday ASMS Meeting 4:45 - 5:30 PM, Hall B3
Enjoy a beverage, hear ASMS Board reports and applaud award recipients.

Thursday Plenary Session 4:45 - 5:30 PM, Hall B3
The Rise and Reign of the Mammals: A New History, from the Shadow of the Dinosaurs to Us
Stephen Brusatte
University of Edinburgh

Thursday Closing Event
ADVANCE PURCHASE TICKET REQUIRED
TICKET SALES CLOSE AT 12PM (noon), MONDAY, JUNE 5
Buy your ticket online via Registration portal. If you purchase after printing your name badge, you will need to re-print your badge.

The event is at the Houston Museum of Natural Science on Thursday, June 8, 7:00 - 10:00 pm. Buffet dinner is included. Cash bars available. Enjoy the INCREDIBLE paleontology and gem exhibitions at the museum. Closing plenary speaker, Steve Brusatte, will attend the event and provide additional Q&A in the Morian Hall of Paleontology.

There is no organized transportation to/from the event. Attendees with the closing event icon on their badge have round-trip light rail included. Please wear your badge in case there is ticket control. Engineers will identify your closing event icon as your paid ride. Light rail instructions are included in the app and will be emailed to all who have purchased the closing event.

The Houston Museum of Natural Science is located at 5555 Hermann Park Drive, Houston TX 77030.
If you do not wish to take the light rail, Uber/Lyft or taxis are available at standard rates.

Consult online planner or mobile app for detailed program.
**General Information**

**Oral Sessions** are 8:30 - 10:30 am and 2:30 - 4:30 pm Monday through Thursday. All session rooms are on Level Three.

- Session A (MOA, TOA, WOA, ThOA) .................Hall B3
- Session B (MOB, TOB, WOB, ThOB) ...............Ballroom A
- Session C (MOC, TOC, WOC, ThOC) ..............Ballroom B
- Session D (MOD, TOD, WOD, ThOD)..............Ballroom C
- Session E (MOE, TOE, WOE, ThOE)..............Room 332
- Session F (MOF, TOF, WOF, ThOF)..............General Assembly A
- Session G (MOG, TOG, WOG, ThOG)............General Assembly B
- Session H (MOH, TOH, WOH, ThOH)...General Assembly C

**Oral Presentations.** Speakers are required to use the ASMS computers for their presentations. ASMS will have a PC and MAC available in each session room for presentations.

**Speakers** must load presentations at least one day prior to their talks. The speaker ready room is Room 330 AB. The room is open with a technician according to this schedule:

- Sunday 10:00 am - 8:00 pm
- Monday through Wednesday 7:30 am - 6:00 pm
- Thursday 7:30 am - 2:30 pm

**Posters and Exhibit Booths,** Halls BC (Level One). The Hall is open:

- Sunday Welcome Reception ....7:45 pm - 9:00 pm
- for Exhibit Booths & Undergrad Poster Competition
- Monday - Wednesday ...............6:30 am - 8:00 pm
- find exhibit booths staffed 9am-5pm
- Thursday ........................................6:30 am - 2:30 pm
- find exhibit booths staffed 9am-2pm

**Poster Set-Up** is by 8:30 am on the day scheduled. A counter for poster supplies is inside the main entrance to the Hall (Level One).

**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. This schedule allows for a one-hour non-overlapping lunch break. All presenters are now scheduled for 3 hours (authors are welcome to attend the full four hours).

- 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.

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 at 2:30 pm.

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

**Workshops** are 5:45 - 7:00 pm on Monday, Tuesday, and Wednesday. Light refreshments are provided.

**Free WiFi Access** is available throughout the convention center, look for the ASMS network on your device and use password asms2023.

**Career Center** is located in Room 352DEF (Level Three). The Career Center is open to all conference attendees. Applicants and employers must enter resumes and employment opportunities online. There are computers in the center for searching the database of candidates and positions. Interview rooms are available nearby and should be reserved one-day in advance.

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

**Gender Neutral Restrooms** locations throughout the convention center. Please ask at the Information counter near badge printing on Level One if you need assistance finding these locations.

**Mother’s Lounge** is available for use by nursing mothers. For location, please consult General Information in mobile app or ask at the Information counter near badge printing on Level One.

**Thursday Closing Event**

**Advance Purchase Ticket Required**

**Ticket Sales Close at 12PM (noon), Monday, June 5**

Buy your ticket online via Registration portal. If you purchase after printing your name badge, you will need to re-print your badge.

The event is at the Houston Museum of Natural Science on Thursday, June 8, 7:00 - 10:00 pm. Buffet dinner is included. Cash bars available. Enjoy the INCREDIBLE paleontology and gem exhibitions at the museum. Closing plenary speaker, Steve Brusatte, will attend the event and provide additional Q&A in the Morian Hall of Paleontology.

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The Houston Museum of Natural Science is located at 5555 Hermann Park Drive, Houston TX 77030.

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CODE OF CONDUCT

The ASMS Code of Conduct guides the expected, professional behavior of all participants at conferences, short courses, and conference-related activities and events.

**Acceptable behavior includes:**
- Treating everyone with respect and consideration;
- Communicating openly and thoughtfully with others and being considerate of the multitude of views and opinions that may be different from your own;
- Being respectful and mindful in your critique of ideas;
- Being mindful of your surroundings and of your fellow participants.

**Unacceptable behavior includes:**
- Harassment and intimidation, including any verbal, written, or physical conduct designed to threaten, intimidate, or coerce any participant, speaker, exhibitor, conference or event organizer or staff, service provider, volunteer, or guest;
- Discrimination based on gender or gender identity, sexual orientation, age, disability, physical appearance, body size, race, religion, national origin, culture, or any other characteristic provided by law;
- Physical or verbal abuse of any participant, speaker, exhibitor, conference or event organizer or staff, service provider, volunteer, or guest;
- Threats of physical violence against any participant, speaker, exhibitor, conference or event organizer or staff, service provider, volunteer, or guest; and
- Disrespectful disruption of presentations.

**Consequences of unacceptable behavior:**
Anyone who violates this Code may be subject to the consequences. ASMS reserves the right to take action beyond these consequences as necessary based on a participant’s behavior in violation of the Code.
- Anyone requested to stop unacceptable behavior is expected to comply immediately;
- Immediate removal from the meeting or event without warning and potentially without refund; and/or
- Prohibition from attending future meetings or events in the sole determination of ASMS.

**Who to contact:**
ASMS Executive Director, Jennifer Watson, jennifer@asms.org

ASMS is proud of our annual conferences, short courses, and conference-related events and wants everyone to have a positive learning and networking experience. Embracing the above professional behavior will help ensure a great experience for all involved.

Text adapted from https://www.frontiersin.org/articles/10.3389/fmars.2016.00103/full


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CONFERENCE REGULATIONS

**Name badge is required** for all conference sessions, short courses, and conference-related events (hospitality suites, closing event.)

**All devices** must be silenced and screens darkened in oral sessions.

**No photography or recording** is allowed in oral sessions or in the poster hall.

**Publicity Release.** By attending or participating in an ASMS event, attendees agree to allow their names, likenesses, and images, in audio, photographic or video format recorded for the event and onsite, to be used by ASMS for educational, promotional, or marketing of ASMS events or activities.

**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. If you wish to cite an abstract presented at the annual conference, please use the citation guidelines for conference proceedings found at asms.org.

**The placement of advertising** in the meeting area is prohibited. There are poster boards and tables in the Poster/Exhibit Hall for approved announcements. Ask at Registration desk to have your announcement approved.

**Hardware, accessories or any items for sale** may be displayed only in corporate exhibit booths and hospitality suites.

**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 are permitted.

In general, ASMS provides the following advice for parents considering bringing child(ren) or infant(s):
Planned conference sessions and hospitality suites may not be appropriate for children. Please respect the interests of your colleagues 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 with careful supervision by parents. Strollers are prohibited in the hospitality suites.
INFORMATICS HUB
Inside the Poster/Exhibit Hall
daily during poster sessions.

The Informatics Hub is a place where informaticians gather with three aims:
1. to provide their advice, knowledge, and support to ANYONE with a relevant question;
2. to discuss current issues and challenges in mass spectrometry informatics with the entire community;
3. to work on interesting, synergistic projects and to freely exchange tools, algorithms, and know-how with each other, across all labs, seniorities and levels of experience.

SPECIAL 3D PRINT DISPLAY
Inside the Poster/Exhibit Hall

Get inspired for your own design and access useful design files from your colleagues. 3D prints on display represent:
- MS Parts
- LC and other Labware
- Educational items

LOOK
HISTORY POSTERS
Main foyer near entrance to Posters/Exhibit Hall.

NETWORKING OPPORTUNITIES
Special Gap Hour Receptions

Monday, Tuesday & Wednesday 7:00-8:00 PM

Monday, 7pm / Ballroom B
Sponsored by Agilent
Reception immediately following workshop 06 Networking for Scientists: Celebrating Women Mass Spectrometrists. All are welcome to join for networking focused on supporting women in mass spectrometry and the FeMS organization.

Tuesday, 7pm / Ballroom B
Sponsored by SCIEX
Reception immediately following workshop 06 Recognizing the “A” in DEIA: Effective Ways to Improve Accessibility for Mass Spectrometrists. All are welcome to join for networking focused on accessibility, diversity, and inclusion.

Wednesday, 7pm | Ballroom B
Sponsored by SEER
Reception immediately following workshop 06 MS Career Options: How to Kick Start Your Career. All are welcome to join for networking focused on career development.

Funding Agency Office Hours
Inside Posters/Exhibit Hall Monday-Thursday 10:30 am - 2:30 pm. Meet with representatives from various funding agencies. Appointment sign-up sheets will be posted on ‘office’ entry sign (along main entry inside posters-exhibits area).

Attendees are encouraged to take advantage of this valuable resource while at the conference.
CONGRATULATIONS
to these members who are elected to serve on the ASMS Board. Their terms begin July 1, 2023

President
Julia Laskin
Purdue University
West Lafayette, IN

Past President
Susan D. Richardson
University of South Carolina
Columbia, NC

Vice President for Programs
Joseph A. Loo
University of California, Los Angeles
Los Angeles, CA

Vice President for Arrangements
Michael Easterling
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Billerica, MA

Treasurer
Sharon Pitteri
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Palo Alto, CA

Secretary
Jessica Prenni
Colorado State University
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Livia Eberlin
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Member-at-Large for Membership
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USDA Food Safety and Inspection Service
Atlanta, GA

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Stephen Valentine
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Morgantown, PA

Vice President for Arrangements
Patrick Batoon
Agilent Technologies
Santa Clara, CA

Secretary
Stephanie M. Cologna
University of Illinois Chicago
Chicago, IL

Member-at-Large for Publicatins
Kelly M. Hines
University of Georgia
Athens, GA
## Interest Group Coordinators

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## Committees

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<td>Asilomar Conference (ACMS)</td>
<td>Jason Hogan, Susan Richardson</td>
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<td>Audit</td>
<td>Ying Ge, Kevin Bateman, Lijiliana Pasa-Tolic, Sharon Piterri, Michael Easterling</td>
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<td>Corporate Liaison</td>
<td>Jeremy Cook, MOBIlion Systems, Angie Jinks, Melanie Juba, Lance Nicolaysen, Bruce Peat, St John Skilton, Protein Metrics</td>
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<td>Digital Communications</td>
<td>Birgit Schilling, Lauren Stopfer, Thomas Wales, Susan Richardson</td>
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<td>Membership, Diversity, and Inclusion</td>
<td>Candice Ulmer-Holland, Dominic Gostick, Hee-Yong Kim, Baljit Ubhi</td>
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<td>Education</td>
<td>Livia Eberin, Joseph Eschweiler, Lisa O’Callaghan, Stacy Malaker, Ian Webb</td>
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<td>P. Jane Gale, Catherine Fenselau, David Herold, Asher Newsome, Magnus Palmblad, Michael Grayson, ex-officio</td>
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<td>Jennifer Brodbelt, Peggi Angel, Tarun Anumol, Abraham Badu-Tawiah, Touradj Solouki</td>
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<td>Stephen Valentine, Joe Cannon, Vanessa Phelan, Stefanie Thomas, Vicki Wysocki, ex officio</td>
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<td>Sanibel Conference</td>
<td>Richard Rogers, Sarah Rogstad, Sharon Piterri</td>
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JOHN B. FENN AWARD FOR A DISTINGUISHED CONTRIBUTION IN MASS SPECTROMETRY
2023 Recipient: Carol V. Robinson
Award Lecture: 4:45 PM, Monday, Hall B3

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. 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.

Carol V. Robinson is the recipient of the 2023 ASMS John B. Fenn Award for a Distinguished Contribution in Mass Spectrometry for the development of mass spectrometry methods for the analysis and characterization of membrane proteins. Dr. Robinson’s pioneering contributions have improved our fundamental understanding of membrane protein complex structure and the role of lipid binding in membrane protein function. Her work has enabled new knowledge into disease mechanisms and has had tremendous impact in drug discovery. Specific accomplishments include: (1) pioneering development of methods to enable gas phase analysis of membrane protein complexes; (2) the application of ion mobility MS and collision-induced unfolding methods to investigate lipid-membrane protein binding; (3) the application of high-resolution MS to resolve the complexity of lipid-protein binding events; and (4) the innovative development of methods for native analysis of membrane protein complexes and lipid binding.

Her collective achievements have been amplified by her dedication to the dissemination of detailed protocols and troubleshooting advice to the research community – ensuring that others had the necessary information to implement the methods. This outreach has resulted in an active cohort of MS researchers across the globe working on the mass spectrometry of membrane protein complexes.

In 2013 Carol was elevated to the title of “Dame Commander of the Order of the British Empire (DBE)” for services to science and Industry. Professor Dame Carol Robinson is University Chair and Professor of Chemistry, University of Oxford.

BIEMANN MEDAL
2023 Recipient: Brandon Ruotolo
Award Lecture: 4:45 PM, Tuesday, Hall B3

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

Brandon Ruotolo is the recipient of the 2023 ASMS Biemann Medal for his significant contributions in the development and application of novel high performance mass spectrometry technologies for protein and protein complex structure elucidation. Examples of his innovative scientific contributions include: (1) leadership in the development of ion mobility MS (IM-MS) for structural characterization of biopolymers; (2) refinement of collision induced unfolding (CIU) methods that enable determination of the number of autonomously folded domains within proteins and characterization of stability reflective of changes in both local and global protein structure; (3) the use of CIU to probe the relative stability of protein-ligand interactions; (4) the development of chemical cross-linkers to stabilize protein structure in the absence of bulk solvent; (5) integration of IM-MS and other structural MS methods as a high-throughput approach for structural proteomics; and (6) application of IM-MS as a screening tool for therapeutic drug discovery. Dr. Ruotolo has built an impressive research program that is addressing application of high impact to the biology and medical communities.

Dr. Ruotolo is Professor of Chemistry, University of Michigan.
The Al Yergey MS Scientist Awards are sponsored by ASMS to recognize dedication and significant contributions to mass spectrometry-based science by "unsung heroes." The awards are named in memory of Al Yergey a well-respected scientist who was known as a dedicated mentor. Each award is conferred at the ASMS Annual Conference with $1,000 cash award and a recognition memento.

**Eduard Denisov** (Thermo Fisher Scientific) is one of key people whose hard and creative work over the last two decades was crucial for making Orbitrap mass spectrometry the leading technique in high resolution mass spectrometry. He took a leading part in experimental development of all major elements of the Orbitrap technology. Over all these years he remained a reliable, modest and at the same time a very passionate enthusiast of Orbitrap technology, who really cares that every user of this technology is getting the best results.

**Jodie Johnson** (University of Florida) is so extremely valuable to MSREC, the University of Florida, and the larger MS community. No matter where you are in your MS career, from novice to 20 years of experience, one can learn invaluable knowledge from Dr. Johnson. He is a dedicated mentor and his knowledge is expansive in areas of chromatography and mass spectrometry. He loves to share his knowledge and loves to engage in research discussions.

**Amina Woods** (NIDA IRP, NIH) has made significant contributions to MS-based science and her dedication to the field of mass spectrometry is amply featured by her record of research, service and teaching. Amina has willingly offered her knowledge through many venues. Biological mass spectrometry became an integral component of her research activities in the early 1990s when she became affiliated with the late Bob Cotter using plasma desorption MS to characterize biological molecules. From then on, mass spectrometry has been at the heart of much of her research portfolio and her community participation in many mass spectrometry organizations including ASMS.

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**The Ron Hites Award** recognizes an outstanding publication of original research published in JASMS. 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 plaque for principal author and certificates for co-authors.

**Joshua Sharp** (University of Mississippi) is recipient of the 2023 Hites Award along with co-authors Emily E. Chea, Sandeep K. Misra, Ron Orlando, Maria Popov, Robert W. Egan, David Holman, and Scot R. Weinberger for their paper "Flash Oxidation (FOX) System: A Novel Laser-Free Fast Photochemical Oxidation Protein Footprinting Platform", 2021, 32, 1601-1609.
Postdoctoral Career Development Awards in the amount of $5,000 promote professional career development of postdoctoral fellows in the field of mass spectrometry.

- Emma Guiberson, Stanford University
- Haiyan Lu, University of Wisconsin-Madison
- Melanie Odenkirk, Colorado State University
- Suttipong Suttapitugsakul, Beth Israel Deaconess Medical Center
- Yixuan Xie, Washington University School of Medicine

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 for the recipient’s proposed research, are fully funded by Bruker, Thermo Fisher Scientific, and Waters Corporation and are made to the institution of each recipient.

- Kelly Marie Hines, University of Georgia
- Jesse Meyer, Cedars-Sinai Medical Center
- Stacy Malaker, Yale University

Research At Primarily Undergraduate Institution (PUI) Award promotes academic research in mass spectrometry by faculty members and their students at primarily undergraduate institutions (PUIs). The Award of $20,000 for the recipient’s proposed research is fully funded by Agilent and is made to recipient’s institution.

- Erica Jacobs, St. Johns University

### 2023 GRADUATE STUDENT TRAVEL AWARDS

**Award Presentations: ASMS Meeting, 4:45 PM, Wednesday, Hall B3**

<table>
<thead>
<tr>
<th>Name</th>
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<tr>
<td>Elizabeth Bayne</td>
<td>University of Wisconsin-Madison</td>
</tr>
<tr>
<td>Danielle Caefer</td>
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<tr>
<td>Hsin-Hsiang Chung</td>
<td>National Taiwan University</td>
</tr>
<tr>
<td>Steven DeFiglia</td>
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</tr>
<tr>
<td>Sarah Dowling</td>
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<tr>
<td>Viraj Gandhi</td>
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<tr>
<td>Yanting Guo</td>
<td>University of Oklahoma</td>
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<tr>
<td>Kejun Yin</td>
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### 2023 UNDERGRADUATE STUDENT TRAVEL AWARDS

**Award Presentations: ASMS Meeting, 4:45 PM, Wednesday, Hall B3**

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<td>Megan Bindra</td>
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<td>Kejun Yin</td>
<td>Georgia Institute of Technology</td>
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[Images of award recipients]
**DOWNTOWN HOTELS**

1. Aloft Houston Downtown  
   0.5 miles — 15 min. walk
2. Cambria  
   0.6 miles — 15 min. walk
3. Courtyard by Marriott  
   0.5 miles — 15 min. walk
4. Embassy Suites Hotel  
   0.3 miles — 10 min. walk
5. Four Seasons  
   0.5 miles — 15 min. walk
6. Hampton Inn  
   0.3 miles — 10 min. walk
7. Hilton Americas Houston  
   Connected to GRB via Skybridge
8. Homewood Suites  
   0.3 miles — 10 min. walk
9. Le Meridien  
   0.5 miles — 15 min. walk
10. Marriott Marquis  
    Connected to GRB via Skybridge
11. Residence Inn Houston  
    0.6 miles — 15 min. walk
12. Springhill Suites  
    0.6 miles — 15 min. walk
13. The Laura  
    0.5 miles — 15 min. walk
### MEDIA EVENTS (PRESS CONFERENCES) AT HILTON AMERICAS

All members of the press are invited to attend these events at the Hilton Americas.

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<th>Time</th>
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<td>Shimadzu</td>
<td>Grand Ballroom GHI</td>
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<tr>
<td>9:30 - 10:30 am</td>
<td>Bruker Daltonics</td>
<td>Americas Ballroom AB</td>
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<td>11:00 am - 12:00 pm</td>
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<td>1:30 - 2:30 pm</td>
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<td>3:00 – 4:00 pm</td>
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<tr>
<td>4:30 – 5:30 pm</td>
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### BREAKFAST SEMINARS AT CONVENTION CENTER & HILTON AMERICAS

Breakfast Seminars are hosted by Corporate Members at the George R. Brown Convention Center and the Hilton Americas. Pre-registration (RSVP) is recommended. Please look for Breakfast Seminars page on www.asms.org and in the online planner / mobile app to find online registration links for these events.

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<td>Biognosys</td>
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<tr>
<td>Bruker</td>
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<td>The Metabolomics Innovation Centre</td>
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<td>Thermo Fisher Scientific</td>
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<td>Zef Scientific, Inc.</td>
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</table>

ASMS is grateful for the support of all Corporate Members. Technologies and services developed by these companies are vital to the ASMS community and the field of mass spectrometry.
PROGRAM ACKNOWLEDGEMENTS

Vice President for Programs

Joseph A. Loo
University of California, Los Angeles
Vice President for Programs

STUDENT ASSISTANTS

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

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Jinhui Zhang
Xueyun Zheng
Mowei Zhou
### PROGRAM OVERVIEW

#### SATURDAY

<table>
<thead>
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<th>Time</th>
<th>Short Courses</th>
<th>Name Badge Printing &amp; Information</th>
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<tr>
<td>9:00 AM - 5:00 PM</td>
<td>(Badge printing for short courses is 8-9am)</td>
<td>Level One Lobby (outside Hall B)</td>
</tr>
<tr>
<td>2:00 - 5:00 PM</td>
<td><strong>ATTENTION:</strong> First-time Graduate Students and Undergraduate Students</td>
<td>Level One Lobby (outside Hall B)</td>
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**Level One Lobby (outside Hall B)**

#### SUNDAY

<table>
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<th>Time</th>
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<td>9:00 AM - 4:30 PM</td>
<td>(Badge printing for short courses is 8-9am)</td>
<td>Level One Lobby (outside Hall B)</td>
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<tr>
<td>10:00 AM - 8:00 PM</td>
<td><strong>ATTENTION:</strong> First-time Graduate Students and Undergraduate Students</td>
<td>Level One Lobby (outside Hall B)</td>
</tr>
<tr>
<td>4:00 - 4:45 PM</td>
<td><strong>ATTENTION:</strong> First-time Graduate Students and Undergraduate Students</td>
<td>Level One Lobby (outside Hall B)</td>
</tr>
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</table>

**Level One Lobby (outside Hall B)**

#### TUTORIAL SESSION I, Hall B3 (5:00 – 5:45 pm)

**Mass Spectrometry and Medicine**

Livia Eberlin
*Baylor College of Medicine*

#### TUTORIAL SESSION II, Ballroom A (5:00 – 5:45 pm)

**Mass Spectrometry and Anti-Doping Research**

Mario Thevis
*Institute of Biochemistry, Center for Preventive Doping Research, German Sport University Cologne*

#### SPECIAL KEYNOTE SESSION, Hall B3 (5:45 - 6:30 PM)

**Activism in Houston - Boots on the Ground: Progress & Challenges**

Jeremy Edwards
*Chair, Houston LGBTQ Advisory Committee*

#### CONFERENCE OPENING PLENARY, Hall A (6:45 - 7:45 PM)

**Welcome, Joseph A. Loo, University of California, Los Angeles**

ASMS Vice President for Programs

**From Human Genome Project to Precision Medicine - A Journey in Chemistry and Technology**

Richard A. Gibbs
*Baylor College of Medicine*

#### WELCOME RECEPTION, Posters-Exhibits Hall (Level One) (7:45 - 9:00 PM)

Join us to celebrate the conference opening, visit exhibit booths. The Undergraduate Student Poster Competition is conducted during the reception. Competition posters are displayed beginning on poster board 001.
### 7:00 AM Corporate Breakfast Seminars, Convention Center (Level Three) and Hilton Americas

### 7:30 AM - 5:00 PM Name Badge Printing & Information, Level One Lobby (outside Hall B)

### 8:30 AM - 10:30 AM Oral Sessions
- **MOA am**: Top Down Protein Analysis, Hall B3
- **MOB am**: Imaging: Instrumentation & Method Development, Ballroom A
- **MOC am**: Clinical Analysis: Innovations, Ballroom B
- **MOD am**: Small Molecules: Structural Characterization and Quantitation, Ballroom C
- **MOE am**: Food Safety & Chemistry: Foodomics, Allergens, Bacteria, Foods, and Supplements, Room 332
- **MOF am**: Covalent Labeling and Chemical Crosslinking, General Assembly A
- **MOG am**: Polymers, General Assembly B
- **MOH am**: Informatics: Metabolomics and Lipidomics, General Assembly C

### 10:30 AM - 2:30 PM Poster Session and Exhibits, Monday Posters, Halls BC
- **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
- 11:30 am - 1:00 pm: Undergraduate students look for reserved tables and free lunch vouchers to Meet the Experts

### 2:30 PM - 4:30 PM Oral Sessions
- **MOA pm**: Single Cell Omics, Hall B3
- **MOB pm**: Ion Mobility: Instrumentation & Method Development, Ballroom A
- **MOC pm**: Structural Biology, Ballroom B
- **MOD pm**: Data-Independent Acquisition and Multiplexing: Lipidomics and Metabolomics, Ballroom C
- **MOE pm**: Food Safety & Chemistry: Innovations, Room 332
- **MOF pm**: Cancer Research, General Assembly A
- **MOG pm**: Fundamentals: Unconventional Approaches in MS, General Assembly B
- **MOH pm**: High Throughput MS, General Assembly C

### 4:45 PM - 5:30 PM Award Lecture, Hall B3
- **John B. Fenn Award for a Distinguished Contribution in Mass Spectrometry** preceded by Al Yergey MS Scientist Awards Presentations
- **Carol V. Robinson**
  *University of Oxford*

### 5:45 PM - 7:00 PM Workshops
- **There are light refreshments in foyers, 5:30 - 5:45 pm.**
- 01 The Role of Mass Spectrometry in Emerging Energy Technologies Development, Room 310 A
- 03 Research and Funding Opportunities at the FDA: Mass Spectrometry for Drug Product Quality, Room 320 A
- 04 Global participatory efforts to characterize the biochemical composition of food: The Periodic Table of Food Initiative and The Proteomes that Feed the World, Room 320 BC
- 05 Single-Cell Proteomic Standardization: From Study Design to Data Analysis, Ballroom A
- 06 Networking for Scientists: Celebrating Women Mass Spectrometrists, Ballroom B
- 08 Ion traps as reaction vessels, Room 332
- 09 Career Opportunities for Chinese Students and Scholars, General Assembly A
- 10 Making Top-Down Mass Spectrometry Easier to Develop and Apply: Ways to Work Together and How Everyone Can Contribute, General Assembly B
- 11 New Aspects in the Development and Implementation of Multi-Attribute Method (MAM), General Assembly C
- 12 Data quality in the core lab: Preventing, catching, reporting and sometimes even fixing! suboptimal "bad data" in a omics core facility aka the "Bad data Workshop", Room 340 AB
- 13 Emerging Techniques for Rapid Fabrication in MS Laboratories, Room 351 ABDE
- 14 Cannabis & Hemp Science: The Importance of Mass Spectrometry, Room 351 CF
- 15 Mind the (Translation) Gap, Room 360 ABDE
- 16 Exposome research: overcoming challenges to deliver answers, Room 360 CF
- 17 Using Casanovo for de novo peptide sequencing, Room 361 ABDE

### 7:00 PM - 8:00 PM Special Gap Hour Reception sponsored by Agilent, Ballroom B
- Reception immediately following workshop 06 Networking for Scientists: Celebrating Women Mass Spectrometrists. All are welcome to join for networking focused on supporting women in mass spectrometry and the FeMS organization.

### After 8:00 PM Corporate Hospitality Suites at Hilton Americas
### TUESDAY

<table>
<thead>
<tr>
<th>Time</th>
<th>Event Description</th>
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<tbody>
<tr>
<td>7:00 AM</td>
<td><strong>Corporate Breakfast Seminars</strong>, Convention Center (Level Three) and Hilton Americas</td>
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<tr>
<td>7:30 AM - 5:00 PM</td>
<td><strong>Name Badge Printing &amp; Information</strong>, Level One Lobby (outside Hall B)</td>
</tr>
<tr>
<td>8:30 - 10:30 AM</td>
<td><strong>Oral Sessions</strong>&lt;br&gt;TOA am: Instrumentation: New Developments in Ionization and Sampling (In Memory of Marvin Vestal), Hall B3&lt;br&gt;TOB am: Biomarkers: Quantitative Analysis, Ballroom A&lt;br&gt;TOC am: Fundamentals: Native MS and Structures of Large Ions, Ballroom B&lt;br&gt;TOD am: Informatics: Peptide and Protein Identification, Proteomics, Ballroom C&lt;br&gt;TOE am: Exposomics, Toxicology, and Health Outcomes, Room 332&lt;br&gt;TOF am: Neurodegenerative Disease Research, General Assembly A&lt;br&gt;TOG am: Drug Metabolism and Pharmacokinetics, General Assembly B&lt;br&gt;TOH am: Imaging: Spatially-Resolved Omics, General Assembly C</td>
</tr>
<tr>
<td>10:30 AM - 2:30 PM</td>
<td><strong>Poster Session and Exhibits</strong>, Tuesday Posters, Halls BC&lt;br&gt;Odd-number posters present: 10:30 - 11:30 am PLUS 12:30 – 2:30 pm&lt;br&gt;Even-number posters present: 10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm</td>
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<tr>
<td>4:45 - 5:30 PM</td>
<td><strong>Award Lecture</strong>, Hall B3&lt;br&gt;Biemann Medal Lecture preceded by Research Award Presentations&lt;br&gt;Brandon Ruotolo&lt;br&gt;University of Michigan</td>
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<tr>
<td>5:45 - 7:00 PM</td>
<td><strong>Workshops</strong>&lt;br&gt;There are light refreshments in foyers, 5:30 - 5:45 pm.&lt;br&gt;01 Open and Reproducible Data Analysis for FT-MS, Room 310 A&lt;br&gt;02 Accelerator Mass Spectrometry (AMS): Current Utility and Future Opportunities, Room 310 BC&lt;br&gt;03 Constructing an Individual Development Plan (IDP), Room 320 A&lt;br&gt;04 The NIH and NSF Review and Funding Process, Room 320 BC&lt;br&gt;05 From data to biology: using -omics datasets to generate an unbiased hypothesis, Ballroom A&lt;br&gt;06 Recognizing the “A” in DEIA: Effective Ways to Improve Accessibility for Mass Spectrometrists, Ballroom B&lt;br&gt;07 Data Independent Acquisition: After the Acquisition, Ballroom C&lt;br&gt;08 FAIR Data Sharing Principles and Barriers: the New NIH Data Management and Sharing (DMS) Policy, Room 332&lt;br&gt;09 Kahoot Trivia! LCMS (and other topics), General Assembly A&lt;br&gt;10 Lipidomics: What does International Lipidomics Society offer to the lipidomic community?, General Assembly B&lt;br&gt;11 Native MS: new approaches to enable discovery in academia and industry, General Assembly C&lt;br&gt;12 New fragmentation methods as seen through the lens of radical ion chemistry, Room 340 AB&lt;br&gt;13 Non-target analysis (NTA): Modern tools for unknown analysis, Room 351 ABDE&lt;br&gt;14 Trans-Proteomic Pipeline: Recent Advances and Future Directions, Room 351 CF&lt;br&gt;15 Imaging MS: Isomer Differentiation in Biological Imaging, Room 360 ABDE&lt;br&gt;16 Mass Spectrometry Support for Extractables and Leachables and Biocompatibility testing, Room 360 CF&lt;br&gt;17 Mass Spectral Tools to Enhance Characterization and Identification of Forensic Evidence, Room 361 ABDE</td>
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<td>7:00 - 8:00 PM</td>
<td><strong>Special Gap Hour Reception sponsored by SCIEX</strong>, Ballroom B&lt;br&gt;Reception immediately following workshop 06 Recognizing the “A” in DEIA: Effective Ways to Improve Accessibility for Mass Spectrometrists. All are welcome to join for networking focused on accessibility, diversity and inclusion.</td>
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<tr>
<td>AFTER 8:00 PM</td>
<td><strong>Corporate Hospitality Suites at Hilton Americas</strong></td>
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## PROGRAM OVERVIEW

### WEDNESDAY

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<th>Event</th>
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<tbody>
<tr>
<td>7:00 AM</td>
<td><strong>Corporate Breakfast Seminars</strong>, Convention Center and Hilton Americas</td>
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<tr>
<td>7:30 AM - 5:00 PM</td>
<td><strong>Name Badge Printing &amp; Information</strong>, Level One Lobby (outside Hall B)</td>
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<tr>
<td>8:30 - 10:30 AM</td>
<td><strong>Oral Sessions</strong>&lt;br&gt;WOA am: Instrumentation: New Hybrid and Multimodal Approaches, Hall B3&lt;br&gt;WOB am: Biotherapeutics: Characterization and Quantitation, Ballroom A&lt;br&gt;WOC am: Drug Discovery and Development: Qualitative and Quantitative Analysis, Ballroom B&lt;br&gt;WOD am: Artificial Intelligence in MS Instrumentation and Applications, Ballroom C&lt;br&gt;WOE am: Industry: Trace Analysis, Quality Control, and Automation, Room 332&lt;br&gt;WOF am: Lipidomics: New MS Technologies and Applications, General Assembly A&lt;br&gt;WOG am: Stable Isotope Labeling: Applications, General Assembly B&lt;br&gt;WOH am: Fundamentals: Ion Activation and Dissociation (Honoring Jean Futrell), General Assembly C</td>
</tr>
<tr>
<td>10:30 AM - 2:30 PM</td>
<td><strong>Poster Session and Exhibits</strong>, Wednesday Posters, Hall BC&lt;br&gt;&lt;br&gt;Odd-number posters present: 10:30 - 11:30 am PLUS 12:30 – 2:30 pm&lt;br&gt;Even-number posters present: 10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm</td>
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<tr>
<td>4:45 - 5:30 PM</td>
<td><strong>ASMS Meeting</strong>, Hall B3. Awards, board reports, wine, beer, soft drinks - and more!</td>
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<tr>
<td>5:45 - 7:00 PM</td>
<td><strong>Workshops</strong>&lt;br&gt;01 High throughput screening mass spectrometry - current status and future landscape, Room 310 A&lt;br&gt;02 Late-Night Lightning Lectures!, Room 310 BC&lt;br&gt;03 Utilizing GC/MS Technologies and Associated Software Tools to Address Challenging Applications in the Flavor, Fragrance and Foodstuffs Laboratory, Room 320 A&lt;br&gt;04 Biomarkers Development: How Mass Spectrometry Is Changing the Field, Room 320 BC&lt;br&gt;05 Ion Mobility Spectrometry: From Data to Structure, Ballroom A&lt;br&gt;06 MS Career Options: How to Kick Start Your Career, Ballroom B&lt;br&gt;07 Ambient Ionization in Application Fields: What is Required, Desired, and Provided?, Ballroom C&lt;br&gt;08 Target Protein Degradation and MS-based Proteomics, Room 332&lt;br&gt;09 What are the future needs of photoionization mass spectrometry for complex mixture analysis?, General Assembly A&lt;br&gt;10 Houston, We Have a Microbiome Problem (...and how the Metaproteomics Initiative aims to solve it!), General Assembly B&lt;br&gt;11 Hispanics and Latinx in Mass Spectrometry, General Assembly C&lt;br&gt;12 Polymeric materials: tackling hydrocarbon-based polymers, Room 340 AB&lt;br&gt;13 ProteomicsML: An online educational platform for machine learning in proteomics, Room 351 ABDE&lt;br&gt;14 Art, Museums, and Archaeology, Room 351 CF&lt;br&gt;15 Remote Sample Collection and Microsampling is Driving New Mass Spectrometry Analytical Solutions, Room 360 ABDE&lt;br&gt;16 Knowledge Share and Instrumentation Donations for Developing World Outreach, Room 360 CF</td>
</tr>
<tr>
<td>7:00 - 8:00 PM</td>
<td><strong>Special Gap Hour Reception sponsored by SEER</strong>, Ballroom B&lt;br&gt;Reception immediately following workshop 06 MS Career Options: How to Kick Start Your Career. All are welcome to join for networking focused on career development.</td>
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<tr>
<td>After 8:00 PM</td>
<td><strong>Corporate Hospitality Suites at Hilton Americas</strong></td>
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## PROGRAM OVERVIEW

### THURSDAY

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<th>Time</th>
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<td>7:30 AM - 2:00 PM</td>
<td><strong>Name Badge Printing &amp; Information</strong>, Level One Lobby (outside Hall B)</td>
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<tr>
<td>8:30 - 10:30 AM</td>
<td><strong>Oral Sessions</strong></td>
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<tr>
<td></td>
<td>ThOA am: Instrumentation: Ambient Ionization and Applications, Hall B3</td>
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<td>ThOB am: Glycopeptides, Glycoproteins, and Glycomics (Honoring Catherine E. Costello), Ballroom A</td>
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<td>ThOC am: Metabolomics: Untargeted Profiling, Ballroom B</td>
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<td>ThOD am: Data-Independent Acquisition and Multiplexing: Proteomics, Ballroom C</td>
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<td></td>
<td>ThOE am: Fundamentals Beyond Mass Analysis: Structural Characterization of Isomers, Room 332</td>
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<td>ThOF am: Protein-Ligand and Protein-Protein Interactions, General Assembly A</td>
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<td>ThOG am: Microbes and the Microbiome, General Assembly B</td>
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<td>ThOH am: Nucleic Acids and Oligonucleotides, General Assembly C</td>
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<tr>
<td>10:30 AM - 2:30 PM</td>
<td><strong>Poster Session and Exhibits</strong>, Thursday Posters, Halls BC</td>
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<td>Odd-number posters present: 10:30 - 11:30 am PLUS 12:30 – 2:30 pm</td>
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<td>Even-number posters present: 10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm</td>
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<tr>
<td>2:30 - 4:30 PM</td>
<td><strong>Oral Sessions</strong></td>
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<tr>
<td></td>
<td>ThOA pm: Instrumentation: Innovative Separation Approaches Coupled to MS, Hall B3</td>
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<td></td>
<td>ThOB pm: Biotherapeutics: Proteins, Antibodies, and Antibody/Drug Conjugates, Ballroom A</td>
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<td>ThOC pm: Imaging: Pharmaceuticals, Metabolites, Lipids, and Glysans, Ballroom B</td>
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<td></td>
<td>ThOD pm: Fundamentals: Ion Structures and Energetics, Ballroom C</td>
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<tr>
<td></td>
<td>ThOE pm: Environmental: Innovative Approaches and Instrumentation, Room 332</td>
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<tr>
<td></td>
<td>ThOF pm: Lipidomics: Targeted and Untargeted, General Assembly A</td>
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<td></td>
<td>ThOG pm: Forensics: Innovations and Applications, General Assembly B</td>
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<td>ThOH pm: Informatics: Innovations, General Assembly C</td>
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<tr>
<td>4:45 - 5:30 PM</td>
<td><strong>Plenary Lecture</strong>, Hall B3</td>
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<td>The Rise and Reign of the Mammals: A New History, from the Shadow of the Dinosaurs to Us</td>
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|            | **Stephen Brusatte**  
|            | **University of Edinburgh**                                         |
| 7:00 – 10:00 PM | **Closing Event at the Houston Museum of Natural Science**         |
|            | Advance purchase ticket is required.                                |
|            | Ticket sales CLOSE on Monday, June 5 at 12pm (noon).                |
|            | Buy your ticket online via Online Registration portal (you can add-on to your existing conference registration). If you purchase after printing your name badge, you will need to re-print your badge. |
|            | Buffet dinner is included. Cash bars available. Enjoy the INCREDIBLE paleontology and gem exhibitions at the museum. Closing plenary speaker, Steve Brusatte, will attend the event and provide additional Q&A in the Morian Hall of Paleontology. |
|            | There is no organized transport to/from the event. Attendees with the closing event icon on their badge have round-trip light rail included. Please wear your badge in case there is ticket control. Engineers will identify your closing event icon as your paid ride. Light rail instructions are included in the app and will be emailed to all who have purchased the closing event. |

The Houston Museum of Natural Science is located at 5555 Hermann Park Drive, Houston TX 77030.

If you do not wish to take the light rail, Uber/Lyft or taxis are available at standard rates.
### MOA am: Top Down Protein Analysis
Hall B3
Session Chair: Frederik Lermty (Technical University of Darmstadt)

**MOA am 08:30**
Proteoforms - how can we transfer them intact from tissues into mass spectrometers? 1,2 Hartmut Schüller 1; Jan Hahn 1; Manuela Moritz 2; Hannah Voss 1; Marcel Kwiatkowski 2; UK-E - Section Mass Spectrometry and Proteomics, University of Hamburg, Hamburg, Germany; 3Functional Proteo-Metabolomics, Department of Biochemistry, University of Innsbruck, Innsbruck, Austria

**MOA am 08:50**
Native top-down for sequencing G protein-coupled receptors and related complexes directly from native membranes; Corinne Lutomski 1,2; Tarick El-Baba 1; Jack L. Bennett 1,2,3; Sophie AS Lawrence 1,2; Joshua D Hinkle 4; Idlir Liko 5; Andrew Dolan 1,2; Christopher Muller 6; John E. P. Syka 1,2; Carol V Robinson 1,2; 1Kavli Institute for Nanoscience Discovery, University of Oxford, Oxford, United Kingdom; 2School of Chemistry, UNSW Sydney, Sydney, Australia; 3Thermo Fisher Scientific, San Jose, California; 5OMass Therapeutics, Oxford, United Kingdom; 6Thermo Fisher Scientific, San Jose, CA

**MOA am 09:10**
Native top-down mass spectrometry approaches to determine the FraB/FrlB substrate binding sites and conformational changes induced by substrate binding; Yuan Gao 1; Sraya Kovvali 1; Jamison Law 1; Venkat Gopalani 1; Vicki H Wysocki 1; 1The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH; 2The Ohio State University-Department of Microbiology, Columbus, OH

**MOA am 09:30**
Parameter-free Deconvolution and Visualization of Peptide and Protein Fragmentation Mass Spectra; Adrian L Guthals 1; Derrill Sturgeon 1; Alexander Gavrilenko 1; Blake Hakkila 1; Stephanie Sturgeon 1; Jhnyia Gavrilenko 1; Rachel Franklin 1; Yury Vasiliev 1; Joseph Meeuwsen 1; Valery Voinov 1; Joseph Beckman 1; 1eMSion, Corvallis, OR

**MOA am 09:50**
Internal Fragment Assignment Challenges in Top-Down Electron Capture Dissociation Tandem Mass Spectrometry; Neven N. Mikawa 1; Carolina Rojas Ramirez 1; Brandon T. Ruotolo 1; Kristina Hakansson 1; 1University of Michigan, Ann Arbor, Michigan

**MOA am 10:10**
Unravelling proteoform footprints of proteasome subtypes using top-down mass spectrometry; Angelique Sanchez Dafun 1; Dusan Zvivkovic 1; Stephen Ardford 2; Leon Icaza 3; Sophie Moeller 3; Carine Froment 1; Delphine Bonnet 4; 1ADME, GmbH 1, 2; 2Institute of Medical Biochemistry and Molecular Biology, University Medicine Greifswald, Greifswald, Germany; 3IRSD, Université de Lyon, INSERM, INRA, INP ENVTT, Université de Lyon 3 Paul Sabatier, Toulouse, France; 4Internal medicine department of digestive disease, Rangueil Hospital, Université de Toulouse - Paul Sabatier (UPS), Toulouse, France; 5NIH/NIH, Bethesda, MD; 6CNRS, Toulouse, France

**MOA am 08:30**
Enhancements in the use of water secondary ion mass spectrometry (SIMS) for multi-omic biomolecular mass and structural analysis; Felicia M Green 1; Sadia Sheraz 1,2,3; Elena Castelfani 1,2; Zoltan Takacs 1; Nick Lockyer 1; 1Rosalind Franklin Institute, Harwell, Didcot, United Kingdom; 2University of Manchester, Manchester, United Kingdom; 3University of Oxford, Dept. of Chemistry, Oxford, United Kingdom; 4Imperial College London, London, United Kingdom

**MOA am 08:50**
Design and performance characterisation of a novel MALDI-2-MSI ionisation source with transmission and reflective mode capabilities; Andrei Groic 1; Benjamin Bartels 1; Alexandros Lekkas 1; Diamantis Koundiss 1; Elias Panagiotopoulos 1; Dimitris Papanastasiou 1; Ron M.A. Heeren 1; Shane R. Ellis 1,3,4; 1M4 - Maastricht Multimodal Molecular Imaging Institute, Maastricht University, Maastricht, Netherlands; 2Fasimtech, NCSR Demokritos, Athens, Greece; 3Molecular Horizons and School of Chemistry and Molecular Bioscience, University of Wollongong, Wollongong, Australia; 4Illawarra Health and Medical Research Institute, Wollongong, Australia

**MOB am: Imaging: Instrumentation & Method Development**
**Ballroom A**
Session Chair: Chris Anderton (Pacific Northwest National Lab)

**MOB am 08:30**
Structural Characterization of Non-Microbial Ions in Urinary Tract Infections by MALDI-TOF MS Lipidomics; Linda K Narthy 1; Abanoub Mikhail 1; Helena Petrosova 1; Michael X Chen 1; Robert K Ernst 2; David R Goodlett 1; 1University of Victoria, Victoria, BC; 2UBC, Vancouver, BC; 3University of Maryland, Baltimore, MD

**MOB am 08:50**
Rapid LC-MS/MS First-Tier Newborn Screening Assay with Throughput Equivalent to FIA-MS/MS; Samantha L Isenberg 1; C. Austin Pickens 1; Adrienne Manning 1; Carla Githure 1; Konstantinos Petritzis 1; Centers for Disease Control and Prevention, Atlanta, GA; 2Katherine A. Kelley State Public Health Laboratory, Rocky Hill, CT

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**MOB am: Imaging: Instrumentation & Method Development**
**Ballroom B**
Session Chair: Jean Van Eyk (Cedars Sinai Medical Center)

**MOB am 08:30**
Multimodal IR-Guided MALDI Imaging of Biological Samples at High Spatial Resolution; Ethan Yang 1; Peng L. Yang 1; Joshua L Fischer 1; Thomas Tang 2; Marten Seebä 3; Hans-Christian Koch 1; Tim Rider 1; Katherine Stumpo 1; Michael Easterling 1; 1Bruker Daltonics, Billerica, MA; 2Bruker Optics Inc, Billerica, MA; 3Bruker Optics GmbH & Co. KG, Ettlingen, Germany

**MOB am 09:10**
Harnessing the Power of Unit Resolution: Separating Isobars and Isomers using Tandem Mass Spectrometry Imaging; Miranda R. Weigand 1; Daisy M. Unshuay Vila 1; Manxi Yang 1; Hang Hu 1; Shane Tichy 1; Julia Laskin 1; 1Purdue University, Dept. of Chemistry, West Lafayette, IN; 2Agilent Technologies, Santa Clara, CA

**MOB am 09:50**
Probing Spatially Resolved Intact Macromolecular Complexes and Proteoforms Directly from Tissue using Native and Denatured Proteoform Imaging Mass Spectrometry; Viyaa Lakshmi Kanchustammbham 1; Pei Su 2; Jared O. Kafader 1; Neil L. Kelleher 1; 1Northwestern University, Evanston, IL

**MOB am 10:10**
DESI imaging at the cellular level through the application of nano-flow and multi-focus approaches; Emily A. Jones 1; Emre Hyes 1; Scott Trinkle 1; Richard Chapman 1; Waters, Milwslow, United Kingdom; 2Waters Corporation, Milwslow, United Kingdom; 3Waters, Milford, MA; 4Waters Corporation, Milford, MA
MOD am 09:10 | Rapid ICP-MS Analysis of Dried Blood Spots via Direct Microextraction from Solid Substrates; P. Kenneth Marcus¹; Cameron J. Stouffer¹; ¹Clemson University, Clemson, SC

MOD am 09:30 | A generic loading strategy for automated sample loading of Evotips for robust and high throughput analysis on the Evoque One; Magnus Huusfeldt¹; Dorte B. Bekker-Jensen¹; Jacob Poder¹; Moritz Heusel¹; Lasse Falkenby¹; Nicolai Bache¹; ¹Evoque, Odense, Denmark

MOD am 09:50 | On-site Breast Cancer Diagnosis Using Paper Spray Ionization Miniature Mass Spectrometry; Cheng-Chih Hsu¹; Hou-Chun Huang¹; Hsin-Hsiang Chung¹; Jia-Yue Yu¹; Bo-Rong Chen²; Ming-Yang Wang³; ¹Department of Chemistry, National Taiwan University, Taipei City, Taiwan; ²Department of Surgery, National Taiwan University Hospital, Taipei City, Taiwan

MOD am 10:10 | Spatial chemistry of the developing brain with defective mitochondria; Carlos Rodriguez-Nava³; Md Amir Hossen³; Mohamed Boutaghou³; Arif Kocabas³; Manuel Gonzalez³; Isaac Marin-Valencia³; ¹Ichahn School of Medicine at Mount Sinai, New York, NY; ²Shimadzu Scientific Instrument, Columbia, MD

MOD am: Small Molecules: Structural Characterization and Quantitation | Ballroom C
Session Chair: Athula Attygalle (Stevens Institute of Technology)

MOD am 08:30 | Gas phase cationization for pesticide analysis: charge-solvated vs. protonated salt for cypermethrin diastereomers distinction under resonant excitation conditions; Kam Eng Trinh¹; Sophie Liu¹; Chenqin Cao¹; Ekaterina Danil¹; Jean-Claude Tabes¹; ²Annelaure Damont¹; François Fenaillé¹; Olivier Firmesse¹; Jacques-Antoine Hennekinne²; Chanthadary Inthavong²; Gwenaelle Lavain-Bompard²; ¹Pesticides and Marine Biotoxins unit (PBM), Laboratory for Food Safety, French Agency for Food, Environmental and Occupational Health & Safety (ANSES), Université Paris-Est; ²Maison-Affort, France; ³CEA-INRA, Laboratoire Innovations en Spectrométrie de Masse pour la Santé (LI-MS), DRF / Institut Joliot / DMTS / SPI, MetaboHUB, CEA Saclay - Université Paris Saclay, Gil-sur-Yvette, France; ²Génomique métabolique, Genoscope, Institut Français Jacob, CEA, CNRS, Université Evry, Université Paris-Saclay, Evry, France; ³Faculté des Sciences et de l’Ingenierie, Institut Parisien de Chimie Moléculaire (IPCM), Sorbonne Université, Paris, France

MOD am 08:50 | Distinguishing between common mold types in mandarins by SPME-SICRIT-MS; Taylor Hayward¹; Allie Ferranti¹; Thomas Wolf¹; Jan-Christoph Wolf¹; ¹Plasmion, Skillman, NJ; ²Plasmion, Augsburg, Germany

MOD am 09:10 | A machine learning method for predicting the origin of biological foreign substances from spectra acquired by MALDI TOF MS; Hiroki Saito¹; Asahi Quality & Innovations; ¹Kanagawa, Japan

MOD am 09:30 | Monitoring Global Soybean Production Using Elementomics to Combat Rainforest Destruction; Brian Quinn¹; Yunhe Hong¹; Nicholas Birse¹; Chris Elliott¹; ¹Queen’s University Belfast, Belfast, United Kingdom

MOD am 09:50 | A comparative untargeted metabolomics analysis of açai (Euterpe oleracea Mart.) fruit, food powder, and botanical dietary supplement extracts; Karle L. Heck¹; Lauren E. Fogel¹; Yuyan Yi¹; Jingyi Zheng¹; Angela I. Calderon¹; ¹Department of Drug Discovery and Development, Auburn University, Auburn, AL; ²Department of Mathematics and Statistics, Auburn University, Auburn, AL

MOD am 10:10 | --Characterization of common foodborne microorganisms via the Combination of LC-MS and GC-MS Based Molecular Fingerprinting; Rui Xu¹; Hong Chen¹; Huan Zhang¹; ²Michael W. Crowder²; Jiangjiang Zhu¹; ¹The Ohio State University, Columbus, OH; ²Miami University, Oxford, OH

MOD am: Covalent Labeling and Chemical Crosslinking | General Assembly A
Session Chair: Richard Scheltema (Utrecht University)

MOD am 08:30 | Custom isobaric labeling strategies for quantitative chemoproteomics; Keriann Backus¹; ¹Icahn School of Medicine at Mount Sinai, New York, NY; ²Arkansas for Medical Sciences, Little Rock, AR

MOD am 08:50 | Analysis of Thyroxine enantiomers in Pharmaceuticals by Ion Mobility Analysis based on molecular imprinted polymers; Fangling Wu¹; Chuan-Fan Ding²; ¹Ningbo University, Ningbo, China; ²Ningbo University, Ningbo, China

MOE am: Food Safety & Chemistry: Foodomics, Allergens, Bacteria, Foods, and Supplements | Room 332
MOF am 09:10  Footprinting integral membrane proteins in their native environment; Jie Sun; Mierixiati Saimi; Qing Zhao; Don L. Rempel; Mengqi Chai; Weikai Li; Michael L. Gross; 1 Washington University in St. Louis, St. Louis, MO; 2 Washington University School of Medicine, St. Louis, MO; 3 Washington university in St louis, St Louis, MO

MOF am 09:30  qXLC-MS elucidation of membrane protein unfolding to visualize membrane complexes dynamics; Anna Bakhtina; Sung-Gun Park; Martin M. Mathay; James E. Bruce; 1 University of Washington, Seattle, WA

MOF am 09:50  Defining the Structures and Interactions of the Human Platelet Secretome using Chemical Crosslinking; Michelle Cleele; Jemma Fenwick; Fay Ghan; Freda H Passam; Mark Larance; 1 Charles Perkins Centre, University of Sydney, Sydney, Australia

MOF am 10:10  Characterizing Glycan-Induced Structural Changes and Binding Interfaces for IgG1-C1q Complex using Hydroxyl Radical Protein Footprinting; Emily Chea; Zhi Cheng; Jiana Duan; Tyler Fletcher; Scot Weinberger; 2 GenNext Technologies, Half Moon Bay, CA

MOF am 09:30  Characterization of Macroyclic and Ring Architectures by Collision Induced Unfolding; Calum Bochenek; Kayla N Williams-Pavlantos; Andrew S McGee; Chrys Wesdemiotis; 1 The University of Akron, Akron, OH

MOF am 09:50  Assessing Degradaability of Poly(Lactic-co-Glycolic Acid) Chains using Reactive Desorption Electrospray Ionization Mass Spectrometry; Laurence Charles; Thierry NJ Fouquet; Jean-Arthur Amalian; Isare Sergent; Pierre Giusti; Didier Gigmes; 1 Aix-Marseille University, Marseille Cedex 20, France; 2 Bausch+Lomb, Rochester, NY; 3 Sanofi, Aramon, France; 4 Aix Marseille Université, CNRS, Institut de Chimie Radicariale, MARSEILLE, France; 5 TotalEnergies OneTech R&D, TotalEnergies Research & Technology, Contreille, France; 6 International Joint Laboratory - iC2MC: Complex Matrices Molecular Characterization, TRTG, Harfluer, France

MOF am 09:10  The MS/MS of the dendrimers, hyperbranched polymers, and linear polymers of bis-MPA; Scott M. Grayson; Mckenna J. Redding; Kayla N Williams-Pavlantos; Oluwapelumi O. Kareem; Chrys Wesdemiotis; 1 Tulane University, New Orleans, LA; 2 University of Akron, Akron, OH

MOF am 09:30  Characterization of Modified Hyaluronic Acid Materials and Their Interaction with Contact Lenses; Michelle L Pietrowski; Andrew J. Hotaling; 1 Bausch+Lomb, Rochester, NY

MOF am 09:50  LDIO-TOF MS and Graphical Data Analysis of Mesophas Pitch Samples used in Carbon Fiber Production; Mark A Arnould; Aparna Annamraju; Ercan Cakmak; Frederic Vautard; 1 Bruker Scientific, LLC, Billerica, MA; 2 Oak Ridge National Laboratory, Oak Ridge, TN

MOF am 10:10  Structural identification of PET (Polyethylene terephthalate) insoluble polyester polymers and microplastics by chemical depolymerization & advanced mass spectrometry; Bayan Almasri; Ahmed Mazzah; Yousef Bakkour; Christian Rolando; 1 Miniaturization for Synthesis, Analysis & Proteomics (MSAP), USR 3290, CNRS, University of Lille, Faculty of Sciences & Technologies, 59655 Villeneuve d'Ascq cedex, France; 2 Laboratory of Applied Chemistry (LAC), Lebanese University, Faculty of Sciences, Tripoli, Lebanon; 3 College of Applied Medical Sciences, King Khalid University, Abha, Saudi Arabia; 4 Shrieking Sixties, 1-3 Allée Lavosier, 59655 Villeneuve d’Ascq, France

MOH am: Informatics: Metabolomics and Lipidomics General Assembly C
Session Chair: Corey Broekeling (Colorado State University)

MOH am 08:30  Network Topology Construction for Molecular Networking; Xianguo Wang; 1 University of California, Riverside, Riverside, CA; 2University of California, Riverside, Riverside, CA

MOH am 08:50  An Automated Workflow Composition System In LC-MS Metabolomics Data Processing; Xinzong Du; Farhad Dastmalchi; Matthew A. Diller; Mathias Brochhausen; Timothy J. Garrett; William R. Hogan; Dominick J. Lemas; 1 University of Florida, Gainesville, FL; 2University of Arkansas for Medical Sciences, Little Rock, AR

MOH am 09:10  Comparing the Use of Internal Standards Against Other Approaches for Normalization of LC-MS Lipidomics Data; Kelly Stratton; Rachel Richardson; Jennifer E. Kyle; Josie G. Eder; Kristin M Engbrecht; Athena A. Schepmoes; Bobbie-Jo Webb-Robertson; Lisa M Bramer; 1 Pacific Northwest National Laboratory, Richland, WA

MOH am 09:30  A Machine Learning Model for Chemical Formula Prediction Using Tandem Mass Spectra of Compounds; Yuhui Hong; Haixu Tang; 1 Indiana University Bloomington, Bloomington, IN

MOH am 09:50  Development of Aggregated Molecular Phenotype (AMP) Scores to Associate and Visualize Molecular Changes; Jessie Chappell; Mary King; Rachel Dehoog; Livia S. Eberlin; David Reil; Erin S. Baker; 1 North Carolina State University, Raleigh, NC; 2 Baylor University, Waco, TX; 3 National Institute of Environmental Health and Sciences, Raleigh, North Carolina; 4 University of North Carolina at Chapel Hill, Chapel Hill, NC

MOH pm 02:30  Reaction-centered multi-omics integration of metabolomics data for mechanistic hypothesis generation; Nikolai Köhler; Vivian Würf; Josch K Pauling; 1 LipiTUM, Technical University of Munich, Freising, Germany

MOH pm 02:30  Speeding up proteomics using a micro-flow LC timSOF-HT; Johanna Tüshaus; Claire Delbridge; Eike Mucha; Christoph Krißp; Jürgen Schlegel; Bernhard Kuster; 1 Technical University of Munich, Munich, Germany; 2 Bruker Daltonics GmbH & Co.KG, Bremen, Germany; 3 Bruker Dalton’s GmbH & Co KG, Bremen, Germany
### MONDAY ORALS

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<th>Time</th>
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<tr>
<td><strong>MOA pm: Single Cell Omics</strong></td>
<td><strong>Hall B3</strong></td>
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<td><strong>Session Chair: Yu Gao (University of Illinois, Chicago)</strong></td>
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<td><strong>MOA pm 02:30</strong></td>
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<td>Single-shape proteomics with an ultra-high sensitivity workflow and preserving spatial context in organs</td>
<td>Matthias Mann, Florian A. Rosenberger, Marvin Thierien, Maximilian T. Strauss, Katherine Madden, Constantin Ammar, Sophia C. Maedler, Lisa Schweizer, Andreas Metoussi, Patricia Skowronek, Maria Wahle, Edwin Rodriguez, Thierry M. Nordmann, Andreas Mund, Max Planck Institute of Biochemistry, Martinsried, Germany; Novo Nordisk Foundation Center for Protein Research, Copenhagen, Denmark</td>
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<td><strong>MOA pm 02:50</strong></td>
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<td>Using single cell mass spectrometry to evaluate CRISPR/Cas9 gene editing results</td>
<td>Trang Nguyen, Lindue Martin, Zongkai Peng, Rakhi Rajan, Zhibo Yang, University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK</td>
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<td><strong>MOA pm 03:00</strong></td>
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<td>Separations with Selective Ion Leveraging High Sensitive and Robust High-field Electrophoresis Enables Ultrasensitive Proteomics</td>
<td>Randolph V. Norheim, Scripps Research, La Jolla, CA; Advanced Clinical Biosystems Research Institute, The Smidt Heart Institute, Cedars Sinai Medical Center, Los Angeles, CA</td>
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<td><strong>MOA pm 03:10</strong></td>
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<td>Capturing Cardiomyocyte Cell-to-Cell Heterogeneity via Shotgun Top-Down Proteomics</td>
<td>Fabio P. Gomes, Blandine Chazarian, Aleksandra Binek, Jolene K. Diedrich, Jennifer E. Van Eyk, John R. Yates III, Scripps Research, La Jolla, CA; Advanced Clinical Biosystems Research Institute, The Smidt Heart Institute, Cedars Sinai Medical Center, Los Angeles, CA</td>
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<td><strong>MOA pm 03:30</strong></td>
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<td>Robust label-free single-cell proteome analysis through in-capillary sample preparation (inCapS): Adela-Eugenie Vrsanova, Syed Azmal Ali, Mathias Käbdorf, Jeroen Krijgsveeld, German Cancer Research Center, Heidelberg, Germany; Cellzone GmbH (a GSK company), Heidelberg, Germany</td>
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<td><strong>MOA pm 03:50</strong></td>
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<td>Electrophoresis-Correlative Mass Spectrometry Enables Ultrasensitive Proteomics</td>
<td>Edwin Rodriguez, University of Utah, Salt Lake City, UT; Adam L. Hollerbach, Kavli Institute for Nanoscience and Cryo-electron Microscopy, University of Groningen, Groningen, The Netherlands; Aniruddha Panda, Iowa State University, Department of Chemistry, Ames, IA</td>
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<td><strong>MOA pm 04:10</strong></td>
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<td>Sensitive and robust high-throughput workflow for qualitative and quantitative single-cell/single cell like analysis</td>
<td>Tabbwang N. Arrey, Bernard Delanghe, Santosh Renuse, Jeff Op De Beeck, Paul Jacobs, Nicolaie Eugen Damoc, Thermo Fisher Scientific, Bremen, Germany; Thermo Fisher Scientific, San Jose, California; Thermo Fisher Scientific - Belgium, Ghent, Belgium</td>
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### MOB pm: Ion Mobility: Instrumentation & Method Development

**Ballroom A**  
Session Chair: Hélène Lavanant (Université de Rouen Normandie)

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<tr>
<td><strong>MOB pm 02:30</strong></td>
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<td>Use of dendrimers to calibrate ion mobility cross section measurements</td>
<td>Jens Sommerfurth, Emily R. Sekera, Bela Paizs, Zoltan Takats, Arpad Somogyi, Polymer Factory Sweden, Stockholm, Sweden; The Ohio State University, Columbus, OH; Rosalind Franklin Institute, Harwell, Didcot, United Kingdom</td>
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<td><strong>MOB pm 02:50</strong></td>
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<td>Hydrazide derivatization in conjunction with cyclic ion mobility-based collision cross section measurements for the improved characterization of human milk oligosaccharides</td>
<td>Sanaz C Habibi, Gabie Nagy, University of Utah, Salt Lake City, UT</td>
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<td><strong>MOB pm 03:10</strong></td>
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<td>Development of an Array of Ion Traps in Structures for Lossless Ion Managements (SLIM): Adam P. Huntley, Adam L. Hollerbach, Anesh S. Prabhakaran, Cameron M. Giberson, Randolph V. Norheim, Richard D. Smith, Yehia M. Ibrahim, Pacific Northwest National Laboratory, Richland, WA</td>
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<td><strong>MOB pm 03:30</strong></td>
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<td>Leveraging High-Resolution SLIM-IMS Separations with Selective Ion-Neutral Clustering, HDX, and Cryogenic IR Spectroscopy</td>
<td>Vasya Yatsyna, Brian H Clowers, Thomas Rizzo, Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland; Washington State University Department of Chemistry, Pullman, WA</td>
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<td><strong>MOB pm 03:30</strong></td>
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<td>In-cell D Gandhi, JiHyeon Lee, Christopher J. Hogan, Carlos Larriba-Andaluz, Indiana University Purdue University - Indianapolis, Indianapolis, IN; Purdue University, Lafayette, IN; University of Minnesota, Minneapolis, MN; Indiana University Purdue University Indianapolis, Indianapolis, IN</td>
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<td><strong>MOB pm 03:50</strong></td>
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<td>Native mass spectrometry on a modified timsTOF Pro</td>
<td>Yu Fu Lin, Ervin Panyczyk, Benjamin Jones, Mark Ridgeway, Arpad Somogyi, Desmond Kaplan, Melvin Park, Vicki Wysocki, The Ohio State University, Columbus, OH; Bruker Daltonics, Billerica, MA; KapiScience LLC, TEWKSBURY, MA</td>
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<td><strong>MOB pm 04:10</strong></td>
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<td>Investigating the effect of high field inelastic collisions using a DMA-FAIMS Hybrid Method for Improved Ion Mobility characterization</td>
<td>Viraj D Gandhi, JiHyeon Lee, Christopher J. Hogan, Carlos Larriba-Andaluz, Indiana University Purdue University - Indianapolis, Indianapolis, IN; Purdue University, Lafayette, IN; University of Minnesota, Minneapolis, MN; Indiana University Purdue University Indianapolis, Indianapolis, IN</td>
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### MOC pm: Structural Biology

**Ballroom B**  
Session Chair: Lan Huang (University of California, Irvine)

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<th>Session</th>
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<tr>
<td><strong>MOC pm 02:30</strong></td>
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<td>In-cell Crosslinking Mass Spectrometry combined with AlphaFold-Multimer to discover and predict the structures of novel protein complexes</td>
<td>Francisco J O'Reilly, Andrea Graziaide, Christian Forbrig, Rica Bremenkamp, Jörg Stülke, Juri Rappsilber, NCI NIH, Frederick, MD; Technische Universität Berlin, Berlin, Germany; Human Technopole, Milan, Italy; University of Göttingen, Göttingen, Germany</td>
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<tr>
<td><strong>MOC pm 02:50</strong></td>
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<td>An integrative structural interactomics approach to reveal protein organization, topology and structure of intact Giant virus particles</td>
<td>Lars Muehllberg, Boris Bogdanow, Kenta Okamoto, Liu Fan, Leibniz-Forschungsinstitut für Molekulare Pharmakologie (FMP), Berlin, Germany; Uppsala University, Upplands, Sweden</td>
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<td><strong>MOC pm 03:10</strong></td>
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<td>Deciphering the mode of interaction for novel insulin receptor partial agonists by HDX-MS and cryo-EM: Haihong Zhou, Giovanna Scapin, Yacob Gomez Llorente, Terri Kelly, David McLaren, Songnian Lin, James Mu, Merck &amp; Co., Inc., Kenilworth, New Jersey</td>
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<td><strong>MOC pm 03:30</strong></td>
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<td>Unravelling the Mechanism of Rotavirus Viral Factory Formation using Structural Mass Spectrometry</td>
<td>Alice Colyer, Julia Acker, Xinyu Wang, Alexander Borodavka, Antonio Calabrese, University of Leeds, Leeds, United Kingdom; University of Cambridge, Cambridge, United Kingdom</td>
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<td><strong>MOC pm 03:50</strong></td>
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<td>Direct determination of membrane protein complexes from cellular membranes</td>
<td>Vanhuyak Jung, Anrudhda Panda, Kailoi Gupta, Yale School of Medicine, Department of Cell Biology, New Haven, CT</td>
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<td><strong>MOC pm 04:10</strong></td>
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<td>Barcoded nanobodies for the capture and characterization of native membrane protein complexes from human brain</td>
<td>Tarick J El-Baba, Corinne A Lutomski, Jack L Bennett, Sophie AS Lawrence, Andrew Dolan, Joshua D Hinkle, Christopher Mullen, John E.P. Syka, Carol V Robinson, Kavli Institute for Nanoscience Discovery, University of Oxford, Oxford, United Kingdom; Physical and Theoretical Chemistry Laboratory, Department of Chemistry, University of Oxford, Oxford, United Kingdom; Department of Chemistry, University of Oxford, Oxford, United Kingdom</td>
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MONDAY ORALS

MOD pm: Data-Independent Acquisition and Multiplexing: Lipidomics and Metabolomics
Ballroom C
Session Chair: TBD

MOD pm 02:30 Untargeted and Targeted DIA-SWATH Mass Spectrometry for the Characterization of Metabolite and Xenobiotics in Pediatric Chronic Kidney Disease Urine Samples; Maria Fernanda Cluenteer Girard1; Gérard Hopfgartner; *University of Geneva, Geneva, Switzerland

MOD pm 02:50 Deep Structural Lipidomics using Ozone-Induced Dissociation in a High-Throughput Data-Independent Analysis Workflow; Jesse A Michael1; Alan T Maccarone2; Todd W Mitchell1; Christer S Ejsing3, 4; Shane R. Ellis1; *School of Chemistry and Molecular Bioscience, University of Wollongong, Wollongong, Australia; 2Department of Biochemistry and Molecular Biology, Villum Center for Bioanalytical Sciences, University of Southern Denmark, Odense, Denmark; 3Cell Biology and Biophysics Unit, European Molecular Biology Laboratory, Heidelberg, Germany

MOD pm 03:10 Creating Deconvoluted Open-Source Files from Data-Independent Analysis Files using IonDecon; Nandarani Abril1; Jeremy Koelmel2; Michael Kummer1; Ralph Hindle1; Kathy Hunt2; Stephen Baumann2; Krystal J Godri Pollitt1; Emma E Rennie1; 1Innovative Omics, Sarasota, FL; 2Yale University, New Haven, CT; 3Vogon Labs, Cochrane, Alberta; 4Agilent Technologies, Santa Clara, CA

MOD pm 03:30 Analysis of yeast lipids exposed to low temperature stress using data-independent acquisition-based lipidomics; Daiki Har1; Nobuyuki Okahashi2, 3; Atsuhiko Toyama4; Junko lida3; 1Fumio Matsuda; 2, 3Japan; 4University of Nebraska-Lincoln, Lincoln, NE

MOD pm 03:50 A powerful single method for sensitive quantification and targeted/non-targeted identification of cell culture media (CCM) components using accurate mass spectrometry; Marialuce Maidini1; Antonella Chiapparino2; Eshani Nandita3; 1SCIX, Milano, Italy; 2SCIEX, Darmstadt, Germany; 3SCIEX, Redwood City, CA

MOD pm 04:10 Plasma Lipidomics using diapASEF Demonstrates Improved Capabilities of Quantification using MS2 Data; Premy Shanthamorporathy1; Hannes Roest1; 1University of Toronto, Toronto, ON

MOD pm: Food Safety & Chemistry: Innovations Room 332
Session Chair: Boniek Vaz (Universidade Federal de Goiás, Brazil)

MOE pm 02:30 Photoionization MS as tool to predict product sensory information as well as physical and chemical product attributes in real time; Jan Heide1, 2; Hendryk Czech3; Sven Ehret3; Andreas Walz1; Ralf Zimmermann1, 2; 1Photonion GmbH, Schwerin, Germany; 2Joint Mass Spectrometry Centre, Chair of Analytical Chemistry, University of Rostock, Rostock, Germany; 3Department for Science and Technology of Life, Light and Matter (LL&M), University of Rostock, Rostock, Germany

MOE pm 02:50 Novel mass spectrometry method for the detection and quantification of peanut protein in processed food matrices; Sara K Schlange1; Justin T Marsh1; Melanie L Downs1; Philip E Johnson1; 1University of Nebraska-Lincoln, Lincoln, NE

MOE pm 03:10 Isotopologue ratio analysis in organic compounds: caffeine in complex sample matrices; Nils Johanne Kuhlbusch1; 2; Dieter Juchelka1; Issaku Edward Koh1; Andreas Hilkert1; Heiko Hayen1; 1University of Muenster, Muenster, Germany; 2Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; 3Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany

MOE pm 03:30 A novel reactivc platform to retrieve reactive carbonyl species (RCS) and their interaction with polyphenols; Changhong Hu1; Miao Yu2; Yantao Zhao2; Yingdong Zhu1; Shengmin Sang1; 1North Carolina A&T State University, Kannapolis, NC; 2The Jackson Laboratory, Bar Harbor, ME

MOE pm 03:50 Cooking food in microwaveable plastic containers: in situ formation of a new chemical substance and increased migration of polypropylene polymers; Francisco José Díaz-Galiano1; Maria José Gómez-Ramos1; Icíar Beraza-Gómez2; María Murcia-Morales1; Amadeo Rodriguez Fernandez-Alba3; 1University of Almería, Department of Chemistry and Physics, Agrifood Campus of International Excellence (ciiA3), Almería, Spain

MOE pm 04:10 Regioselective dissociation by collisional activation of alkali-cationized cereulide in gas phase, coexisting charge-solvated vs. protonated salt forms; Sophie Liu1; Kam Eng Trinh1; Chenqin Cao2; Ekaterina Dari1; Annelaura Damont1; Jean-Claude Tabet1; Yves Gimbert1; François Fenaux1; Yasmine Makri2; 1Chanthadary Inthavong3; Gwenaëlle LAVISON-BOMPARD4; Jacques-Antoine Hennekinne1; Olivier Firmesse1; 1Staphylococcus, Bacillus and Clostridium unit (SBCL), Laboratory for Food Safety, French Agency for Food, Environmental and Occupational Health & Safety (ANSES), Université Paris-Est, Maisons-Alfort, France; 2Pesticides and Marine Biotoxins unit (PBM), Laboratory for Food Safety, French Agency for Food, Environmental and Occupational Health & Safety (ANSES), Université Paris-Est, Maisons-Alfort, France; 3CEA-INRA, Laboratoire Innovations en Spectrométrie de Masse pour la Santé (LI-MS), DRF / Institut Joliot / DMT2 / SPI, Météobius, CEA Saclay - Université Paris-Saclay sur Yvette, France; 4Génomique métabolique, Genoscope, Institut François Jacob, CEA, CNRS, Univ Evry, Université Paris-Saclay, Evry, France; 5Faculté des Sciences et de l’ingénierie, Institut Parisien de Chimie Moléculaire (IPCM), Sorbonne Université, Paris, France; 6Département de Chimie Moléculaire, UMR CNRS 5250, Université Grenoble Alpes, Grenoble, France

MOF pm: Cancer Research General Assembly A
Session Chair: Sarah Totten (Lycia Therapeutics)

MOF pm 02:30 Immunopeptidomics identifies tumor associated antigens in pancreatic ductal adenocarcinoma--; Eva Verzan1; Zackery Ely1; Karl R Clausen1; Susan Klaeger1; Zachary Kulstad2; Andrew Aguirre1, 3, 4; William A Freed-Pastor4, 4; Jennifer G Abel1; Tyler Jacks2; Steven A Carr2; 1Broad Institute of MIT and Harvard, Cambridge, MA; 2Massachusetts Institute of Technology, Cambridge, Massachusetts; 3Harvard Medical School, Boston, MA; 4Dana-Farber Cancer Institute, Boston, MA
**MONDAY ORALS**

**MOF pm 02:50**
Proteome Imaging Mass Spectrometry to Interrogate the Ovarian Cancer Microenvironment; Nathaniel Henning, Vijaya Lakshmi Kanchustambham, Pei Su, Michael Caldwell, Jared O. Kafader, Thomas Conrads, Neil L. Keiser, "Chemistry of Life Processes Institute, Northwestern University, Evanston, IL; The Proteomics Center of Excellence, Northwestern University, Chicago, IL; Women’s Health Integrated Research Center at Inova Health System, Annandale, Virginia.

**MOF pm 03:10**
Characterization of Metabolic Variabilities Associated to Glioblastoma to Identify Patient Specific Combination Therapies using Liquid Chromatography-Tandem Mass Spectrometry; Stellena Mathiaparanam, Olga Zaslaver, Michelle Kushida, Trevor Pugh, Peter Dirks, J. Rafael Montenegro-Burke, Hannes Röst, "University of Toronto, Toronto, ON; The Hospital for Sick Children, Toronto, ON; Princess Margaret Cancer Centre, Toronto, ON; Helen Diller Family Comprehensive Cancer Center, University of California, San Francisco, CA.

**MOF pm 03:30**
Employing Top-down Mass Spectrometry to Examine RAS Proteoforms in Malignant Cell Lines; Caroline Dehart, Robert A. D’ippolito, Kanika Sharma, Nicole Fer, Brian Smith, Mackenzie Meyer, Scott Eury, Katie Powell, Vanessa Wall, William Burgan, Dominic Esposti, Anna E. Maciag, Frank McCormick, Dwight V. Nissley, Frederick National Laboratory for Cancer Research, Frederick, MD; Helen Diller Family Comprehensive Cancer Center, University of California, San Francisco, CA.

**MOF pm 03:50**
Optimization of peptide purification and DDA-PASEF method for increased sensitivity of MHC class II peptide identification; Raghothama Chakrai, Li Dai, Kristina Archer, Abby J. Chiang, Lisa H. Cazes, Rajat Varma, Mark Cobbold, Sonja Hess, AstraZeneca R&D, Gaithersburg, Maryland.

**MOH pm: High Throughput MS General Assembly C**
Session Chair: John Tran (Genentech)

**MOH pm 02:50**
Robust and High-Throughput Analytical Flow Proteomics Analysis of Cynomolgus Monkey and Human Matrices with Zeno SWATH Data Independent Acquisition; Weiwen Sun, Yu Li, Yue Huang, Joselyn Chan, Sonia Terrillon, Anton I. Rosenbaum, Kevin Contrepois, AstraZeneca, South San Francisco, CA.

**MOH pm 03:30**
Next generation high-throughput multiplexed chemoproteomics in 96-well plates on a high resolution accurate mass platform with a new mass analyzer; Qing Yu, Ka Yang, Kevin Dong, Martin Zeller, Graeme C McAlister, Joao A Paulo, Hamish Stewart, Christian Hock, Nicolea Eugen Damoc, Vlad Zabrouskov, Joshua J. Coon, University of Wisconsin-Madison, Madison, WI; Thermo Fisher Scientific, Bremen, Germany; Thermo Fisher Scientific, San Jose, California; Morgridge Institute for Research, Madison, WI.

**MOG pm 03:50**
Ultra-high-throughput Intact Protein Analysis for Drug Discovery Using Acoustic Ejection Mass Spectrometry; Xiujuan Wen, Kiersten Tovar, Adway O. Zacharias, Chang Liu, Richard Johnstone, Ryan Loy, Lyle Burton, Thomas R. Covey, Markus Koglin, Kevin P. Bateman, Mary Jo Wildey, David G. McLaren, Merck & Co, Kenilworth, NJ; SCIEX, Concord, ON; Merck, West Point, PA.

**MOH pm: High Throughput MS General Assembly B**
Session Chair: Leslie Hicks (University of North Carolina, Chapel Hill)

**MOH pm 02:30**
Miniature, Monolithic, Fully Additively Manufactured Glass-Ceramic Quadrapole Mass Spectrometers for Portable Mass Spectrometry; Colin Eckhoff, Nicholas K. Lubinsky, Luis F. Velasquez-Garcia; MIT, Cambridge, MA.

**MOH pm 02:50**
Real-time Pressure Control Algorithm Enables Vacuum Design for Miniature mass spectrometer; Ningxi Li, Zhijun Cai, Xiaoyou Zhou, Zheng Ouyang; Tsinghua University, Beijing, China.

**MOH pm 03:10**
The Wisconsin Oscillator: A Low-Cost Circuit for Powering Ion Guides, Traps, Funnels, and Ion Mobility Spectrometers; Steven J Krepel, Blaise J Thompson, Gilbert M. Nathanson, Timothy H. Bertram, University of Wisconsin-Madison, Department of Chemistry, Madison, WI.

**MOH pm 03:30**
Mass Spectrometer Observing Lunar Operations (MSolo); Roberto Aguilar Ayala, Matthew L. Hancock, Alexander W. Jarnot, Janine E. Captain, Jacqueline W. Quinn, National Aeronautics and Space Administration, Kennedy Space Center, FL; University of Central Florida, Orlando, FL.

**MOG pm 03:50**
Machine learning-derived charge state assignments with better accuracy than human experts; Heather Desaire, David Hua, Hanna Nguyen, Eden Go, University of Kansas, Lawrence, KS.

**MOG pm 04:10**
TOA am: Instrumentation: New Developments in Ionization and Sampling (In Memory of Marvin Vestal)
Hall B3
Session Chair: Brian Musselman (Bruker)

TOA am 08:30
Electroless ionization mass spectrometry (ELI-MS), a plug-and-play ambient technique for ultrafast ionization: Stefan Kooij1; Aleksandra Chojnacka2; Garry L. Corlhals2; Cees Van Rijn1; 1Van der Waals Zeeman Institute, Amsterdam, Netherlands; 2Van ’t Hoff Institute for Molecular Sciences, Amsterdam, Netherlands; Quantitative Analysis of GC/MS in DBS: Working Towards Decentralizing the Patient Clinical Trial Experience: Brendan Tierney1; Ting-Wen Cheng1; Savion Vigil2; Matthew Blatnik3; 3Pfizer, Groton, CT

TOA am 08:50
MS SIEVE – pushing the limits for low-abundant (bio)molecules: Nina Mønner1; Kudratullah Karimi1; Jonathan Zöller1; Tommy Hofmann1; Rene Zangl1; 1Goethe-University, Institute of Physical and Theoretical Chemistry, Frankfurt am Main, Germany; 2Proteomics, Max-Planck-Institute for Brain Research, Frankfurt am Main, Germany; 3HALOChem, Institute of Biochemistry and Biotechnology, Martin Luther University Halle-Wittenberg, Halle, Germany; 4Department of Chemistry – Biochemistry, Johannes Gutenberg University Mainz, Mainz, Germany

TOA am 09:10
DON’T SLEEP ON SAMPLING – IF YOU DON’T GRAB IT YOU CAN’T SEE IT: Dan Carmpany1; Paul Demond1; Patrick W. Fedick2; Elizabeth Dhummakupar1; Excelsior Gunpowder, MD; 2U.S. Army DEVCOM Chemical Biological Center, Aberdeen Proving Ground, MD; 3EXCECT Incorporated, Edgewood, MD; 4Naval Air Warfare Center, United States Navy Naval Air Systems Command (NAV/AFR), China Lake, CA

TOA am 09:30
Miniaturized plasma-based ionization source for LC-MS detection of multiclass explosives: Priscilla Rocci Bautista1; Marcos Bouza Areces2; Sebastian Brandt2; Joachim Fränkel3; Antonio Molina Diaz1; Juan Francisco Garcia Reyes3; 1Universidad de Jaen, Jaen, Spain; 2University of Jaen, Jaen, Spain; 3ISAS: Leibniz Institut für Analytische Wissenschaften, Dortmund, Germany; 4University Research Institute for Olives Grove and Olive Oil, University of Jaen, Jaen, Spain

TOA am 09:50
The newly designed "Aim" soft chemical ionization reactor for direct, real-time measurement of inorganic acids, organics, and PFAAs in air: Abigail Koss1; Matthieu Riva2; Felipe Lopez-Hilliker1; 1Tofwerk AG, Thun, Switzerland

TOA am 10:10
cVSSI-APCI-MS for rapid identification of drugs and their metabolites in serum: Madison Pursell1; Liam P. Poole2; Kaitlyn J. Aggar2; Stephen Valentine2; Peng Li3; 1West Virginia University, Morgantown, WV; 2West Virginia University- C. Eugene Bennett Department of Chemistry, Morgantown, WV

TOA am: Biomarkers: Quantitative Analysis
Ballroom A
Session Chair: Norelle Wibburger (AstraZeneca)

TOA am 08:30
Histone post-translational modifications as determinants for drug outcome in T-cell acute lymphoblastic leukemia: Laura Corveley1; Lien Prove2; Bart Van Puyvelde3; Dieter Deforce4; Pieter Van Vlierberge5; Maarten Dhaenens6; 1Lab of Pharmaceutical Biotechnology, Ghent University, Ghent, Belgium; 2Department of Biomedical Medicine, Ghent University, Ghent, Belgium

TOA am 08:50
Absolute quantification of IgA1 immune-complex proteins in serum of patients with IgA nephropathy: Mary A. Cunningham1; Ellenore P. Crain1; Alyssa L. Hansen1; Stacy Hall1; Dana V. Ritz1; Bruce A. Julian1; Jan Novak1; Matthew B. Renfrow2; 1University of Alabama at Birmingham, Birmingham, AL; 2Quantitative Analysis of GC/MS in DBS: Working Towards Decentralizing the Patient Clinical Trial Experience: Brendan Tierney1; Ting-Wen Cheng1; Savion Vigil2; Matthew Blatnik3; 3Pfizer, Groton, CT

TOA am 09:00
Ultra-fast SARS-CoV-2 peptide detection using peptid-immunoaffinity enrichment combined with Acoustic Ejection Mass Spectrometry (AEMS): Bart Van Puyvelde1; Christie Hunter2; Yang Oliver Wang3; Estelle Hoedt4; Maxim Zhgamadze5; Koen Raedschelders3; Qin Fu6; Dieter Deforce7; Maarten Dhaenens1; Jennifer Van Eyk7; 1Ghent University, Laboratory of Pharmaceutical Biotechnology, Ghent, Belgium; 2SCIEX, Redwood city, CA; 3Cedars-Sinai Medical Center, Los Angeles, CA

TOA am 09:50
D-Amino Acids Quantification by LC/MS/MSMRM in Type 1 Diabetes-Affected Human Serum: Shuangshuang Chen1; Cindy J. Lee2; Stanislav S. Rubakhin1; Jonathan V. Sweedler1; 1University of Illinois Urbana Champaign, Urbana, IL

TOA am: Fundamentals: Native MS and Structures of Large Ions
Ballroom B
Session Chair: Boris Krichel (University of Siegen / CSSB Hamburg)

TOA am 08:30
Native Top-Down MS with Orbitrap-Based Capture Dissociation Reveals Higher Order Structure Information for Protein Complexes: Boyu Zhao1; Carter Lantz2; Benqian Wei3; Rachel R. Ogorz1; Andrew A. T. R. Quinlan1; 1Center for Protein Therapeutics (CPT), Morrisville, NC; 2Peking University, Beijing, China; 3Shenzhen Bay Laboratory, Shenzhen, China; 4Tsinghua University, Beijing, China

TOA am 08:50
Sensitive characterization of native protein complexes from biological samples using biofunctionalized dissociable hydrogel microbeads: Xinyang Shao1; 1Tianjin University, Tianjin, China; 2Nanjing Tech University, Nanjing, China

TOC am 09:00
MS analysis of free, circulating 20S proteasomes from blood: Gili Ben-Nissim1; David Morgenstern1; Yegor Leushkin2; 1Weizmann Institute of Science, Rehovot, Israel; 2Can We Really Correctly Assign Charge States of Large Oligomeric Complexes? Spectral Interferences in Native MS of Macromolecular Assemblies: Victor Yin1; Janet C Saunders2; Paul WA Devine2; Nicholas J Bond2; Albert J.R. Heck1; 1Utrecht University, Utrecht, Netherlands; 2AstraZeneca, Cambridge, United Kingdom

TOC am 09:30
Can We Really Correctly Assign Charge States of Large Oligomeric Complexes? Spectral Interferences in Native MS of Macromolecular Assemblies: Victor Yin1; Janet C Saunders2; Paul WA Devine2; Nicholas J Bond2; Albert J.R. Heck1; 1Utrecht University, Utrecht, Netherlands; 2AstraZeneca, Cambridge, United Kingdom

TOC am 09:50
Unleashing the power of CE-MS: from the separation of ~106 Da multimeric protein assembly conformers to their in-depth structural characterization: Anne-Lise Marie1; Somak Ray2; 1Van Vliet Laboratory, Utrecht, Netherlands; 2AstraZeneca, Cambridge, United Kingdom
TUESDAY ORALS

TOE am 09:10
Development of a sensitive high-resolution LC-MS/MS approach for global profiling of urinary mercapturic acid conjugates; Kevin Murray1; Dylan McKeon1; Chiara Lecchi1; Peter W. Villalta2; Silvia Balbo1; Masonic Cancer Center; University of Minnesota, Minneapolis, MN; Robert N Cole1; 1Department of Environmental Health and Engineering, Bloomberg School of Public Health, Johns Hopkins University, Baltimore, MD; 2Department of Biological Chemistry, Johns Hopkins University School of Medicine, Baltimore, MD; 3Department of Anesthesiology, School of Medicine, Johns Hopkins University, Baltimore, MD.

TOE am 09:30
Detecting temporal changes in the serum albumin adductome following bariatric surgery using Pan-Protein Adductomics; Joshua W Smith1; Robert N O'Meally2; Sean M Burke3; Robert H Brown1; John D Groopman3; Robert N Cole1; 1Department of Environmental Health and Engineering, Bloomberg School of Public Health, Johns Hopkins University, Baltimore, MD; 2Department of Biological Chemistry, Johns Hopkins University School of Medicine, Baltimore, MD; 3Department of Anesthesiology, School of Medicine, Johns Hopkins University, Baltimore, MD.

TOE am 10:10
Assessing Per- and Polyfluoroalkyl Substances (PFAS) and Lipidomic Alterations in Plants Grown in Contaminated Soil; Rebecca L Beres1; Sarah Doydora1; Kaylie I Kirkwood2; Allen Li3; Owen Duckworth4; Erin S Baker5; 1Department of Chemistry, University of North Carolina at Chapel Hill; Chapel Hill, NC; 2Department of Crop and Soil Sciences, North Carolina State University; Raleigh, NC; 3Department of Chemistry, North Carolina State University; Raleigh, NC; 4Institute of Plant Protection, Chinese Academy of Agricultural Sciences, Beijing, China.

TOE am 09:05
Chemical exposome in brain cancer: An exploratory study; Ruben Gil-Solsona1; Albert Pons-Escoda2; Daniel Gutierrez-Martín1; Jordi Bruna3; Noemi Vidal-Sarro3; Carles Majos5; Pablo Gago Ferreiro1; 1Institute of Environmental Assessment and Water Research - Spanish Council for Research (IDAEA-CSIC); Barcelona, Spain; 2Department of Neuroradiology, Hospital Universitari de Bellvitge, C. Feixa Llarga SN, 08907 L’Hospitalet de Llobregat, Spain; 3Hospital de Llobregat, Spain; 4Unit of Neuro-Oncology. Hospital Universitari de Bellvitge-ICo, Barcelona, Spain; 5Department of Neurobiology, Institute Hospital de Bellvitge, Barcelona, Spain.

TOE am 09:50
Fragment ion intensity prediction improves the identification rate of non-tryptic peptides in TimsTOF; Charlotte Adams1; Wissam Gabrie2; Kris Laukens3; Wout Bittremieux1; Mathias Wilhelm1; Kurt Boonen1; 1University of Antwerp, Antwerpen, Belgium; 2Technical University of Munich, Munich, Germany.

TOE am 09:30
A modular and open workflow for the extraction and quantification of peptides in synchro-PASEF experiments; Georg Wallmann1; Patricia Skowronek2; Marvin Thiele1; Corazon Ericka Mae Itang1; Sander Willems3; 1The Ohio State University, Columbus, OH; 2Proteome Software, Portland, OR.

TOE am 09:10
Library-free analysis of DIA experiments using a feature-centric approach; J. Sebastian Paz1; Carolyn Allen1; Lindsay K Pino1; Daniele Canzani1; William E Fondrie1; Talus Bioscience, Seattle, WA.

TOE am 10:05
A systematic characterization of LC-MS features sheds light on the full potential of DIA identification; Grzegorz Skoraczynski1; Tejas Gandhi1; Oliver M Bernhardt2; Lukas Reiter1; Biognosys AG, Schlieren, Switzerland.

TOE am 10:10
TOF am: Neurodegenerative Disease Research A General Assembly A Session Chair: Judith Steen (Boston Children’s Hospital)

TOE am 08:30
Multi-omics profiling of human induced pluripotent stem cells (iPSCs) to investigate the mechanisms of splicing dysfunction in AD pathogenesis; Zhen Wang1; Ping-Chung Chen2; Junmin Peng3; 1St. Jude Children’s Research Hospital, Memphis, TN.

TOE am 10:00
Machine Learning Models Predict Mild Traumatic Brain Injury Using Lipid Mass Spectrometry Imaging Data; Dimitry Leonovsky1; Alexis N Pulliam2; David A Gaul3; Michelle C Laplace4; Facundo M Fernandez5; 1School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA; 2Coulter Department of Biomedical Engineering, Georgia Institute of Technology/Emory University, Atlanta, GA.

TOE am 09:30
Analysis of Brain Protein Stability Changes in Mouse Models of Normal Aging and Alzheimer’s Disease; Joshua W Smith1; Robert N O’Meally2; Sean M Burke3; Robert H Brown1; John D Groopman3; Robert N Cole1; 1Department of Environmental Health and Engineering, Bloomberg School of Public Health, Johns Hopkins University, Baltimore, MD; 2Department of Biological Chemistry, Johns Hopkins University School of Medicine, Baltimore, MD; 3Department of Anesthesiology, School of Medicine, Johns Hopkins University, Baltimore, MD.

TOE am 08:30
Exposomic approaches for next-generation human biomonitoring; Benedikt Warth1; University of Vienna, Vienna, Austria.

TOE am 09:00
Medication Read-out in Untargeted Metabolomics Using a MS/MS Library of Drugs and Metabolites Propagated from Repository-scale Molecular Networking; Haoqi Nina Zhao1; Wout Bittremieux1; Corinna Brungs2; Robin Schmid3; Simone Zufla1; Pieter C Dorrestein1; 1University of California San Diego, San Diego, CA; 2University of Antwerp, Antwerpen, Belgium; 3Institute of Organic Chemistry and Biochemistry of the CAS, Prague, Czech Republic.

TOE am 09:00
Session Chair: Olga Vitek (Northeastern University)

TOE am: Informatics: Peptide and Protein Identification, Proteomics Ballroom C

TOE am 08:30
Detecting and removing interference in precursor quantification; Brian C Searle1; Ariana E Shannon1; Damien B Wilburn1; 1The Ohio State University, Columbus, OH; 2Proteome Software, Portland, OR.

TOE am 08:50
Session Chair: Yinsheng Wang (University of California, Riverside)

TOE am 08:50
A systematic characterization of LC-MS features sheds light on the full potential of DIA identification; Grzegorz Skoraczynski1; Tejas Gandhi1; Oliver M Bernhardt2; Lukas Reiter1; Biognosys AG, Schlieren, Switzerland.

TOE am 09:00
Chemical exposome in brain cancer: An exploratory study; Ruben Gil-Solsona1; Albert Pons-Escoda2; Daniel Gutierrez-Martín1; Jordi Bruna3; Noemi Vidal-Sarro3; Carles Majos5; Pablo Gago Ferreiro1; 1Institute of Environmental Assessment and Water Research - Spanish Council for Research (IDAEA-CSIC); Barcelona, Spain; 2Department of Neuroradiology, Hospital Universitari de Bellvitge, C. Feixa Llarga SN, 08907 L’Hospitalet de Llobregat, Spain; 3Hospital de Llobregat, Spain; 4Unit of Neuro-Oncology. Hospital Universitari de Bellvitge-ICO, Barcelona, Spain; 5Department of Neurobiology, Institute Hospital de Bellvitge, Barcelona, Spain.

TOE am 09:00
Session Chair: Judith Steen (Boston Children’s Hospital)

TOE am 09:30
Detecting temporal changes in the serum albumin adductome following bariatric surgery using Pan-Protein Adductomics; Joshua W Smith1; Robert N O’Meally2; Sean M Burke3; Robert H Brown1; John D Groopman3; Robert N Cole1; 1Department of Environmental Health and Engineering, Bloomberg School of Public Health, Johns Hopkins University, Baltimore, MD; 2Department of Biological Chemistry, Johns Hopkins University School of Medicine, Baltimore, MD; 3Department of Anesthesiology, School of Medicine, Johns Hopkins University, Baltimore, MD.

TOE am 09:10
Development of a sensitive high-resolution LC-MS/MS approach for global profiling of urinary mercapturic acid conjugates; Kevin Murray1; Dylan McKeon1; Chiara Lecchi1; Peter W. Villalta2; Silvia Balbo1; Masonic Cancer Center; University of Minnesota, Minneapolis, MN; Robert N Cole1; 1Department of Environmental Health and Engineering, Bloomberg School of Public Health, Johns Hopkins University, Baltimore, MD; 2Department of Biological Chemistry, Johns Hopkins University School of Medicine, Baltimore, MD; 3Department of Anesthesiology, School of Medicine, Johns Hopkins University, Baltimore, MD.

TOE am 08:50
Mass spectrometry reveals ATP production defects in Niemann-Pick disease, type C1 mouse brain myelin and human oligodendrocytes; Chandimal Pathmasiri1; Stephanie M Cologna4; 1University of Illinois at Chicago, Chicago, IL.

TOE am 09:10
TOF am: Neurodegenerative Disease Research A General Assembly A Session Chair: Judith Steen (Boston Children’s Hospital)

TOE am 08:30
Multi-omics profiling of human induced pluripotent stem cells (iPSCs) to investigate the mechanisms of splicing dysfunction in AD pathogenesis; Zhen Wang1; Ping-Chung Chen2; Junmin Peng3; 1St. Jude Children’s Research Hospital, Memphis, TN.

TOE am 08:50
Mass spectrometry reveals ATP production defects in Niemann-Pick disease, type C1 mouse brain myelin and human oligodendrocytes; Chandimal Pathmasiri1; Stephanie M Cologna4; 1University of Illinois at Chicago, Chicago, IL.
TUESDAY ORALS

TOF am 09:50

BrainProt: An Omics based knowledgebase towards the understanding of Human Brain and diseases; Deepak Biswas1; Sanjoy Vinayak Shenoy1; Arifin Chauhan1; Advait Padhye1; Sanjeeva Srivastava1; IIT Bombay, Mumbai, India

TOF am 10:10

Employing LCMS-based system-wide quantification of N-glycosylation to determine the effects of fatty acids on a neuroinflammation cell model; Sherly Joyce B. Grijaldo2; Michael Russell S. Alvarez2; Ryan Lee Schindler1; Armin Oloomi1; Tristan Alexander Seales2; Siyu Chen1; Nikita P. Bacalzo1; Radu C. Nacario1; Gladys C. Completo1; Carito B. Lebrilla2; 1University of the Philippines Los Baños, Los Baños, Laguna, Philippines; 2University of California, Davis, Davis, CA; 3University of the Philippines Manila, Manila, Philippines

TOF am: Drug Metabolism and Pharmacokinetics

General Assembly B

Session Chair: Josh Yu (Gilead)

TOG am 08:30

Automated High-Resolution Mass Spectrometry Data Processing Meets/Beats QQK for Drug Quantification Studies; Kevin Bateman1; Fabien Fontaine3; Bernard Choi1; Luca Morettoni2; Ismael Zamora3; 1Preclinical Development, Merck Research Lab, Meck & Co. Inc, West Point, PA; 2Lead Molecular Design, S.L., Sant Cugat del Valles, Spain; 3Molecular Discovery, Elstree Borehamwood, United Kingdom

TOG am 08:50

Confident characterization and identification of glucuronide metabolites using diagnostic fragments from orthogonal MS/MS data; Rahul Baghla1; Eshani Nandita1; SCIEX, Redwood City, CA

TOG am 09:10

Quantitative Analysis of Liver mARCl in Different Species Using Reagent Free-Automatic High pH Fractionation Enrichment (RF-auto HpH) and LC-MS; Xue Dong1; Julie Lade2; Fang Xie2; Zhe Wang3; Xiaoming Shen1; 1Amgen, Inc., South San Francisco, CA

TOG am 09:30

Accelerator Mass Spectrometry @ Boehringer-Ingelheim – implementing ultrahigh sensitivity 14C analysis for routine microtracer studies in DMPK; Ralf Laux1; Stefan Blech1; Boehringer Ingelheim Pharma, Biberach, Germany; 2Boehringer Ingelheim Pharma, Biberach, Germany

TOG am 09:50

Intact Protein Mass Analysis throughout Covalent Drug Discovery, including Pharmacokinetics/Pharmacodynamics, Tissue Distribution, Route of Administration, Dose Estimation, and Efficacy; Md Amin Hossain1; Rutuli R. Brahme1; Brandon C. Miller1; Jakal Amin1; Jared R. Auclair1; Qingping Wang2; David J. Greenblatt3; Roman Manetsch1; Jeffrey N. Agar1; 1Northeastern University, Boston, MA; 2Sanofi, Cambridge, MA; 3School of Medicine, Tufts University, Boston, MA

TOG am 10:10

Quantitative Proteomics supports characterization of complex translational in vitro models for oral prodrugs; Xue Wang1; Liang Jin1; Abhinav Sharma2; David Stresser1; Yu Tian2; 1AbbVie Bioresearch Center, Worcester, MA; 2AbbVie Inc., North Chicago, IL

TOH am 08:30

Exploring cellular heterogeneity within human pancreas by 3D-MALDI imaging of intact proteoforms; Kevin J Zemalics1; Dušan Velicković1; David J Degnan2; James M Fulcher3; Lye Meng Markille3; Yu Mi Kwon3; Dehong Hu4; Yen-Chen Liao4; Sarah M Williams5; Lisa M Bramer6; Ying Zhi7; William Kew8; Wei-Jun Qian9; Mowi Zhou10; Lijiliana Paša-Tolić11; 1Pacific Northwest National Laboratory, Richland, WA

TOH am 08:50

Spatial Proteomics of the Skeletal Matrix in Osteoarthritis via MALDI-MSI Reveals Molecular Delineations in Disease Severity and New Biomarkers; Charles E. Churchill1; Jonathan N. Tao1; Jonathun J. Woo2; Tamara Alliston3; Peggi M. Angel4; Birgit Schilling1; 1Buck Institute for Research on Aging, Novato, CA; 2Braker Daltonics, San Jose, CA; 3University of California San Francisco, Department of Orthopaedic Surgery, San Francisco, CA; 4Medical University of South Carolina, Charleston, SC

TOH am 09:09

Deep Visual Proteomics and spatial transcriptomics uncover the landscape of cancer malignancy in borderline ovarian cancer; Lisa Schweizer1; Rahul Krishnan2; Aasa Shimizu1; Andreas Metousis1; Hilary Kenny1; Lisha Zhu1; Thierry Nordmann2; Florian Rosenberger3; Agnes Julia Bilecz4; Rachelle Mendoza5; Sanaa Nakad6; Ralf Borrego7; Marvin Thielert7; Sophia Mädler8; Andreas Mund9; Mengjie Chen9; Ricardo Lastra10; Matthias Mann11; Ernst Lengyel12; 1Max Planck Institute of Biochemistry, Martinsried, Germany; 2Department of Obstetrics and Gynecology/Section of Gynecologic Oncology, University of Chicago, Chicago, Illinois; 3Medicine/Section of Genetic Medicine, The University of Chicago, Chicago, Illinois; 4Department of Pathology, The University of Chicago, Chicago, Illinois; 5Proteomics Program, Novo Nordisk Foundation Center for Protein Research, Faculty of Health and Medical Sciences, University of Copenhagen, Copenhagen, Denmark

TOH am 09:30

Correlating Tissue Biomechanics and Molecular Information – The Combination of physiological AFM and MALDI MSI; Martina Marchetti-Deschmann1; Martin Handelshauser2; Aleksandra Lebedeva2; Crestis Andreiots; Philipp Thurner3; 1TU Wien, Vienna, Austria

TOH am 09:50

MALDI Imaging of Post-Mortem COVID-19 Lungs; Caitlin Tressler1; Gargye B. Yagnik2; Karl Smith3; Nicole M. Jenkins4; Chad Weissman5; Kenneth J. Rothschuld6; Mark J. Lim7; David Nauen8; Kristine Glunde1; 1Johns Hopkins University School of Medicine, Baltimore, MD; 2AmberGen, Inc., Billerica, MA; 3Leibniz-Institut für Analytische Wissenschaften—ISAS—e.V., Dortmund, Germany; 4National High Magnetic Field Laboratory, Tallahassee, FL

TOH am 10:10

Software workflow and statistical analysis tools for evaluating multiomics MALDI MSI studies; Tobias Boskamp1; Sören-Oliver Deininger2; Mark Lim2; Gargye Yagnik2; Nathalie Agar2; Sylwia Stopka1; Richard R. Drake1; Stacy A. Malaker1; Rachel Stubler1; Kenneth J. Rothschuld3; 1Braker Daltonics GmbH & Co. KG, Bremen, Germany; 2AmberGen, Inc., Billerica, MA; 3Harvard Medical School, Boston, MA; 4Medical University of South Carolina, Charleston, SC; 5Yale University, New Haven, CT; 6Boston University, Dept. of Physics and Photonics Center, Boston, MA

TOH am: Imaging: Spatially-Resolved Omics

General Assembly C

Session Chair: Elizabeth Neumann (University of California, Davis)
<table>
<thead>
<tr>
<th>Time</th>
<th>Title</th>
<th>Authors</th>
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<tbody>
<tr>
<td>TOB pm 02:30</td>
<td>Enhanced resolving power using multiple passes of a multi-reflecting time-of-flight mass analyser</td>
<td>William Johnson, Martin E. Palmer, Peter Nixon</td>
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<tr>
<td>TOB pm 02:50</td>
<td>Pushing the boundaries of quantitative proteomics with data independent acquisition using a novel high-resolution mass analyzer</td>
<td>Lilian R. Heij, Nicolaie Eugen Damoc, Tabiwang N. Arrey, Anna Pashkova, Chris Hsu, Christine C. Wu, Philip M. Remes, Hamish Stewart, Christian Hook, Michael Senko, Vlad Zabrouskov, Michael J. MacCoss, University of Washington, Seattle, WA; Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; Thermo Fisher Scientific, San Jose, CA</td>
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<tr>
<td>TOB pm 03:01</td>
<td>Combining TIMS-ToF and FT-ICR: A prototype TIMS-FT-ICR MS instrument capable of deep characterisation of complex samples</td>
<td>Christopher Andrew Wootton, Alina Theisen, Gregory Brabeck, Carlos Schat, Claudia Kriete, Roland Jertz, Bruker Daltonics, Bremen, Germany</td>
</tr>
<tr>
<td>TOB pm 03:30</td>
<td>High Resolution Analysis of Megadalton Sized DNA using Charge Detection Mass Spectrometry</td>
<td>Lothar Miller, Polycorp Oegbu, Benjamin Draper, Martin F. Jarrold, Indiana University Bloomington, Bloomington, IN</td>
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<tr>
<td>TOB pm 04:10</td>
<td>Performance demonstration of an in situ laser desorption/ionization Orbitrap mass spectrometer</td>
<td>Adrian Southard, Soumya Ray, Ricardo Arevalo, Jr., Amy M. McKenna, Greg T Blakney, Michael W. Senko, Christopher L. Hendrickson, National High Magnetic Field Laboratory, Tallahassee, FL; Thermo Fisher Scientific, San Jose, CA</td>
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<td>TOB pm 02:50</td>
<td>A novel paradigm for kinase-associated disorders: Multiplexed phosphoproteomic analysis of kinase specificity rewiring in patient-derived samples of rare neurodevelopmental disorder</td>
<td>Danielle M. Caefer, Jeremy Balsbaugh, Jennifer Liddle, Anastasios Tzingounis, Daniel Schwartz, University of Connecticut, Storrs, CT</td>
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<tr>
<td>TOB pm 03:10</td>
<td>Investigating T-cell Activation Using the Phosphorylation Integrated Thermo Shift Assay</td>
<td>Brandon M. Gassaway, Alison E. Ringel, Emily M. Huntsman, Jared L. Johnson, Lewis C. Cantley, Edward L. Huttlin, Steven P. Gygi, Marcia C. Haigis, Harvard Medical School, Boston, MA; MIT, Cambridge, MA; Weill Cornell Medicine, New York, NY</td>
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<td>TOB pm 03:30</td>
<td>Time-resolved deoxyribonucleotidyl polymorphism for protein degraders: Ishwar Kohale, Aman Makajru, Han-Yin Yang, Bradford Gibson, Daryl N. Bulloch, Amgen, South San Francisco, CA; Amgen, Thousand Oaks, CA</td>
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<td>TOB pm 03:50</td>
<td>A quantitative and site-specific atlas of the in vivo citrullination reveals widespread expansion of citrullination</td>
<td>Alexandra Stropp, A. Hendriks, Sara C. Buch-Larsen, Jonas D. Elsborg, Rebecca Kirsch, Nadezhda T. Doncheva, Lars J. Jensen, Maria Christophorou, Michael L. Nielsen, NNF Center for Protein Research, Univ of Copenhagen, Copenhagen N, Denmark; Babraham Institute, Cambridge, United Kingdom</td>
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<tr>
<td>TOB pm 04:10</td>
<td>PTKExchange : Globally harmonized re-analysis and sharing of data on post-translational modifications</td>
<td>Kerry A. Rambottom, Oscar M Camacho, Zhi Sun, Emily Bowler-Barnett, Jun Fan, Ananth Surappa, Narayanappa, Deepi Kundu, Yasset Perez-Riverol, Maria-Jesus Martin, Antonio J. Vizcaino, Eric W. Deutsch, Andrew R Jones, University of Liverpool, Liverpool, United Kingdom; Institute for Systems Biology, Seattle, WA; EMBL's European Bioinformatics Institute (EMBL-EBI), Wellcome Genome Campus, Hinxton, United Kingdom</td>
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<td>TOB pm 02:30</td>
<td>New High-Resolution Accurate Mass (HRAM) Platform Enables Rapid and Deep Human Phosphoproteomics</td>
<td>Noah M. Lancaster, Trenton M. Peters-Clarke, Tabiwang N. Arrey, Anna Pashkova, Nicholas Arp, Jing Fan, Evgenia Shishkova, Michael S. Westphall, Hamish Stewart, Eugen Damoc, Vlad Zabrouskov, Joshua J. Coon, Department of Chemistry, University of Wisconsin-Madison, Madison, WI; Department of Biomedical Chemistry, University of Wisconsin-Madison, Madison, WI; Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; Morgridge Institute for Research, Madison, WI; Cellular and Molecular Biology Graduate Program, University of Wisconsin-Madison, Madison, WI; Department of Nutritional Sciences, University of Wisconsin-Madison, Madison, WI; National Center for Quantitative Biology of Complex Systems, Madison, WI; Thermo Fisher Scientific, San Jose, CA</td>
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<td>TOB pm 02:50</td>
<td>Spontaneous Breakup of Charged Aqueous Nanodrops: Dynamics of Rayleigh Fission in the Submonolayer Range</td>
<td>Emeline Hanzin, Conner C Harper, Matthew S. McPartlan, Evan R. Williams, University of California Berkeley, Berkeley, CA</td>
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<td>TOB pm 03:01</td>
<td>Transition metal identification and speciation by MALDI FT-ICR MS as salen complexes</td>
<td>Elena Giaretti, Farah Salma, Davide Corini, Caterina Bordin, Manal Ridany, Mariaelisa Crestoni, Christian Rolandi, Department of Sciences &amp; Technologies, University of Venice, Villeneuve d’Ascq, France; Faculty of Science III, Lebanese University, Tripoli, Lebanon; Dipartimento di Chimica e Tecnologie del Farmaco, Sapienza - Università di Roma, Roma, Italy; Shreiking Sixties - 1-3 Allee Lavosier, Villeneuve d’Ascq, France</td>
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<tr>
<td>TOB pm 03:30</td>
<td>Effect of gas-phase on reactant ions, ionization and fragmentation in dielectric barrier discharge</td>
<td>Elysia S. Gallagher, Baylor University, Waco, TX</td>
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</table>
Unravelling the Mechanisms of Magic Number Custer Formation During Electrospray Ionization: Lars Konermann1, Yousef Haidar1, Vida Alinezhad1, Elnaz Aliyari2, 1Univ. of Western Ontario, London, ON

Use of Acoustic Energy to Disrupt Exosomes for Direct Compositional Analysis by MS: Ashton N Taylor1, Cheyenne Sircher1, Yuqi Huang1, Venkata Bhethanabotla1, Theresa Evans-Nguyen1, 1University of South Florida, Tampa, FL

TOD pm 03:50

TOD pm 04:10

Direct Compositional Analysis by MS

Lars Konermann1, Yousef Haidar1, Vida Alinezhad1, Elnaz Aliyari2, 1Univ. of Western Ontario, London, ON

Use of Acoustic Energy to Disrupt Exosomes for Direct Compositional Analysis by MS: Ashton N Taylor1, Cheyenne Sircher1, Yuqi Huang1, Venkata Bhethanabotla1, Theresa Evans-Nguyen1, 1University of South Florida, Tampa, FL

Session Chair: Sonja Hess (AstraZeneca)

ProtPipe: An informatic pipeline for mass spectrometry-based proteomics and peptidomics; Ziyi Li1, 2; Nicholas Johnson1, 2; Syed Shah1, 1; Cory A. Weller1, 2; Ying Hao1; Jessica Roberts1; Rahul Bezabih1; Mark R. Cookson1; Michael E. Ward1; Andrew B. Singleton1; Mike A. Nalls1, 2; Yue A. Qi1; Center for Alzheimer’s and Related Dementias, National Institute of Health, Bethesda, MD; 2Department of Biomedical Medicine, Faculty of Health Sciences and Medicine, Ghent, Belgium; 3Interuniversity Institute of Bioinformatics in Brussels, ULB-VUB, Brussels, Belgium; 4Structural Biology Brussels, Vrije Universiteit Brussel, Brussels, Belgium

ProtPipe: An informatic pipeline for mass spectrometry-based proteomics and peptidomics; Ziyi Li1, 2; Nicholas Johnson1, 2; Syed Shah1, 1; Cory A. Weller1, 2; Ying Hao1; Jessica Roberts1; Rahul Bezabih1; Mark R. Cookson1; Michael E. Ward1; Andrew B. Singleton1; Mike A. Nalls1, 2; Yue A. Qi1; Center for Alzheimer’s and Related Dementias, National Institute of Health, Bethesda, MD; 2Department of Biomedical Medicine, Faculty of Health Sciences and Medicine, Ghent, Belgium; 3Interuniversity Institute of Bioinformatics in Brussels, ULB-VUB, Brussels, Belgium; 4Structural Biology Brussels, Vrije Universiteit Brussel, Brussels, Belgium

Session Chair: Sonja Hess (AstraZeneca)

TOD pm 02:10

TOD pm 03:10

Multi-omic microsampling for the profiling of lifestyle-associated changes in health: Xiaotao Shen1, Ryan Kellogg2, Daniel Pardy1, 2; Michael E. Ward1, 2; Andrew B. Singleton1, 2; 1Department of Biomedical Medicine, Faculty of Health Sciences and Medicine, Ghent, Belgium; 2Department of Biomedical Medicine, Faculty of Health Sciences and Medicine, Ghent, Belgium

TOD pm 02:30

Multi-omic microsampling for the profiling of lifestyle-associated changes in health: Xiaotao Shen1, Ryan Kellogg2, Daniel Pardy1, 2; Michael E. Ward1, 2; Andrew B. Singleton1, 2; 1Department of Biomedical Medicine, Faculty of Health Sciences and Medicine, Ghent, Belgium; 2Department of Biomedical Medicine, Faculty of Health Sciences and Medicine, Ghent, Belgium

TOD pm 03:30

Mass spectrometry-based multi-omics identifies sarcopenia-associated molecular landscape perturbations in rhesus monkey skeletal muscle; Melissa R Pergande1, Yutong Jin1, Kalina J Rossler1, Gaëtan Misson1, 1University of Wisconsin-Madison, Madison, WI

TOD pm 03:30

Mass spectrometry-based multi-omics identifies sarcopenia-associated molecular landscape perturbations in rhesus monkey skeletal muscle; Melissa R Pergande1, Yutong Jin1, Kalina J Rossler1, Gaëtan Misson1, 1University of Wisconsin-Madison, Madison, WI

TOD pm 03:50

Development of a Tumor Immunopeptidome database for T cell-based therapies: Yulan Chiu1, Ke Pan1, Cassian Yue1, The University of Texas MD Anderson Cancer Center, Houston, TX

TOD pm 03:50

Development of a Tumor Immunopeptidome database for T cell-based therapies: Yulan Chiu1, Ke Pan1, Cassian Yue1, The University of Texas MD Anderson Cancer Center, Houston, TX

TOD pm 04:10

Deep Human Proteome Sequencing for Global Detection of Mutations and Alternative Splicing; Pavel Simcik1, 2, Alicia L. Richards1, 2, Robert J. Weatheritt1, 2, Daifeng B. Brandon3, 4, Jesse Meyer3, 5, Michael S. Westphal3, 5, Evgenia Shishkova6, 7, Benjamin J. Blencowe1, 10, Juergen Cox1, Joshua J. Coon3, 4, 7, 9, Computational Systems Biochemistry Research Group, Max-Planck Institute of Biochemistry, Martinsried, Germany; 2Morgannide Institute for Research, Madison, WI; 3National Center for Quantitative Biology of Complex Systems, Madison, WI; 4Department of Chemistry, University of Wisconsin-Madison, Madison, WI; 5EMBL Australia and Garvan Institute of Medical Research, Darlinghurst, Australia; 6School of Biotechnology and Biomolecular Sciences, University of New South Wales, Sydney, Australia; 7Department of Biomolecular Chemistry, University of Wisconsin - Madison, Madison, WI; 8Department of Microbiology and Ecosystem Science, University of Vienna, Vienna, Austria; 9Donnelly Centre for Cellular and Biomolecular Research, Toronto, ON; 10Department of Molecular Genetics, University of Toronto, Toronto, ON

TOD pm: Informatics: Multimics Integration and Applications

Session Chair: Sonja Hess (AstraZeneca)

TOC pm 03:50

TOC pm 03:10

TOE pm 03:10

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TOE pm 03:50

TOE pm 04:10

TOC pm 02:50

TOC pm 02:50

TOE pm 02:30

TOE pm 02:30

TOE pm: Plants and Natural Products

Room 332

Session Chair: Joshua Kellogg (Pennsylvania State University)

TOD pm 02:50

A tissue specific post-translational modification (PTM) map of human proteome; Pathmanaban Ramasamy1, 1; Hanne Devos2, 2; Wim F. Vranken2, 3, Lennart Martens1, 2, 1VIB-UGent Center for Medical Biotechnology, Gent, Belgium; 2Department of Biomedical Medicine, Faculty of Health Sciences and Medicine, Ghent, Belgium; 3Interuniversity Institute of Bioinformatics in Brussels, ULB-VUB, Brussels, Belgium

Identifying chia oil in Colonial Mexican art materials using multi-omics approaches; Aleksandra Popowich1, Jose Luis Lazarte Luna2, Catherine Gilbert3, Monica Katz1, Ronda Kasl1, Christopher Mason1, Caroline Tokarski2, Julie Arslanoglu2, 3MetroPac Museum of Art, New York, NY; 2University of Aberdeen, Aberdeen Proving Ground, United Kingdom; 3GEOMAR Helmholtz Centre for Ocean Research Kiel, Germany; 4Federal Institute of Science and Technology of Maranhão, Timor, Brazil

Pathogen-oriented platform for large-scale discovery of drug-like natural products discovers novel and highly potent small molecule drug-resistant Candidiasis; Bahar Behsaz1, Andres Mauricio Caraballo-Rodriguez2, Pieter C Dorrestein1, Hosein Mohimani1, 1Carnegie Mellon University, Pittsburgh, PA; 2University of California San Diego, San Diego, CA

Profiling of the Polyphenol Content of Honey and its Relationship to Geographical Origins using HPLC-MS/MS; Kate Nyarko1, Kaitlyn Boozerr1, Michael Greenfield1, 1University of Missouri-Columbia, Columbia, MO

Single-protoplast and tissue-specific proteomics of agronomic-relevant plant systems using a nanodroplet processing platform; Saral M Williams1, James M Fulcher1, William Christopher Liyu Andrey1, Lye Meng Markille1, Vimal Kumar Balasubramanian1, Mowei Zhou1, Jaeho Song1, Gary Stacey1, Amy Marshall-Colon1, John Mullet1, Amirhossein H. Ahkami1, Ljiljana Pasa1, Ying Zhu1, Pacific Northwest National Laboratory, Richland, WA; 2University of Missouri, Columbia, MO; 3University of California Davis, Davis, CA; 4Texas A&M University, College Station, TX; 5Genentech Inc., South San Francisco, CA

Looking into the small and fragile – highly resolved, matrix-free MSI of the floating fern Azolla and its specialized metabolites: Benjamin Bartels1, Erbl Gungor2, Sara Tortorella1, Ismael Zamora1, Henriette Schueppmann1, Ron M.A.
TOF pm: Ion Mobility: Structure Determination & Applications

Session Chair: Thanh Do (University of Tennessee, Knoxville)

TOF pm 02:30 Solution and Gaseous Ensembles of α-Synuclein: Towards a Biophysical Understanding of “Unstructured” Protein IM/MS; Melanie Cheung See Kit1; Tyler C Cropsey2; Frank Sobott3; Christian Biehhler4; Ian K. Webb5; 1Indiana University Purdue University Indianapolis, Indianapolis, IN; 2Florida State University, Tallahassee, FL; 3University of Leeds, Leeds, United Kingdom

TOF pm 02:50 Cyclic ion mobility-mass spectrometry and electron capture dissociation probe dimerization of aggregation-prone IAPP; Aisha Ben-Younis1; Alexander Zhvyoloup1; Hannah Britt2; Daniel Raleigh1; 1Konstantinos Thalassinos3; 1University College London, London, United Kingdom; 2Stony Brook University, Stony Brook, NY

TOF pm 03:30 Ion Mobility – Mass Spectrometry Evaluates the Effects of Lipid Bidders On Membrane Protein Structure and Stability; Iliana Levesque1; Aniruddha Panda2; Kalliop Gupto3; Brandon T Ruotolo4; 1University of Michigan, Ann Arbor, MI; 2Yale University, New Haven, CT

TOF pm 03:50 Resolving regio- and stereo-isomer complexity using cyclic ion mobility coupled to mass spectrometry; Stephen J Blankety1; Berwyck Pool1; Reuben S. E. Young2; Lachlan Jeknavor3; Felicia Hansen1; Thi Phuong Do1; Hendrik Frisch1; Michael Pfund1; David L Marshall1; Kathleen Mullen1; 1Queensland University of Technology, Brisbane, Australia; 2University of Wollongong, Wollongong, Australia

TOF pm 04:10 High-Resolution Ion Mobility Mass Spectrometry in Separation of Oligonucleotide Impurities; Nenfa N. Dieke1; Joshua Shipman1; Cynthia Sommers1; Jason Rodriguez1; Deyi Zhang2; Darby Kozak2; Kui Yang3; 1U.S. Food and Drug Administration, Saint Louis, MO; 2U.S. Food and Drug Administration, Silver Spring, MD

TOH pm: H/D Exchange: Innovations and Applications

Session Chair: Martial Rey (Institut Pasteur)

TOH pm 02:30 Folding of prestin’s anion-binding site and implications to electromotility and hearing as revealed by HDX-MS; Xiaojuan Lin1; Patrick Haller1; 2Navid Bavi1; 2Nabil Faruk1; Eduardo Perozo1, 3, 4; Tobin R Sosnick1, 4, 5; 1Department of Biochemistry and Molecular Biology, The University of Chicago, Chicago, IL; 2Center for Mechanical Excitability, The University of Chicago, Chicago, IL; 3Institute for Neuroscience, The University of Chicago, Chicago, IL; 4Institute for Biophysical Dynamics, The University of Chicago, Chicago, IL; 5Pritzker School for Molecular Engineering, The University of Chicago, Chicago, IL

TOH pm 03:10 Distinguishing Isomeric Disaccharides with Intenselectrospray Ionization Hydrogen/Deuterium Exchange Mass Spectrometry (in-ESI HDX-MS); Anna V. Quintero1; O. Tara Liyanage1; Elyssia S. Gallagher1; 1Baylor University, Waco, TX

TOH pm 03:30 Transient structural dynamics during allosteric activation and inhibition of glycocon phosphorylation from non-equilibrium millisecond HDX-MS; Monika Kish1; Dylan P Ivory1; Jonathan J Phillips1; 1Living Systems Institute, University of Oregon, Exeter, Exeter, United Kingdom

TOH pm 04:10 Selective protein capture under HDX-MS quench conditions for probing complex biological systems; Dietmar Hammerschmid1; Anthony Keesee2; Polina Healey1; Mark Howarth1; Eamonn Reading1; 1Department of Chemistry, King's College London, London, United Kingdom; 2Department of Pharmacology, University of Cambridge, Cambridge, United Kingdom

TOH pm 02:30 Mass Spectrometry for the Underserved: A Chemical Signal Amplification Strategy for Asymptomatic Malaria Detection; Abraham Kwame Badu-Tawiah1; Ayehsa Seth2; Muralikrishnan Girish3; Kingsley Badu1; 1The Ohio State University, Columbus, OH; 2Ohio State University, Columbus, OH; 3Kwame Nkrumah University of Science and Technology, Kumasi, Ghana

TOH pm 02:50 Development of a Lead and Heavy Metal ICP-MS Assay from Quantitative Dried Blood Spots; Donald H. Chace1; Daniel Magiera2; Nesta Bortey-Sam1; Jerry Vockley1; Capitainer AB, Solna, Sweden; 1MMS Diagnostics, Warwick, RI; 2University of Pittsburgh, Pittsburgh, PA; 3University of Pittsburgh Medical Center, Pittsburgh, PA

TOH pm 03:10 Tackling challenges in clinical plasma proteomics studies; Jana Zecha1; Junmin Wang1; Stefani N. Thomas2; Ventzislava A. Hristova3; Sonja Hess4; 1Dynamic Omics, Centre for Genomics Research (CGR), Discovery Sciences, Biopharmaceuticals R&D, Gaithersburg, MD; 2Data Sciences & Quantitative Biology, Discovery Sciences, Biopharmaceuticals R&D, AstraZeneca, Waltham, MA; 3Department of Laboratory Medicine and Pathology, University of Minnesota, Minneapolis, MN

TOH pm 03:30 Targeted proteomics enables multiplex quantification of immunomodulatory and DNA mismatch repair proteins in FFPE tissue specimens; Jeff Whiteaker1; Lei Zhao1; Uliana Voytovich1; Jacob J. Kennedy2; George Miles1; Galen Hostetter3; Chelsea Newton2; Scott Jewell1; Yongchao Dou1; Xuying Liao1; Bing Zhang1; Andy
TOH pm 03:50

Plasma Catecholamines by LC-MS/MS: Use of In-column Ion Pairing for Reverse Phase Retention and Interference Separation; Stephen D Merrigan¹; Preejith P. Vachali¹; Elizabeth L. Frank²; ARUP Laboratories, Salt Lake City, UT; University of Utah, Salt Lake City, UT

TOH pm 04:10

Using robotic automation to advance standardisation and traceability in clinical diagnostics; Tabatha Hambidge¹,²; Emily Whyte¹,²; Camilla Liscio³; Steven Corless¹; Patrick Sears³; Chris Hopley¹; LGC, Teddington, United Kingdom; University of Surrey, Guildford, United Kingdom; Element Materials Technology, Cambridge, United Kingdom
WOB am 08:30  Omnimitrap-Orbitrap performance enhancement via unreduced data processing; Anton N. Kozhinov1; Konstantin O. Nagornov; Camille Garcia2; Tingting Fu3; Julia Chamot-Rooke2; Yury O. Tsybin; 1Spectroswiss, Lausanne, Switzerland; 2Mass Spectrometry for Biology Unit, Institut Pasteur, Paris, France

WOB am 08:50  Rapid Characterization of Antibodies via Automated Flow Injection Coupled with Online Microdroplet Reactions and Native-pH Mass Spectrometry; Hao Chen1; Harsha P. Gunawardena2; Yongling Ai1; Jinshan Gao2; Richard N Zare3; 1New Jersey Institute of Technology, Newark, NJ; 2Janssen Research & Development, Spring House, PA; 3Montclair State University, Montclair, NJ; 4Stanford University, Stanford, CA

WOB am 09:10  The Use of Mass Spectrometry in Therapeutic Protein Biologics License Applications: A Retrospective Review Revisited. Jamie Mans1; Mercy Ogun1; Bethel Jesdale1; Cynthia Sommers1; Sarah Roostead2; 1US Food and Drug Administration, Saint Louis, MO; 2US Food and Drug Administration, Silver Spring, MD

WOB am 09:30  Host cell protein (HCP) profiling and quantitation in gene therapy products on a novel high-resolution accurate mass platform; Josh Smith1; Sara Carillo2; Kristina Szrenicz; Tabiwang N. Arrey2; Anna Pashkova2; 1The National Institute for Bioprocessing Research & Training, Mount Merrion, Ireland; 2Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; 3Thermo Fisher Scientific, Reinach, Switzerland; 4Thermo Fisher Scientific, Hemel Hempstead, United Kingdom; 5University College Dublin, Belfield, Ireland

WOB am 09:50  Pulsed Mode Charge Detection Mass Spectrometry Allows Selective Analysis of Gene Therapy Products in Unpurified Samples; Daniel V. Botamanenko1; Benjamin E. Draper1; Martin F. Jarrold1; 1Megadalton Solutions, Bloomington, IN; 2Indiana University Bloomington, Bloomington, IN

WOB am 10:10  Oligonucleotide Mapping via LC-UV-MS/MS to Enable Comprehensive Primary Structure Characterization of an mRNA Vaccine Against SARS-CoV-2; Andrew William Dawdy1; Brian C. Gau2; Leah Hanrili Wang2; Carlos H Castaneda3; Olga V Fries4; Matthew S Thompson2; Thomas F Lerch1; 1Brady, 2Bruker Daltonics, Billerica, MA; 3Research & Training, Mount Merrion, Ireland; 4Montclair State University, Chesterfield, MO

WOB am: Instrumentation: New Hybrid and Multimodal Approaches Hall B3 Session Chair: Benjamin Garcia (Washington University School of Medicine)

WOB am 08:30  Ambient soft-lending enables cryo-EM sample preparation and structural elucidation of native proteins in electrified droplets; Jingjin Fan1; Zi Yang2,3; Xiao Fan2,3; Hongwei Wang2,3; Xiaoyu Zhou1; Zheng Ouyang1; 1Tsinghua University, Beijing, China; 2Department of Precision Instrument, Beijing, China; 3Tsinghua University, Beijing University Joint Center for Life Sciences, Beijing, China

WOB am 08:30  High-Throughput Bioanalytical Analyses of Therapeutic Antibodies Using FAIMS Combined with the SampleStream Platform and Intact Protein Mass Spectrometry; Rachel Liueing Shi1; Michael A. Dillon1; Philip D. Compton2; Christoph Spiess1; Jonathan L. Josephs1; John C. Tran1; 1Genentech Inc, South San Francisco, CA; 2Integrated Protein Technologies Inc., Carlsbad, CA

WOB am: Biotherapeutics: Characterization and Quantitation Ballroom A Session Chair: Pavel V. Bondarenko (Amgen)

WOB am 08:30  Multi-omic analysis reveals changes in cellular pathways following MARC1 knockdown in mouse models of NASH; David Chow1; Yuanjun Guo1; Edward Lagory1; Han-Yin Yang1; Bradford Gibson1; Matthew Rardin1; 1Amgen, Inc., South San Francisco, CA

WOB am 08:50  Deciphering Deubiquitination Ubiquitin Signaling and Substrate Degradation by DIA-PASEF; He Zhu1; Guillaume Adelmant1; Indrajit Sahu4; Nour Alharbi5; Uwai Puyamurtu5; Scott B. Fellner5; Sara J. Buhrlage1; Jarrod A. Marto1; 1Dana-Farber Cancer Institute, Boston, MA; 2Department of Cancer Biology, Department of Oncologic Pathology, Blais Proteomics Center, Dana-Farber Cancer Institute, Boston, MA; 3Department of Cancer Biology and the Linde Program in Cancer Chemical Biology, Dana-Farber Cancer Institute, Boston, Massachusetts

WOB am 09:09  Developing high-throughput screening MALDI-TOF MS cellular assays for drug discovery in non-alcoholic fatty liver disease; Ruth H Walker1; José Luis Marin-Rubio1; Frank H. Büttner1; Matthias Trosi1; Maria Emilia Dueràs1; 1Biosciences Institute Faculty of Medical Sciences, Newcastle University, NE2 4HH, Newcastle Upon Tyne, United Kingdom; 2Bruker Daltonics, Billerica, MA; 3Bruker Daltonik GmbH, Bremen, Germany; 4Chemical Biology, DIB, University of Texas at Austin, Austin, TX; 5Indiana University Bloomington, Bloomington, IN
WOG am 08:50
Spatially and temporally probing distinctive phospholipid alteration in Alzheimer’s disease mouse brain via high-resolution ion mobility-enabled sn-position resolved lipidomics; Shuling Xu¹; Zhijun Zhu¹; Daniel G. Delafield¹; Michael J. Rigby¹; Luigi Pugielli¹; Lingjun Li¹; ¹University of Wisconsin-Madison, Madison, WI

WOF am 09:10
In-Situ Droplet-Based Tissue Derivatization for Lipid Isomer Characterization Using LEISA; Dallas P. Freitas¹; Xi Chen¹; Erin A. Hirtzel¹; Madison E. Edwards¹; Jooohan Kim¹; Hongying Wang¹; Yuxiang Sun¹; Klaudia I. Kocurek¹; David Russell¹; Xin Yan¹; ¹Texas A&M, College Station, TX

WOF am 09:30
Microscopy-directed Imaging Mass Spectrometry for Rapid High Spatial Resolution Molecular Imaging of Gliomei; Allison B Esselman¹,²; Nathan Heath Patterson¹,²; Lukasz G Migas¹; Martin Dufresne¹,²; Katerina V Djambazova¹,³; Madeline E Colley¹,³; Mark P De Caestecker¹; Rab Van De Plas²,³,⁴; Jeffrey M Spragins¹,²,³; ²Department of Chemistry, Vanderbilt University, Nashville, TN; ³Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; ⁴Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; ²Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; ³Division of Nephrology, Department of Medicine, Vanderbilt University, Nashville, TN

WOF am 09:50
Decreasing Relapse in Esogastic Cancer by Improved Diagnostic with SpiderMass Technology; Léa Ledoux¹; Yanis Ziremi⁴; Florence Renaud⁴; Michel Salzet⁴; Isabelle Fournier⁴; ¹Laboratoire PRISM, Université de Lille, Villeneuve d’asq, France; ²PRISM Inserm U1192 - University of Lille, Villeneuve d’asq Cedex, France; ³UMR-S 1192, Lille, France

WOF am 10:10
Integrated morphometric and molecular classification of central nervous system cancers using a unified platform with picosecond infrared laser mass spectrometry; Alexa Fiorante¹; Michael Woolman¹; David Munoz¹; Gérald Zadeh¹; Sunit Das¹; Howard Ginsberg¹; ¹University of Toronto, Toronto, ON

WOG am 08:30
A novel strategy for the systematic analysis of protein degradation identifies direct targets of molecular glue degraders; Marco Jochem¹; Anna Schrmpf²; Lina-Marie Wagner¹; Georg Winter²; Jeroen Krijgsveid³; ¹German Cancer Research Center (DKFZ), Heidelberg, Germany; ²CeMM Research Center for Molecular Medicine, Vienna, Austria

WOG am 08:50
Chiral Pair Isobaric Labeling Strategy for Multiplexed Absolute Quantitation (CHRISTMAS) Revealed Alteration of Enantiomeric DL-Amino Acids in Alzheimer’s Disease Progression; Zhijun Zhu¹; Shuling Xu¹; Zicong Wang¹; Daniel G. Delafield¹; Michael J. Rigby¹; Gaoyuan Lu¹; Ting-Jia Gu¹; Peng-Kai Liu¹; Xin Ma¹; Luigi Pugielli¹; Lingjun Li¹; ¹University of Wisconsin-Madison, Madison, WI

WOG am 09:10
Deep Proteome Turnover in human iPSC-derived Neurons; Ashley Frankenfield¹; Jiawei Ni¹; Jamison Shi¹; Noah Smeriglio¹; Ling Hao¹; ¹George Washington University, Washington, DC

WOG am 09:30
Aziridination-Based 2-Aminopyridine Isotopic (AAPI) and Temporally Enables Lipid Accurate Quantitation with Isomer Resolving Power; Shuli Tang¹; Syuan-Ting Kuo¹; Hongyuan Yang¹; Luchen Wuyang¹; Jiaxin Feng¹; Xin Yan¹; ¹Texas A&M University, College Station, TX

WOG am 09:50
Spatial Neutron-Encoded Stable Isotopic Labeling of Three-Dimensional Multicellular Spheroids; Arbel Lopez¹; Nicole C. Beller¹; Amanda B Hummon¹; ¹The Ohio State University, Columbus, OH

WOG am 10:10
Design and application of a plate-based, proteome-wide reactive cysteine profiling platform using vastly reduced starting protein amounts; Ka Yang¹; Qing Yu¹; Shane Lillis Dawson¹; Joao A. Paulo¹; Steven P. Gygi¹; ¹Harvard Medical School, Boston, MA

WOG am: Stable Isotope Labeling: Applications General Assembly B
Session Chair: Fei Xia Chu (University of New Hampshire)

WOG am 08:30
A novel strategy for the systematic analysis of protein degradation identifies direct targets of molecular glue degraders; Marco Jochem¹; Anna Schrmpf²; Lina-Marie Wagner¹; Georg Winter²; Jeroen Krijgsveid³; ¹German Cancer Research Center (DKFZ), Heidelberg, Germany; ²CeMM Research Center for Molecular Medicine, Vienna, Austria

WOG am 10:10
Differential labelling and mass spectrometry coupled with 473 nm photo-dissociation analysis for relative quantification of cysteine oxidation in proteins; Marion Giord¹; Jean-Valery Guilaubez²; Jérôme Lemoine¹; ¹University of Lyon, Villeurbanne, France; ²University of California, Irvine, CA
WOA pm: Instrumentation: Detection of High-Mass Analytes
Hall B3
Session Chair: Nina Morgner (Goethe Universität Frankfurt)

WOA pm 02:30 Side by Side Comparison of Orbitrap Direct Mass Technology and Charge Detection Mass Spectrometry; Martin Jarrold, Indiana University; Chemistry Department, Bloomington, IN

WOA pm 02:50 Benefits of ultra-long transients in Orbitrap based charge-detection mass spectrometry; Evolène Desligniere1; Victor Yin1; Amber Rolland1; Eduard Ebberink2; Arjan Barendregt2; Tobias P. Wörner2; Konstantin Nagornov3; Anton Kozhinov3; Kylie L. Fort4; Yury O. Tsybin5; Alexander A. Makarov6; Albert J.R. Heck5; 1Utrecht University, Utrecht, Netherlands; 2Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; 3Spectroswiss, Lausanne, Switzerland

WOA pm 03:10 To 200k m/z and beyond: native electron-capture charge reduction resolves heterogeneous signals in large biopharmaceutical analytes; a new Orbitrap record; Kyle I.P. Le Huray1,2; Tobias P. Woerner2; Maria Reichardt-Szyba2; Kyle L. Fort4; Frank Sobott1; Alexander A. Makarov6; 1University of Leeds, Leeds, United Kingdom; 2Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany

WOA pm 03:30 Differential Ion Mobility Separations of Intact Antibodies and Complexes: Taking FAIMS of Macromolecules Toward the MegaDalton Range; Tobias W. Thurner1; Alexander A. Makarov6; Alexandre A Shyvartsburg2; 1Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; 2Wichita State University, Wichita, KS

WOA pm 03:50 Protein complex heterogeneity and structure revealed by native mass spectrometry with electron capture charge reduction and surface induced dissociation; Jared B. Shaw1; Sophie R. Harvey2; Chen Du3; Vicki H Wysocki3; 1,eMision, Corvallis, OR; 2Resource for Native Mass Spectrometry-Guided Structural Biology, The Ohio State University, Columbus, OH; 3Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH

WOA pm 04:10 Large and In Charge: Rapid Analysis of 300+ MDa Nanoparticles and Biomolecules Using High-Throughput, Filter-less Charge Detection Mass Spectrometry (CDMS); Conner C Harper1; Zachary M. Miller1; Matthew S. McPartlan1; Jacob S. Jordan1; Evan R. Williams1; 1University of California, Berkeley, Berkeley, CA

WOB pm: Metabolomics: New Technologies and Applications
Ballroom B
Session Chair: Facundo Fernandez (Georgia Institute of Technology)

WOB pm 02:30 Current practices in LC-MS untargeted metabolomics: a scoping review on the use of pooled quality control samples; Corey D Broekling1; Richard Beger2; Leo L Cheng3; Raquel Lassiter4; Daniel J Cuthbertson5; Surendra Dasar6; Clay W Davis7; Warwick B Dunn8; Anne M Evans9; Álvaro Fernández-Ochoa10; Kelli D Goodman11; Helen Gika12; Royston Goodacre13; Jon Gonzalco J Gouveia14; Hsu Ping-Ching15; Jennifer A Kiwan16; Dritan Kodra17; Julia Kuligowski18; Lan S Renny19; Maria Eugenia Monge20; Jonathan D Mosley21; Sindhu Nambiar22; Nicole Reisdorph23; Stacy D Sherr24; Georgios Theodoridis25; Candice Z Umer26; Dajana Vuckovic27; Bo Zhang28; 1Colorado State University, Fort Collins, CO; 2National Center for Toxicological Research, Jefferson, AR; 3Harvard Medical School, Boston, MA; 4Institut d’Investigación Sanitaria Pere Virgili, Tarragona, Spain; 5Agilent Technologies, Santa Clara, CA; 6Mayo Clinic, Rochester, MN; 7National Institute of Standards and Technology, Charleson, SC; 8University of Liverpool, Liverpool, United Kingdom; 9Metabolon, Morrisville, NC; 10University of Granada, Granada, Spain; 11Aristotle University of Thessaloniki, Thessaloniki, Greece; 12National Institute of Standards and Technology, Rockville, MD; 13University of Arkansas for Medical Sciences, Little Rock, AR; 14Max Delbrück Center, Berlin, Germany; 15Health Research Institute La Fe, Valencia, Afghanistan; 16Arkansas Children’s Nutrition Center, Little Rock, AR; 17Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET), Buenos Aires, Argentina; 18Environmental Protection Agency, Athens, GA; 19University of Alberta, Edmonton, AB; 20University of Colorado Anschutz, Denver, CO; 21Vanderbilt University, Nashville, TN; 22USDA-FSIS, Athens, GA; 23Concordia University, Montreal, QC; 24Olaris, Framingham, MA

WOB pm 02:50 Development of a High-Coverage and Quantitative Metabolomics Assay for Targeted Analysis of Multiple Pathways: Shuang Zhao1; Liang Li2; Shuang Zhao1; 1The Metabolomics Innovation Centre (TMIC) - University of Alberta, Edmonton, AB; 2University of Minnesota, Minneapolis, MN

WOB pm 03:10 Mass spectrometry-related tools expand the underappreciated diversity of bile acids and their biological implications; Helena Manniche Rius2; Ispta Mohanty1; Yasin El Abiad3; Joshua V Schweer1; Robin Schmid1; Simone Zuffa3; 1Wissenschaftszentrum Berlin für Sozialforschung, Berlin, Germany; 2University of Copenhagen, Copenhagen, Denmark; 3University of Innsbruck, Innsbruck, Austria
Integrating quantification of low abundant targets into nontargeted LC-MS/MS screening using Simultaneous Quantitation and Discovery (SQUAD): Elvise Rodriguez1; Uri Keshet2; Bashar Amer2; Suramaditha Yeld2; Brandon Bills2; Tong Shen1; Susan Bird2; Oliver Fiehn1; University of California Davis, Davis, CA; Thermo Fisher Scientific, San Jose, California; ThermoFisher Scientific, San Jose, CA

Introducing Owlstone’s Breath Biopsy VOC Atlas: Identification of breath VOCs with TD-GC-Orbitrap high resolution accurate mass spectrometry: Shane Swann1; Wisenave Arulvasan1; Ace Hatch1; Julia Greenwood1; Dominic Roberts1; Billy Boyle1; Max Allsworth1; Owlstone Medical, Cambridge, United Kingdom; Thermo Fisher Scientific, Manchester, United Kingdom

Development of a multi-omic approach for microorganism identifications: Jana M Carpenter1; Kingsley Bimphe1; Hannah Hynds1; Kelly Hines1; University of Georgia, Athens, GA

Structural Elucidation of Lipolysaccharides using Field Asymmetric Ion Mobility Spectrometry and Kendrick Mass Defect Plots: Abarouba Mikhail1,2; Darryl Hardie1; Drek Smith1; Helena Petrosova1; Robert K Ernst2; David R Goodlett1,3; University of Victoria Genome British Columbia Proteomics Center, Victoria, BC; 2University of Maryland, Baltimore, MD; 3University of Victoria, Victoria, BC

Analysis of high-resolution mass spectrometric data from non-terrestrial materials: Joseph Frye-Jones1,2; Martha L Chacón-Patío3; Ryan P Rodgers1,2; Alan G Marshall1,2; Florida State University, Tallahassee, FL; National High Magnetic Field Laboratory, Tallahassee, FL

Enhancing Hydrophilic Metabolite Detection and Quantifiability via Derivatization-Assisted Sample Preparation and Dispersive Liquid-Liquid Microextraction (DLLME) Techniques: Olga L Riusch1; Lijun Li1; University of Wisconsin, Madison, WI

Structural elucidation of lipopolysaccharides using field asymmetric ion mobility spectrometry and kendrick mass defect plots: Abarouba Mikhail1; Darryl Hardie1; Drek Smith1; Helena Petrosova1; Robert K Ernst2; David R Goodlett1,3; 1University of Victoria Genome British Columbia Proteomics Center, Victoria, BC; 2University of Maryland, Baltimore, MD; 3University of Victoria, Victoria, BC

Comprehensive impurities profiling in synthetic oligonucleotides by high-resolution mass spectrometry intact mass data processing: A M Abdulla1; Cynthia Sommers1; Jason Rodriguez1; Deyi Zhang1; Darby Kozak1; Kui Yang1; US Food and Drug Administration, Saint Louis, MO; 2US Food and Drug Administration, Silver Spring, MD

Advancing to ultra-high throughput for broad plasma proteome profiling using a novel high-throughput accurate mass platform: Qin Fu1; Tabiwang N. Arrey2; Niveda Sundararaman1; Eugen Damoc2; Yue Xuan2; Jennifer E. Van Eyk1; Cedars Sinai Medical Center, Los Angeles, CA; 2Thermo Fisher Scientific, Bremen, Germany

Polymer Analysis on a High-Resolution Quadrupole-Multi Reflecting Time-Flight Mass Spectrometer: Bryan C. Katzenmeyer1; Dale A. Cooper-Shepherd1; Martin E. Palmer4; Waters Corporation, Millford, MA; 2Waters Corporation, Wilmslow, United Kingdom; 3Waters, Wilmslow, United Kingdom
WEDNESDAY ORALS

WOF pm 03:10
A multidimensional proteomic atlas of replicative aging in budding yeast; Mario Leuten1; Joe Armstrong1; Anja R Ollodrat2; Kyle N Hess2; Michael Muir3; Richard A Rodriguez-Miras; Matt Kaeberlein4; Maitrey Dunham4; Judit Villien4; 1Department of Genome Sciences, University of Washington, Seattle, WA; 2Department of Laboratory Medicine and Pathology, University of Washington, Seattle, WA

WOF pm 03:30
Mapping communication dynamics between physically interacting cells using HySiC; Kelly E Stecker1; Sofia Ibanez-Molero2; Tatiana M. Shamorkina3; Rosa Viner3; Daniel S. Peepers3; Maarten A.F.M. Alteaa1; 1Utrecht University, Utrecht, Netherlands; 2Netherlands Cancer Institute, Amsterdam, Netherlands; 3Thermo Fisher Scientific, San Jose, CA

WOF pm 03:50
Evaluation of the Relative Quantitative Performance Using Tandem Mass Tags on a New High-Resolution Accurate Mass Platform; Martin Zeller1; Jenny Ho2; Amirmansoori Hakimi3; Maowei Dou4; Ryan Bomgaarder5; Rosa Viner2; Bernd Hagedorn2; Ankit Dwivedi2; Nicolaie Eugen Damo4; 1Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; 2Thermo Fisher Scientific, Hemel Hempstead, United Kingdom; 3Thermo Fisher Scientific, San Jose, CA; 4Thermo Fisher Scientific, Rockford, IL

WOF pm 04:10
The day after the drug: understanding persister-derived cells to uncover the mechanisms underlying non-genetic cancer resistance; Bianca J Kuhn1; Natalie Clark1; D. R. Mani1; Adi Goldstein2; Yara Orren3; Steven A Carr4; Namrata D Udeshi2; 1Broad Institute of MIT and Harvard, Cambridge, MA; 2Tel Aviv University, Tel Aviv, Israel

WOF pm 04:10
A New Mechanism for Water Splitting from Gas-Phase Fragmentation of Water Clusters with Holmium Nitrate Complexes; Junseoo Kim1; Idaho National Laboratory, Idaho Falls, ID

WOH pm 02:30
Identifying the Toxins of Harmful Algal Blooms with High Resolution Mass Spectrometry; Logan C Krajewski1; Kirsten A Cottrell2; William A Bragg1; Brady R Cunningham1; Noeland R Bois3; Kristin D Vitory3; Dana L Woodruff4; Karen L Wahl5; David S Wunschel6; Rudolph C Johnson7; Elizabeth I Hamelin1; 1Centers for Disease Control and Prevention, Atlanta, GA; 2Battelle Memorial Institute at the Centers for Disease Control and Prevention, Atlanta, GA; 3Pacific Northwest National Laboratory, Richland, WA

WOH pm 02:50
Library Matching in Real-Time for Guided Data-Dependent HRAM Analysis of Unknown PFAS; Brandon Bills; Sunandini Yedin1; Ed George1; Juan Sanchez1; Tim Stratton1; Ralf Tauteenhahn1; Vlad Zabrouskov1; 1Thermo Fisher Scientific, San Jose, California

WOH pm 03:10
Non-targeted identification of chemical markers to authenticate honey botanical origin using LC-QTOF-MS; Lei Tian1; Shaghig Bilamjian1; Tarun Anumol1; Daniel Cuthbertson1; Stéphane Bayen1; 1McGill University, Ste-Anne-de-Bellevue, QC; 2Agilent Technologies, Santa Clara, CA

WOH pm 03:30
Uncovering the Fate of High Latitude Oil Spills: Non-target LC-Orbitrap Analysis of Hydrocarbon Oxidation Products; Maxwell L. Harsha1; Danielle E. Verna2; Zachary C. Redman3; Josh Wesolowski3; Angelique Fouche4; David C. Podgorski1,3; Patrick L Tomo5,3; 1University of New Orleans, New Orleans, LA; 2Prince William Sound Regional Citizens’ Advisory Council, Valdez, AK; 3University of Alaska Anchorage, Anchorage, AK

WOH pm 03:50
Tissue distributions and metabolism of known and novel PFASs in mice dosed with a complex aqueous film-forming foam (AFFF) mixture; David Duker1; Carrie A McDonough2; 1Stony Brook University, Stony Brook, NY; 2Carnegie Mellon University, Pittsburgh, PA

WOH pm 04:10
Toward wider access availability of a non-targeted standard/quality control mixture for more reliable method development/assessments; Christine M. Fisher1; Ann M. Knollhoff1; 1FDA Center for Food Safety, College Park, MD

WOF pm: Fundamentals: Reactions of Gaseous and Solvated Ions

General Assembly B

Session Chair: David Foreman (Merrick)

WOG pm 02:30
Evidence of the Role of the 5f-Orbitals in An- Reactivity in ICP-MS/MS Reactions with CO2 and NO; Richard Cox1; Amanda D. French2; Kaili M. Melby1; Micah Prange2; Niri Govind1; 1University of New Orleans, New Orleans, LA; 2University of Alaska Anchorage, Anchorage, AK

WOG pm 02:50
Structural differentiation of denatured ubiquitin conformers via gas-phase ion/ion cross-linking reactions coupled with infrared multiphoton dissociation; Woo-Young Kang1; Arup Mondal1; Julia R. Bonney1; Alberto Perez2; Boone M. Prentice1; 1University of Florida, Gainesville, FL

WOG pm 03:10
Variable Temperature H/D Exchange and Ion- Neutral Clustering using FT-IM-MS to Probe Solvation Dynamics; Haley M Schramm1; Tomoya Tamadate1; Christopher J Hagan1; Brian H Clowers1; 1Washington State University Department of Chemistry, Pullman, WA; 2University of Minnesota, Minneapolis, MN

WOG pm 03:30
Theta-capillary-based interfacial microreactor for reaction acceleration and intermediate capture; Madhu M. E Edwards1; Erin A. Hintze2; Dallas Freitas1; Anmesha Sengupta1; Joohan Kim2; Xin Yan3; 1Texas A&M Chemistry, College Station, TX; 2Texas A&M, College Station, TX

WOG pm 03:50
Methanol-Catalysed Isomerism of Aryl-Amine Protomers; Boris Lecur1; Oisín J Shiels1; Alan T Maccarone1; Shane R. Ellis1,2; Stephen J Blanksby3; Adam J Trevitt3; 1University of Wollongong, School of Chemistry, Wollongong, Australia; 2Illawarra Health and Medical Research Institute, Wollongong, Australia; 3Central Analytical Research Facility, Institute for Future Environments, Brisbane, Australia
**THURSDAY ORALS**

**ThOA am 08:30** Melting needles in haystacks: Fast laser heating coupled to solution-phase separations for measuring protein thermal stabilities from complex matrices; Jacob S. Jordan; Evan R. Williams; 1University of California, Berkeley, CA

**ThOA am 08:50** A monolithic microfluidic probe for ambient mass spectrometry imaging of biological tissues; Luxie Jiang; Matthias Polack; Manxi Yang; Xiangtang Li; Detlev Belder; Julia Laskin; 1Purdue University, West Lafayette, IN; 2Texas A&M University, College Station, TX; 3University of California San Diego, San Diego, CA; 1Purdue University, Lafayette, IN

**ThOA am 09:10** Towards Molecular Digital Twins for Oncology Surgery with Real-Time SpiderMass Mass Spectrometry Imaging; Nina Ogrinc; Paul Chaillou; Lea Ledoux; Michel Salzet; Isabelle Foumier; FRISM Inserm U1192 - University of Lille, Villeneuve Dazac Cedex, France

**ThOA am 09:30** Advances in Venturi Easy Ambient Sonic-Spray Ionization; Luan Felipe C Oliveira; David U. Tega; Alessandra Sussulini; Xin Yan; Lane A. Baker; 1Texas A&M, College Station, TX; 2University of Campinas, Campinas, Brazil; 3Texas A&M Chemistry, College Station, TX

**ThOA am 09:50** Temperature-Controllable Spark Probe Ionization for Multi-dimensional Mass Spectrometer Analysis; Ningxi Li; Xinwei Liu; Zhijun Cai; Zongyao Zhang; Xiejun Bu; Simin Cheng; Xiaohiao Ma; Wenpeng Zhang; Xiaoyu Zhou; Zheng Ouyang; 1Tsinghua University, Beijing, China; 2PURSPEC Technologies (Beijing) Inc., Beijing, China

**ThOA am 10:10** Next-generation Portable Ambient Ionization Mass Spectrometer with Integrated 2D MS/MS Capabilities; Dalton Snyder; Leonard Rorrer; Mitch Wells; Megan Guetzloff; Jane Likens; Nicole Huckaby; Harman Casey; Kevin Rosenbaum; Brandon Reese; Austin Stieglitz; Anthony Esheleman; Luther Collins; Brett Atkinson; 1Teledyne FLIR, West Lafayette, IN

**ThOB am 09:30** Discovery of unusual high-mannose N-glycans by new multi-stage tandem mass spectrometry; Chia Yen Liew; 2Hong-Sheng Lu; 4Ting-Yi Yang; 3An-Ti Hung; 5Bryan John Abel Magoling; 6Charles Pin-Kuang Lai; 1Chi-Kung Hsii; 1AMS, Academia Sinica, Taipei, Taiwan; 2International Graduate Program of Science and Technology (MST), National Taiwan University, Taipei, Taiwan; 3Molecular Science and Technology (MST), Taiwan International Graduate Program (TIGP), Taipei, Taiwan; 1Department of Chemistry, National Taiwan Normal University, Taipei, Taiwan; 2Department of Chemistry, National Tsing Hua University, Hsinchu, Taiwan; 3Chemical Biology and Molecular Biophysics Program, Taiwan International Graduate Program, Academia Sinica, Taipei, Taiwan; 4Academia Sinica, Taipei, Taiwan

**ThOB am 09:50** Mass-defect peak fingerprints embedded by 6-plex mSUGAR tag labeling guide targeted high-resolution mass spectrometry for ultra-sensitive glycomic; Min Ma; 3Miyang Li; 2Yinlong Zhu; 3Yingyi Zhao; 2Feixuan Wu; 2Zicong Wang; 2Yu Feng; 1Hung-Yu Chiang; 2Cheng Chang; 2Lingjun Li; 1School of Pharmacy, University of Wisconsin-Madison, Madison, WI; 1Department of Chemistry, University of Wisconsin-Madison, Madison, WI; 1State Key Laboratory of Proteomics, Beijing Proteome Research Center, National Center for Protein Sciences (Beijing), Beijing Institute of LifeSciences, Beijing, China; 1Chongqing Key Laboratory on Big Data for Bio Intelligence, Chongqing University of Posts and Telecommunications, Chongqing, China; 1State Key Laboratory of Proteomics, Beijing Proteome Research Center, National Center for Protein Sciences (Beijing), Beijing Institute of LifeSciences, Beijing, China; 1Biophysics Program, University of Wisconsin-Madison, Madison, WI; 1Research Unit of Proteomics Driven Cancer Precision Medicine, Chinese Academy of Medical Sciences, Beijing, China; 1Department of Chemistry, University of Wisconsin-Madison, Madison, WI

**ThOB am 10:10** Expanding the MSFragger Glyco Toolkit with O-Pair Localization of O-Glycopeptides in FragPipe; Daniel Polaskey; Lei Lu; Fengchao Yu; Guo Ci Teo; 1Michael R. Shortreed; 2Alexey I. Nesvizhskii; 3University of Michigan, Ann Arbor, MI; 2University of California San Francisco, San Francisco, CA; 3University of Wisconsin-Madison, Madison, WI

**ThOC am 08:30** QA/ QC for Untargeted Metabolomics in a Large Core Lab: Current Best Practices and Innovative Strategies; Uli Keshet; Gert Wohlgemuth; Fanzhou Kong; Yuanue Li; Diego Pedrosa; Oliver Fiehn; 1UC Davis, Davis, CA

**ThOC am 08:50** Untargeted metabolomics by high-resolution mass spectrometry as an enhanced tool for food quality classification; Angela Di Canu; Maria Assunta Acquaviva; Carmine Geta; Patrizia Iannece; Rosanna Cirillo; Filomena Leliario; Carmen Tesoro; Roberto Rubino; Giuliana Bianco; 1Università degli Studi della Basilicata, Dipartimento di Scienze, via dell’Ateneo Lucano 10, 85100, Potenza, Italy; 2Università Degli Studi di Salerno, Dipartimento di Chimica e Biologia, Via Giovanni Paolo II 132,84084, Fisciano (SA), Italy; 3ANFoS - Via San Leonardo 62/A, 84131, Salerno, Italy

**ThOC am: Metabolomics: Untargeted Profiling**

**Session Chair: Kirsten Overdahl (National Institute of Environmental Health Sciences (NIEHS))**

**ThOC am 08:30** QA/ QC for Untargeted Metabolomics in a Large Core Lab: Current Best Practices and Innovative Strategies; Uli Keshet; Gert Wohlgemuth; Fanzhou Kong; Yuanue Li; Diego Pedrosa; Oliver Fiehn; 1UC Davis, Davis, CA

**ThOC am 08:50** Untargeted metabolomics by high-resolution mass spectrometry as an enhanced tool for food quality classification; Angela Di Canu; Maria Assunta Acquaviva; Carmine Geta; Patrizia Iannece; Rosanna Cirillo; Filomena Leliario; Carmen Tesoro; Roberto Rubino; Giuliana Bianco; 1Università degli Studi della Basilicata, Dipartimento di Scienze, via dell’Ateneo Lucano 10, 85100, Potenza, Italy; 2Università Degli Studi di Salerno, Dipartimento di Chimica e Biologia, Via Giovanni Paolo II 132,84084, Fisciano (SA), Italy; 3ANFoS - Via San Leonardo 62/A, 84131, Salerno, Italy

**ThOB am: Glycopeptides, Glycoproteins, and Glycomics**

**ThOB am 08:30** Glycosite mapping and structural dynamics of TIM family immune checkpoints enabled by mucinase SME; Joanna Chongvarsitisinuk; Alexandra D. Steigmeier; Keira E. Mahoney; Mia A. Rosenfield; Taryn M. Lucas; Deniz Ince; Fiona L. Kearns; Alexander Battison; Michael J. Ferracane; Rommie E. Amar; Stacy A. Malaker; 1Yale University, New Haven, CT; 2University of California San Diego, San Diego, CA; 3University of Redlands, Redlands, CA

**ThOB am 08:50** Benefits of dual ion routing multiplexes for glycoproteomics; Nicholas M. Bilev; 2Jingjing Huang; David Bergren; William D. Barshop; John E.P. Syka; Jesse D. Canterbury; Vlad Zubarovsk; Graeme C. McAlister; Christopher Mullen; 1Stanford University, Stanford, CA; 2University of Washington, Seattle, WA; 3Thermo Fisher Scientific, San Jose, CA

**ThOB am 09:10** Characterization of multi-glycosylated proteins by combining O-glycoprotease IMPs and 193 nm ultraviolet photodissociation; Amanda Helms; Edwin Escobar; 1Saulius Vainauskas; Christopher H. Taron; Jennifer S. Brodbelt; 1University of Texas at Austin, Austin, TX; 2New England Biolabs, Ipswich, MA

**ThOB am: Glycomics**

**ThOB am 08:30** Glycosite mapping and structural dynamics of TIM family immune checkpoints enabled by mucinase SME; Joanna Chongvarsitisinuk; Alexandra D. Steigmeier; Keira E. Mahoney; Mia A. Rosenfield; Taryn M. Lucas; Deniz Ince; Fiona L. Kearns; Alexander Battison; Michael J. Ferracane; Rommie E. Amar; Stacy A. Malaker; 1Yale University, New Haven, CT; 2University of California San Diego, San Diego, CA; 3University of Redlands, Redlands, CA

**ThOB am 08:50** Benefits of dual ion routing multiplexes for glycoproteomics; Nicholas M. Bilev; 2Jingjing Huang; David Bergren; William D. Barshop; John E.P. Syka; Jesse D. Canterbury; Vlad Zubarovsk; Graeme C. McAlister; Christopher Mullen; 1Stanford University, Stanford, CA; 2University of Washington, Seattle, WA; 3Thermo Fisher Scientific, San Jose, CA

**ThOB am 09:10** Characterization of multi-glycosylated proteins by combining O-glycoprotease IMPs and 193 nm ultraviolet photodissociation; Amanda Helms; Edwin Escobar; 1Saulius Vainauskas; Christopher H. Taron; Jennifer S. Brodbelt; 1University of Texas at Austin, Austin, TX; 2New England Biolabs, Ipswich, MA
**THURSDAY ORALS**

**ThOD am 09:10**

**Dual column chromatography improves non-targeted analysis coverage when assessing rhizosphere chemical communication:**
Alexandra A Bennett1; Çağla Görkem Eroğlu2; Teresa Steininger-Mairinger1; Markus Puschener1; Aurélie Glell1; Judith Wirth1; Stephan HANN1;
1University of Natural Resources and Life Sciences, Vienna, Department of Chemistry, Institute of Analytical Chemistry, Vienna, Austria; 2Agroscope, Department of Plant-Production Systems, Herboligy in Field Crops Research Group, Nyon, Switzerland; 3University of Natural Resources and Life Sciences, Vienna, Department of Forestry, and Soil Sciences, Institute of Soil Research, Vienna, Austria

_Author(s)_

**ThOD am 09:30**

**ThOD am 09:50**

**Real-Time Breath Analysis Towards a Healthy Human Breath Baseline:**
Zachary J. Sasiene1; Erick S. Lebrun1; Eric G. Schaller1; Phillip M. Mach1; Robert M. Taylor1; Trevor G. Glaros1; Justin T. Baca1; Ethan M. McBride1; los Alamos National Laboratory, Los Alamos, NM; 2University of New Mexico, Department of Chemical and Biological Engineering, Albuquerque, NM

_Author(s)_

**ThOD am 09:50**

**Untargeted metabolomics reveals severity biomarkers for Type 2 Diabetes mellitus and related complications in the Indian population:**
Pramod P Wangikar2; Sneha A Rana1; Vivek Mishra1; Prajval Nakrani1; Bhushan Burkal1; Rakesh Kumar Sahay1; Lakshman Kumar1; 1Indian Institute of Technology Bombay, Mumbai, India; 2Clarity Bio Systems India Pvt Ltd, Pune, India; 1osmania medical college, Hyderabad, India

_Author(s)_

**ThOD am 10:10**

**ThOD am 10:10**

**Molecular network-based optimization of annotations in GC-MS:**
Alexander Semenov1; Vladimir Bogoleba1; Alexey Melnik1; Alexander Aksonov2; 1University of Florida, Gainesville, FL; 2University of Central Florida, Orlando, FL; 3University of Connecticut, Storrs, CT

_Author(s)_

**ThOD am: Data-Independent Acquisition and Multiplexing: Proteomics**
Vertigo C

**Session Chair:** Birgit Schilling (Buck Institute)

**ThOe am 08:30**

**Over 5000 proteins quantified in plasma using DIA-PASEF analysis of nanoparticle protein corona on TIMS-TOF MS:**
Hasnain Keshishian1; Michael W. Burgess1; Sebastian Vaca1; Joseph Allen1; Elizabeth D. Lightbody1; Irene M. Gobrial1; D. R. Mani1; Michael A. Gillette2,3; Matt Willetts4; Steven A. Carr5; 1Broad Institute of MIT and Harvard, Cambridge, MA; 2Bruker Scientific, Storrs, CT; 3Dana Farber Cancer Institute, Boston, MA; 4Massachusetts General Hospital, Boston, MA; 5Bruker Scientific, LLC, Billerica, MA

_Author(s)_

**ThOe am 08:50**

**ThOe am 09:00**

**Over 5000 proteins quantified in plasma using DIA-PASEF analysis of nanoparticle protein corona on TIMS-TOF MS:**
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_Author(s)_

**ThOe am 09:30**

**Rapid single-shot proteomics using narrow window DIA on a novel high-resolution accurate mass (HRAM) platform:**
Ana Martinez Del Val1; Ulises H. Guzmán1; Zilu Ye1; Florian Harking1; Ole Østergaard2; Anna Pashkova3; Tabiwang N. Areyy3; Hamish Stewart4; Abhijit Dasgupta1; Junxin Peng2; Eugen Damoc3; Jesper V. Olsen3; 1Novo Nordisk Foundation Center for Protein Research, Copenhagen, Denmark; 2Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany

_Author(s)_

**ThOe am 09:50**

**Extracellular Matrix Proteomics of Human Lungs Enabled by a Photocleavable Surfactant and diaPASEF:**
Elizabeth F Bayne1; Yanlong Zhu2,3; Kevin M. Buck1; Melissa R. Pergande1,2,3; Vanessa Morales-Tirado2; Yupeng He2; Yoga Tian2; Ying Ge2,3; 1Department of Chemistry, University of Wisconsin - Madison, Madison, WI; 2Department of Cell and Regenerative Biology, University of Wisconsin - Madison, Madison, WI; 3Human Proteomics Program, University of Wisconsin - Madison, Madison, WI; 4Discovery Immunology, Abbvie, Wauwatosa, WI; 5Discovery Immunology, Abbvie Bioresearch Center, Worcester, MA; 6Discovery Immunology, Abbvie Bioresearch Center, Worcester, MA

_Author(s)_

**ThOe am 10:10**

**Parkin Activator, PR-364 Protects Cardiomyocytes Post-Heart Attack: Increased Mitochondrial Flux and Translational Reprogramming:**
Lizhou Ai1; Aleksand Stonstad1; Simion Kreimer1; Matthew Ayres1; Juliana De Freitas Germano1; Chengguo Huang1; Tauseef Butt2; Suresh Kumar2; Roberta Gottlieb1; Jennifer Van Eyk1; 1Cedars-Sinai Medical Center, Los Angeles, CA; 2Progenica Inc, Malvern, PA

_Author(s)_

**ThOe am: Fundamentals Beyond Mass Analysis: Structural Characterization of Isomers**
Room 332

**Session Chair:** Gabe Nagy (University of Utah)

**ThOe am 08:30**

**Beyond Mass Spectrometry: Negative Ion Photoelectron Spectra of 1-, 2-, and 3- Cyanonitracene Radical Anions and the Thermochemistry of Cyanonitraceane Isomers:**
Veselko G. Gusev1; Wilson Gichuru2; Aidan J. Usher1; Kie T. Workman1; 1University of Florida, Gainesville, FL; 2Progenra Inc, Malvern, PA

_Author(s)_

**ThOe am 08:50**

**Identification and relative quantification of fatty acid double bond positional isomers in biological tissues using gas-phase charge inversion ion/ion reactions:**
Julia R. Borney1; Boone M. Prentice1; University of Florida, Gainesville, FL

_Author(s)_

**ThOe am 09:10**

**Tracking Isomerizations in High-Energy Adenine and 9-Methyladenine Cation Radicals by UV-Vis Photodissociation Action Spectroscopy and Cyclic Ion Mobility:**
Václav Zima1; Jiahao Wan1; Mikuláš Vlk1; Josef Cvačka2; František Tureček1; 1University of Washington, Seattle, WA; 2Institute of Organic Chemistry and Biochemistry of the CAS, Prague, Czech Republic

_Author(s)_

**ThOe am 09:30**

**Everything but the kitchen sink:**
Combining IMS-IMS, cryogenic IR spectroscopy, and MS to tackle the isomer problem in oligosaccharide analysis; Ali H. Abikhodr1; Stephan Warnke2; Ahmed Ben Faleh2; Vasyly Yatsyna3; Thomas Rizzo3; 1Tennessee Tech University, Cookeville, TN; 2Bruker Scientific, Malvern, PA; 3University of Washington, Seattle, WA

_Author(s)
THURSDAY ORALS

ThOE am 09:50  A universal photosensitizer for isomer-resolved mass spectrometry imaging of lipids using singlet oxygen reaction;  
Sara Amer1; Daisy M Unishuyu Vila2;3; Musthefa Iqfath; Julia Laskin1;  
1Purdue University, West Lafayette, Indiana;  
2University of Pennsylvania, Philadelphia, Pennsylvania;  
3University of Pennsylvania

ThOE am 10:10  Characterization of sialylated N-glycoprotein isomers on reversed phase LC-ESI mass spectrometry;  
Suya Liu1; Zoe Zhang1; Pavel Ryumin1; Takashi Baba1;  
1AB SCIEX, Concord, ON

ThOF am 09:50  Protein Interactions across the Human Interactome;  
Edward L. Hutlin1; Julian Minteris1; Roger Vargas1; Laura Fontana Vailes1; Tyrone Lee1; Sanjukta Guha Thakurta1; Lana D’Addieco1; Fana Gebreab1; Emily Hill1; Danielle Swane2;  
1Department of Cellular and Quantitative Biosciences Institute of MIT and Harvard, Cambridge, MA;  
2Department of Cellular and Quantitative Biosciences Institute of MIT and Harvard, Cambridge, MA

ThOF am 09:30  Characterizing the interactions between the HIV-1 capsid protein and small molecule ligands using native mass spectrometry;  
Sophie Harvey1;2; William M McFadden1; Bruce E Torbett4;5; Stefan G Sarafianos1;6; Vicki H Wysocki2;3;  
1Department of Chemistry and Biochemistry, The Ohio State University, Columbus, Ohio;  
2Resource for Native Mass Spectrometry Guided Structural Biology, Columbus, OH;  
3Center for ViroSciences and Cure, Laboratory of Biochemical Pharmacology, Department of Pediatrics, Emory University School of Medicine, Atlanta, Georgia;  
4Broad Institute of MIT and Harvard, Cambridge, MA;  
5Interline Therapeutics, Brisbane, CA

ThOF am 10:10  Benchmarks and protocols for top-down mass spectrometry of native proteins and complexes: A consortium-based study;  
Tanja Habeck1; Kyle A. Brown2; Benjamin Des Soyé3; Carter Lantz4; Mowei Zhou5; Novera Alam6; Md Amin Hossain7; Wonhyeok Jung1; James E. Keener1; Michael Volny1; Jesse W. Wilson1; Yujia Ying2; Jeffrey N. Agar3; Paul O. Dais1;6,7; Ying Ge9; Neil L. Keilnehmer10; Hulin Li1; Joseph A. Loo1; Michael T. Marty7; Lilijana Paša-Tolić9; Wendy Sandoval1; Frederik Lernyte1;  
1Technical University of Darmstadt, Darmstadt, Germany;  
2University of Wisconsin-Madison, Madison, WI;  
3Northwestern University, Evanston, IL;  
4University of California, Los Angeles, Los Angeles, CA;  
5Pacific Northwest National Laboratory, Richland, WA;  
6Northeastern University, Boston, MA;  
7University of Arizona, Tucson, AZ;  
8Genentech Inc, South San Francisco, CA;  
9Sun Yat-sen University, Guangzhou, China;  
10Consortium for Top-Down Proteomics, Cambridge, MA

ThOG am 08:30  BioPlex 3D: Predicting Structures for Protein-Protein Interactions across the Human Interactome;  
Edward L. Hutlin1; Julian Minteris1; Roger Vargas1; Laura Fontana Vailes1; Tyrone Lee1; Sanjukta Guha Thakurta1; Lana D’Addieco1; Fana Gebreab1; Emily Hill1; Danielle Swane2;  
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2Resource for Native Mass Spectrometry Guided Structural Biology, Columbus, OH;  
3Center for ViroSciences and Cure, Laboratory of Biochemical Pharmacology, Department of Pediatrics, Emory University School of Medicine, Atlanta, Georgia;  
4Broad Institute of MIT and Harvard, Cambridge, MA;  
5Interline Therapeutics, Brisbane, CA

ThOG am 08:30  Untargeted mass spectrometry-based metabolomics reveals responses to high fiber whole-food diets and microbiome composition in mice;  
Jacob J. Haffner1;2; Yi Sun1;4; Daniela Betancurt Anzola1; Evan R. Hutchison1; Eugenio I. Vivas1; Robert L. Kerby1; Nsoua H. Diabaté1; Camila Gosmanov1; Alejandro Reyes Muñoz2; Federico E. Reyes3; Laura-Isobé McCall4;5;6,7;  
1University of Oklahoma, Department of Anthropology, Norman, OK;  
2University of Oklahoma, Laboratories of Molecular Anthropology and Microbiome Research, Norman, OK;  
3University of Wisconsin-Madison, Department of Bacteriology, Madison, WI;  
4Northwest A&F University, College of Food Science and Engineering, Yangling, China;  
5Universidad de los Andes, Departamento de Ciencias Biológicas, Bogotá, Colombia;  
6University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK;  
7University of Oklahoma, Department of Microbiology and Plant Biology, Norman, OK

ThOG am 08:50  MINNO: A new platform for interpreting complex microbial metabolomics data;  
Stephanie L Bishop1; Ayush Mandival1; Mehdi Mohammadi1; Thomas Rydzak1; Ryan A Groves1; Mildred Castellanos1; George Chaconas1; Joern Davidsen1; Ian A Lewis1;  
1University of Calgary, Calgary, AB

ThOG am 08:30  Evaluating the benefit of dia-PASEF approaches and sample-specific database strategies for metaproteomics of very complex microbiomes;  
Thibaut Dumas1; Olivier Pible1; Guylaine Miotello1; Kristina Marx1; Pierre-Olivier Schmitt2,3; Jean Armengaud1;  
1CEA-Marcoule - Laboratory «Innovative technologies for Detection and Diagnostics», Bagnols-sur-Cèze, France;  
2Bruker Daltonics GmbH, Bremen, Germany;  
3Bruker France S.A., Wissembourg, France

ThOG am 09:30  On-chip multi-modal imaging of soil biogeochemical processes using Synthetic Soil Habitats;  
Arumina Bhattacharjee1; Jocelyn Richardson1; Dušan Veličković2; Gregory Vandergeest1; Christopher Anderton1;  
1Pacific Northwest National Laboratory, Richland, WA;  
2Stanford University, Palo Alto, CA

ThOG am 09:50  RAPID ANALYSIS OF PROTEIN-PROTEIN INTERACTIONS USING A NOVEL HIGH-RESOLUTION ACCURATE MASS PLATFORM;  
Lia Serrano1; Danielle Swaney2,3,4; Tabiwang N. Arrey1; Trenton M. Peters-Clarke1; Noah M Lancaster1; Anna Paszkow1; Evgenia Shishkova1; Michael S. Westphall1; Christian Hook1; Nicolaie Eugen Damoc1; Vlad Zabrouskev1; Joshua J. Coon1;  
1University of Wisconsin-Madison, Madison, WI;  
2OBI COVID-19 Research Group (OQRG), San Francisco, CA;  
3Quantitative Biosciences Institute (QBI), University of California San Francisco, San Francisco, CA;  
4Department of Biomedical and Pharmaceutical Sciences, University of California, San Diego, CA

ThOG am 08:30  Untargeted mass spectrometry-based metabolomics reveals responses to high fiber whole-food diets and microbiome composition in mice;  
Jacob J. Haffner1;2; Yi Sun1;4; Daniela Betancurt Anzola1; Evan R. Hutchison1; Eugenio I. Vivas1; Robert L. Kerby1; Nsoua H. Diabaté1; Camila Gosmanov1; Alejandro Reyes Muñoz2; Federico E. Reyes3; Laura-Isobé McCall4;5;6,7;  
1University of Oklahoma, Department of Anthropology, Norman, OK;  
2University of Oklahoma, Laboratories of Molecular Anthropology and Microbiome Research, Norman, OK;  
3University of Wisconsin-Madison, Department of Bacteriology, Madison, WI;  
4Northwest A&F University, College of Food Science and Engineering, Yangling, China;  
5Universidad de los Andes, Departamento de Ciencias Biológicas, Bogotá, Colombia;  
6University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK;  
7University of Oklahoma, Department of Microbiology and Plant Biology, Norman, OK

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Stephanie L Bishop1; Ayush Mandival1; Mehdi Mohammadi1; Thomas Rydzak1; Ryan A Groves1; Mildred Castellanos1; George Chaconas1; Joern Davidsen1; Ian A Lewis1;  
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1CEA-Marcoule - Laboratory «Innovative technologies for Detection and Diagnostics», Bagnols-sur-Cèze, France;  
2Bruker Daltonics GmbH, Bremen, Germany;  
3Bruker France S.A., Wissembourg, France

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Arumina Bhattacharjee1; Jocelyn Richardson1; Dušan Veličković2; Gregory Vandergeest1; Christopher Anderton1;  
1Pacific Northwest National Laboratory, Richland, WA;  
2Stanford University, Palo Alto, CA
ThOG am 09:50 **Reliable and high-resolution 3D MS imaging of complex biofilms**; Yuting Shen1,2; Kangning Ren1; Zongwei Cai1,2; 1State Key Laboratory of Environmental and Biological Analysis, Hong Kong, China; 2Department of Chemistry, Hong Kong Baptist University, Hong Kong, China

ThOG am 10:10 **Mapping Cellular Organization and Molecular Distributions in S. aureus Abscesses**; Jacqueline M Van Ardenne1,2; Lukasz G Migas3; Madeline E Colley4; Martin Dufresne5,6; Jeffrey A Freiberg7; Valeria M Reyes Rui8; Andy Weiss9; Katerina V Djambazova7,10; Katherine N Gibson-Corley6; Martin Dufresne2,5; Jeffrey M Spraggins1,2,5,7; 1Department of Chemistry, Vanderbilt University, Nashville, TN; 2Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; 3Department of Biochemistry, Vanderbilt University, Nashville, TN; 4Department of Microbiology and Immunology, Vanderbilt University Medical Center, Nashville, TN; 5Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; 6Department of Pathology, Microbiology, and Immunology, Vanderbilt University Medical Center, Nashville, TN; 7Department of Biochemistry, Vanderbilt University, Nashville, TN; 8Department of Chemistry, Vanderbilt University, Nashville, TN; 9Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; 10Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN

**ThOH am: Nucleic Acids and Oligonucleotides**

**General Assembly C**

Session Chair: Jennifer Lippens (Janssen Pharmaceutica NV)

ThOH am 08:30 **Identification of critical impurities in starting materials for oligonucleotide therapeutics by derivatization with reactive chromophores**; Rajeswari Lakshmanan1; Andrew Rodriguez1; Phil Olsen1; Dennis Rhodes2; Claus Rentel3; 1Ionis Pharmaceuticals, Inc., Carlsbad, CA

ThOH am 08:50 **Sequence mapping and rapid quality control analysis of mRNA therapeutics using mass spectrometry**; Emma N Welbourne1; Caroline Evans1; Christina Vanhinsbergh1; Mark Dickman1; 1University of Sheffield, Sheffield, United Kingdom

ThOH am 09:10 **LC-HRMS-based Multi-Attribute Method for Oligonucleotides (MAMO)**; Kul Yang1; A M Abdullah1; Md Rabiu Islam1; Nnenna E Dieke1; Cynthia Sommers1; Jason Rodriguez1; Deyi Zhang2; Darby Kozak2; David Keire1; 1US FDA, St. Louis, MO; 2US Food and Drug Administration, Silver Spring, MD

ThOH am 09:30 **Characterisation and sequencing of modified large mRNA products by nanoflow liquid chromatography coupled to high resolution mass spectrometry**; Craig Jakes1; Maikel Gaitkoski1,2; Felipe Guapo1; Silvia Millan Martin1; Sara Carillo1; Jonathan Bones1,2; 1National Institute of Bioprocessing Research and Training, Dublin, Ireland; 2School of Chemical and Bioprocess Engineering, University College Dublin, Dublin, Ireland

ThOH am 09:50 **Ion Trap Collision-induced Dissociation as a Probe of G-quadruplex Formation**; Nicole M Brundridge1; Jonathan Dickerhoff1; Danzhou Yang1; Scott A McLuckey1; 1Purdue University, Dept. of Chemistry, West Lafayette, IN

ThOH am 10:10 **Complete sequencing of large modified peptide-nucleic acids using MALDI TOF MS/MS**; Danil G Ivanov1; John J Thomas2; Dani M Stoltzfus3; Igor A Kaltashov1; 1University of Massachusetts Amherst, Amherst, MA; 2NeuBase Therapeutics, Pittsburgh, PA
THURSDAY ORALS

**ThOA pm 03:00**

**Open Tubular Solid Phase Extraction Columns Enable Simple and Robust Nonlinear Liquid Chromatography for Single-Cell Proteomics**

Kei Webber1, Sigi Huang1, Thuy Truong1, Xiaofeng Xie1, Ryan Kelly1, Brigham Young University, Provo, UT

**Photoinitiator-Integrated Mobile Phases for Protein Disulfide Mapping By LC/MS2 : Intact versus Bottom-up Approach and pH-Eff:**

Shuhui Chen1, Chinh-Ming Kuo2, Fung-Yu Chen3

National Cheng Kung University, Taiwan, Taiwan

**Exploring Charge Detection Mass Spectrometry on Liquid Chromatography Time Scales:**

Lisa Strasser1, Florian Fueßl1, Tomas E. Morgan1, Felipe Guapo1, Sara Carillo1, Jonathan Bones1, 2

NIBRT, Dublin, Ireland; School of Chemical and Bioprocess Engineering, University College Dublin, Dublin, Ireland

**Unifying the Multi-omics World with Microchip Capillary Electrophoresis: Discovering Secrets in Six Dimensions from One Drop of Dried Blood:**

J. Will Thompson1, 2, J. Scott Mellors1, Youwei Chen2, Timothy McMahon2, Matthew W Foster3, 908 Devices Inc, Carrboro, NC; Duke University Medical Center, Durham, NC

**ThOA pm 03:30**

**Enhanced Sensitivity for Low-Load Proteomics Orbitrap Workflows Using Ion Fractionation with Structures for Lossless Ion Manipulation:**

Daniel Debord1, Liulin Deng1, Brian Adamson2, Alan McKenzie-Coe3, Kyle L. Fort4, Tobias Woerner4, Oliver M Bernhardt4, Roland Bruderer4, Tejas Gandhi5, Lukas Reiter5, Eloy R Wouters6, Jean-Jacques Dunyach7, Alexander Makarov7, MOBiLion Systems, Chadds Ford, PA; 2Thermo Fisher Scientific, San Jose, CA; 3Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; 4Biognosys AG, Schlieren, Switzerland

**Rapid and accurate quantitation of therapeutic drugs by coupling capillary electrophoresis with miniature mass spectrometry system:**

Xiao Chen1, Junhan Wu2, Yacon Liu3, Wenpeng Zhang4, Zheng Ouyang4

Tsinghua University, Beijing, China

**ThOB pm 03:30**

**Monoclonal Antibodies and Antibody-drug Conjugates:**

Bengian Wei1, Carter Lantz1, Rachel R. Ogorzalek Loo1, Iain D. G. Campanzano2, Joseph A. Loo1, UCLA, Los Angeles, CA; 2Amgen, Thousand Oaks, CA

**Antibody structural dynamics investigated by covalent labelling and structure-sensitive label:**

Melissa Ann Coxhead1, Dale A. Cooper-Shepherd2, Romina Hofele3, Paul Devine4, Nicholas J. Bond5, Frank Sobott6

University of Leeds, Leeds, United Kingdom; 2Waters Corporation, Stamford Ave, Altrincham Road, Wilmslow, United Kingdom; 3Analytical Sciences, BioPharmaceutical Development, BioPharmaceuticals R&D, AstraZeneca, Gaithersburg, Maryland; 4Analytical Sciences, BioPharmaceutical Development, BioPharmaceuticals R&D, AstraZeneca, Cambridge, United Kingdom

**Glycosylation-dependent stability and aggregation behavior of an immuno-regulatory protein complex revealed by native ion mobility mass spectrometry:**

Philipp Bittner1, Felix Kuhner2, Dietmar Reusch3, Renato Zenobi4, ETH Zurich, Zurich, Switzerland; 2Roche Diagnostics GmbH, Pharma Technical Development, Penzberg, Germany

**ThOB pm 03:50**

**ThOC pm 03:00**

**Mass spectrometry imaging DESI-TQMS for brain biodistribution evaluation of new radiopharmaceuticals:**

Antoine Lefèvre1, Emmanuelme Claudim2, Sylvie Chalon2, Julie Busson2, Johnny Vercoullié3, Freddy Drouyé4, Laurent Galineau4, Patrick Emond5

1University Tours, INSERM, iBrain, UMR 1253, Tours, France; 2Waters Corporation, Wilmslow, United Kingdom; 3Waters Corporation, Guyancourt, France; 4CHRU Tours, Serv Med Nucl Vitro, Tours, France

**Age-related N-glycan changes in human skin biopsies identified by MALDI FTICR imaging:**

Samuele Zorato1, 2, Mirjam Babisi1, 3, Christopher Kremslehner2, 4, Sandra Forestier2, 5, Gaelle Gendronneau2, 5, Florian Gruber2, 4, Martina Marchetti-Deschmann1, 2, TU Vienna, Vienna, Austria; 3Christian Doppler Laboratory for Multimodal Imaging of Aging and Senescence - SKINMAGINE, Vienna, Austria; 4MS Proteomics Research Group, Research Centre for Natural Sciences, Budapest, Hungary; 5Medical University of Vienna, Department of Dermatology, Vienna, Austria; 6Chanel PB, Pantin, France

**ThOC pm 03:05**

**Advancing spatial N-glycomics with MALDI-MSI to reveal molecular signatures of degenerative glomeruli in diabetic kidney disease:**

Dušan Veličković1, Jeffrey Hodgkin2, Theodore Alexandrov3, Kumar Sharma4, Christopher Anderton1, Pacific Northwest National Laboratory, Richland, WA

2University of Michigan Ann Arbor, Ann Arbor, MI; 3EMBL, Heidelberg, Germany; 4University of Texas Health San Antonio, San Antonio, TX

**ThOC pm 03:10**

**Steatoda nobilis Female and Male: A Comparative Study Including Full Body MALDI-FT-ICR Imaging and Deep Venom Characterization:**

Damien Redureau1, John Dunbar2, Antoine Fort2, Virginie Bertrand3, Raphael La Rocca1, Christopher Kune3, Sophie Rappe2, Ronan Sulcic5, Edwin De Pauw2, Michel Dugon2, Loïc Quinton1, 1MS-Lab, MOLSys Research Unit, Switzerland; 2University of Lille, Villeneuve d’Ascq, France; 3University of Sciences and Technologies, Lille, France; 4Biotech France, Lille, France; 5National Institute for Biology, Ljubljana, Slovenia

**ThOC pm 03:20**

**ThOB pm 03:50**
University of Liège, Liège, Belgium; 2 Venom Systems Lab - School of Natural Sciences - University of Galway, Galway, Ireland; 3 Plant Systems Biology Lab, Plant and AgriBiosciences Research Centre, School of Natural Sciences, Ryan Institute, National University of Ireland Galway, Galway, Ireland

**ThOD pm 02:30**
MALDI IMS identifies changes in lipids and metabolites in rat brains following arsenic exposure; E. Ellen Jones; Dustyn Barnette; Laura Schnackenberg; Richard Berger; Andrew Shen; Timothy Flanigan; 1 FDA/NCTR, Jefferson, AR

**ThOD pm 03:10**
Taming Conformational Heterogeneity of N-Methylated Macrocyclic Peptides on an Ion Race Track; Thanh D Do; Hernando J. Olivos; Jonathan K. Martens; Jos Ooms; 1 University of Tennessee, Knoxville, Knoxville, TN; 2 Waters Corporation, Milford, MA; 3 HFML FELIX, Radboud University, Nijmegen, Netherlands

**ThOD pm 03:10**
Conformational heterogeneity of top-down fragment ions analyzed by tandem-trapped ion mobility spectrometry/mass spectrometry (iTIMS/MS); Thais Pedrete; Tyler C Copley; Fanny C Liu; Jusung Lee; Christian Bleiholder; 1 Florida State University, Tallahassee, FL

**ThOD pm 03:30**
Simulations of Surface-Induced Dissociation Mass Spectrometry of a Protein Dimer Essential for Healing; Zachary D Smith; Yu-Fu Lin; Dalton Snyder; Vicki H Wysocki; Marcos Sotomayor; 1 Ohio State University, Columbus, OH; 2 Teledyne FLIR, West Lafayette, IN

**ThOD pm 03:50**
Investigation of Transient Species through Metal Clusters of Triphenylphosphine Chalcogenides with Group I Metals; Brittany Hodges; Jungsoo Kim; Christopher A. Zarrana; 1 Idaho National Laboratory, Idaho Falls, ID

**ThOD pm 04:10**
Coulomb explosion molecular imaging: direct characterization of complex structures through multivariate analysis; Michael Burt; Louis Minion; James Somper; 1 University of Oxford, Oxford, United Kingdom; 2 Imperial College London, London, United Kingdom

**ThOE pm 02:30**
2-Nitrophloroglucinol as an Effective Matrix for Quantitative MALDI MS and Imaging of Fungicide Pyrimethanil in Strawberries; Heather McDonald; Qi Li; Md Ashaduzzaman; Chao Zhao; Shalinli Pan; Gregory J. Szulczewski; Qiaoli Liang; 1 University of West Alabama, Livingston, AL; 2 University of Alabama, Tuscaloosa, AL

**ThOE pm 02:50**
Rapid chemical characterization of microplastics and nanoparticles by thermal desorption and pyrolysis mass spectrometry with semi-supervised learning; Thomas P. Forbes; Eric Pettitbone; Eric Windsor; Diana L. Ortiz-Montalvo; Abigail P. Lindstrom; Joseph M. Conny; Robert A. Fletcher; 1 National Institute of Standards and Technology, Gaithersburg, MD

**ThOE pm 03:10**
Combining high-performance liquid chromatography with chemical ionization tandem mass spectrometry by liquid electron-impact ionization interface to determine per- and polyfluoroalkyl substances; Malvika Dutt; Adriana Arigo; Giorgio Famiglietti; Pierangela Palma; 1, 2 Achille Cappiello; 1, 2 UNIVERSITY OF URBINO CARLO BO, URBINO, Italy; 3 Vancouver Island University, Nanaimo, BC

**ThOE pm 03:30**
Odor profiling and SIFT-MS analysis reveal relationships for perceived odor during wastewater treatment; Michael A McGinley; Olivia Rice; Leslie P. Silva; 1 St. Croix Sensory, Inc., Stillwater, MN; 2 Syft Technologies, Los Angeles, CA

**ThOE pm 03:50**
Resolving halogenated water disinfection by-products (DBPs) isomers of Bisphenol A with ion mobility - mass spectrometry; Mauricio Marques D Amorim; Los Santos; Caixa Li; Shenglan Jia; Shane A Snyder; 1 Nanyang Technological University (NTU); 2 NEWRI, Singapore, Singapore

**ThOE pm 04:10**
Improved target, suspect- and non-target analysis of environmental contaminants using a GC-El&CI-TOF-MS system; Marleen Vetter; Steffen Bräkling; Sonja Klee; 1 TOFWERK, Gwatt (Thun), Switzerland

**ThOF pm: Lipidomics: Targeted and Untargeted**
***Session Chair: Kermit Murray (Louisiana State University)***

**ThOF pm 02:30**
Development of a targeted multiplexed method to measure sphingolipids in CSF samples from patients with multiple sclerosis; Yadira X Perez-Paramo; Dawn Dufield; Rathina Veeramachaneni; Emily Parkhurst; Christopher Harp; Akshaya Ramesh; W. Rodney Mathews; Verónica Anania; 1 Genentech, South San Francisco, CA; 2 KCAS, Olathe, KS

**ThOF pm 02:50**
Quantitative and Structural Elucidation of Intact Brain Sphingolipids with nanoflow HPLC-MS/MS; Ryan L. Schnider; Jennifer Tena; Carlito B. Lebrilla; 1 UC Davis, Davis, CA

**ThOF pm 03:10**
Ultraviolet photodissociation (UVPD) mass spectrometry for structural characterization of lipids in biological matrices on chromatographic time scales; Rahul Ravi Deshpande; Mandy Bowman; Bashar Amer; Thomas Moehring; Susan Bird; 1 Thermo Fisher Scientific, San Jose, California; 2 Thermo Fisher Scientific, Bremen, Germany

**ThOF pm 03:30**
Connecting altered branched fatty acid distributions with membrane fluidity in daptomycin-resistant Staphylococcus aureus; Christian D Freeman; Craig Gatto; Brian J Wilkinson; Vinette K Singh; Kelly M Hines; 1 University of Georgia, Athens, GA; 2 Illinois state
ThOH pm 02:30

**Structural Characterization of Phosphatidylcholine Isoomers Using Collisional Induced Dissociation/Electron Induced Dissociation (CID/EID) in Imaging Mass Spectrometry:** Tingting Yan¹; Zhongling Liang²;
Boone M. Prentice¹; ¹University of Florida, Gainesville, FL

ThOH pm 04:10

**Investigating the lipidome of small extracellular vesicles:** Adriana Zardini Buzzatto¹; Liang Li¹, ²; ¹The Metabolomics Innovation Centre (TMIC), Edmonton, AB; ²University of Alberta, Edmonton, AB

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**SESSION CHAIR:** Xiuxia Du (University of North Carolina at Charlotte)

**SESSION CHAIR:** Alyssa Marsico (University of New Haven)

**THURSDAY ORALS**

**ThOH pm 02:30**

**Forensics: Innovations and Applications General Assembly B**

Session Chair: Alyssa Marsico (University of New Haven)

**ThOH pm 02:30**

Forensic proteomics offers a new minimally invasive and robust tool for discriminating ivory species; Catherine Gilbert¹; Vaclav Krupicka²; Aleksandra Popovich¹; Kaitell Bathany¹; Stéphane Claverol¹; Julie Arsianou²; Caroline Tokarski¹; ¹Institute of Chemistry and Biology of Membrane and NanoObjects (CBMN), CNRS UMR 5248 University of Bordeaux, Bordeaux, France; ²Department of Scientific Research, The Metropolitan Museum of Art, New York City, NY; ³Proteome Platform, University of Bordeaux, Bordeaux, France

**ThOH pm 03:00**

**High Throughput Analysis of Isomeric Drug of Abuse in Human Urine Samples by Liquid Chromatography Vacuum Differential Mobility Spectrometry-Mass Spectrometry:** Maria Fernanda Cifuentes Girard¹; Patrick Knight²; Gerard Hopfgartner¹; ¹University of Geneva, Geneva 4, Switzerland; ²Shimadzu Research Laboratory (Europe), Manchester, United Kingdom

**ThOH pm 03:30**

**A Modified 3D-Printed Cone Spray Ionization (3D-PCSI) Source for On-Site, Trace Forensic Evidence Processing via Integrated Vacuum Collection:** Christopher C. Mulligan¹; Ebenezer E. Bondzie²; Adewale A. Adenhimoye³; Brian T. Molnar¹; Patrick W. Fedick³; ¹Illinois State University, Normal, IL; ²Illinois State University, Normal, IL; ³Naval Air Warfare Center, Weapons Division, China Lake, CA

**ThOH pm 03:50**

**Bayesian statistical modeling reveals missing value mechanisms in label-free Mass Spectrometry-based proteomics experiments:** Devon Kohler¹; Olga Vitek¹; ¹Northeastern University, Boston, MA

**ThOH pm 04:10**

**Boosting workflow efficiency and productivity with instrument intelligence and smart automation:** Emma E. Rennie¹; Huy Bu¹; Patrick Batoon¹; Christian Klein¹; James S. Pyke¹; Li Sun¹; Haopeng Wang¹; George Yetzchak¹; ¹Agilent Technologies, Inc., Santa Clara, CA

**ThOH pm 02:50**

**A Novel Method for Automatically Calibrating GC Retention Index from MS Library Search Results:** Don Kuehl¹; Stacey Simonoff¹; Yongdong Wang¹; ¹Cerino Biosciences, Las Vegas, NV

**ThOH pm 03:10**

**Drug of abuse Screening in nail at 8 Seconds per samples Using LDTD-MS/MS:** Sarah Demers¹; Jonathan Rochon¹; Serge Auger¹; Jean Lacoursière²; Pierre Picard²; ¹Phytronix Technologies, Quebec City, QC; ²Phytronix Technologies Inc., Quebec, CA

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**ThOH pm 02:30**

**LibGen 2.0: fully automated pipeline for cleaning spectral libraries:** Fanzhou Kong¹; Uri Keshet¹; Jeremiah D Wells¹; Oliver Fiehn¹; ¹West Coast Metabolomics Center, University of California, DAVIS, CA

**ThOH pm 02:50**

**Scalable analysis of untargeted LC-HRMS data by means of SQL database archiving:** Marie Mandial¹, ²; Brian Schou Rasmussen¹; Kristian Linnet³; Christian Brinch Mollerup³; ¹Department of Pharmacy, the Arctic University of Northern Norway, Tromsø, Norway; ²Department of Forensic Medicine, University of Copenhagen, Copenhagen, Denmark

**ThOH pm 03:30**

**Molecular networking for the 21st century:** Christoph A. Krettler¹; John T. Prince¹; Daniel G. C. Treen¹; David Healey¹; Joe Rokicki¹; ¹Enveda Biosciences, Boulder, CO

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**ThOH pm 03:50**

**Investigating the lipidome of small extracellular vesicles:** Adriana Zardini Buzzatto¹; Liang Li¹, ²; ¹The Metabolomics Innovation Centre (TMIC), Edmonton, AB; ²University of Alberta, Edmonton, AB

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**ThOH pm 04:10**

**Trace Detection of Styphnate and Fulminate Primary Explosives via LC-MS/MS:** Sarah N. Siipe¹; Haley A. Mulder¹; Courtney A. Cruse¹; Mark L. Miller¹; ¹ORISE Visiting Scientist Program - FBI, Quantico, VA; ²Federal Bureau of Investigation, Quantico, VA

**ThOH pm 03:30**

**A Modified 3D-Printed Cone Spray Ionization (3D-PCSI) Source for On-Site, Trace Forensic Evidence Processing via Integrated Vacuum Collection:** Christopher C. Mulligan¹; Ebenezer E. Bondzie²; Adewale A. Adenhimoye³; Brian T. Molnar¹; Patrick W. Fedick³; ¹Illinois State University, Normal, IL; ²Illinois State University, Normal, IL; ³Naval Air Warfare Center, Weapons Division, China Lake, CA

**ThOH pm 03:50**

**Characterizing the likelihood of misidentifying fentanyl analogs using the NIST23 EI-MS Library:** Arun Moorthy¹; Edward Erisman¹; Anthony Kearns¹; Tuyue Liang¹; Edward Sisco¹; William E. Wallace¹; ¹NIST, Gaithersburg, MD

**ThOH pm 04:10**

**Drug of abuse Screening in nail at 8 Seconds per samples Using LDTD-MS/MS:** Sarah Demers¹; Jonathan Rochon¹; Serge Auger¹; Jean Lacoursière²; Pierre Picard²; ¹Phytronix Technologies, Quebec City, QC; ²Phytronix Technologies Inc., Quebec, CA
Mass spectrometry technology has played a key role over several decades in the development of fossil fuels and to a lesser extent, alternative energies including biofuels. Mass spectrometry allows for the precise analysis of chemical compounds, which provides the detailed molecular composition of energy feedstock materials. The information is essential for optimizing the energy source production and refining processes, leading to more efficient and cost-effective energy generation. Mass spectrometry is beginning to play a role in developing new energy technologies, such as advanced batteries and fuel cells, by enabling scientists to analyze and improve their performance properties.

This workshop will provide the opportunity to discuss the role of mass spectrometry in development of alternative energy technologies. The workshop will feature practitioners who are applying mass spectrometry in alternative energy research to discuss experiences, enablers, challenges, and the outlook of the role of mass spectrometry in emerging energy fields.

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MONDAY WORKSHOPS, 5:45 -7:00 PM

**05 Single-Cell Proteomic Standardization: From Study Design to Data Analysis**  
**Independent**  
**Presiding:** Jennifer Van Eyk, Peter Nemes  
**Ballroom A**

Recent advances in mass spectrometry technology have extended proteomics into single cells. A rapidly growing number of laboratories seek to adapt single-cell mass spectrometry across a broad swath of biology. Technologies based on automated sample preparation, liquid chromatography and capillary electrophoresis as well as mass spectrometry have enabled ultra-high sensitive quantification of hundreds-to-thousands of proteins in various cell types. These studies are revealing previously unknown (and unexpected) paradigms about the molecular organization of the cell. Yet there are many challenges associated with the design, execution and data analysis of single-cell proteomics. To facilitate scientific rigor and reproducibility, we propose a single-cell proteomics workshop. This workshop will fulfill the following aims: (1) Update the scientific community of technological advances with a focus on study design, execution, and data analysis; (2) disseminate single-cell methods and protocols to promote technological adaptation on a focus recent community-wide standards established in single-cell mass spectrometry proteomics; (3) identify remaining challenges in single-cell proteomics; (4) recruit new members to the field. The workshop will focus on challenges and solutions. It will start with each panelist giving a 5 min talk overview of their biggest challenges and solutions and end with a roundtable discussion of panelists, who will solicit and answer questions from attendees. Moderator, Jennifer Van Eyk. Panelists: Nikolai Slavov (Northeastern U.) - Study design and Standards; Lingjun Li (U. of Wisconsin) - Sample prep; Ryan Kelly (Brigham Young Univ.) - sample interrogation with MS; Peter Nemes (U. of Maryland) - MS throughput; Fabio Gomes (Scripps) - Topdown SCP; Olga Vitek (Northeastern Univ.) - Statistics with respect to SCP.

**06 Networking for Scientists: Celebrating Women Mass Spectrometrists**  
**Independent**  
**Presiding:** Stacy Malaker, Aivett Bilbao, Julie Courraud  
**Ballroom B**

This year we plan on having a more interactive networking event. To begin, as in years past, 3-4 new panelists will be introduced and then take time to discuss career paths they have followed, what factors they considered when making big decisions, and advice they would give to a woman and members from underrepresented minorities facing the same challenges. Then, we will ask the attendees to answer questions via Kahoot (or similar polling application), which the panelists will then comment on and discuss. The goal here would be for the participants to see they are not alone in their experiences and/or challenges. Some example questions for this event could include:

- Have you seen improvements to promote gender equality and diversity inclusion within your team/group? Following this, a larger cohort of organizers/volunteers (approximately 15-20) of varying backgrounds and career stages will then lead small group discussions. The attendees will be encouraged to join a group, share their experiences and contact information, then network accordingly. The small group discussions will last for the remainder of the workshop before the gap hour networking sponsored by Agilent.

**07 Exploring the World of Mass Spectral Libraries, Library Search Software and Their Applications**  
**Mass Spectral Libraries Interest Group**  
**Presiding:** Emma Rennie, Xiaoyu Yang, Melinda McFarland  
**Ballroom C**

The growing amount of data produced by mass spectrometry has made the identification of compounds in routine data analysis increasingly challenging. The use of mass spectral (MS) libraries has emerged as a valuable solution for fast and accurate compound identification. This workshop delves into the most recent advancements in MS libraries, exploring their use, application, and accompanying software tools. A panel of leading experts will present on the current state of MS libraries and the software tools they have developed or utilized in their work. They will also provide their perspectives and insights on the development and application of MS libraries. Following their presentations, there will be an opportunity for a brief Q&A session, followed by an interactive discussion on a range of topics, such as: the available MS libraries; library search software; integration with open source software platforms (e.g. Skyline and GNPS); AI applications; data processing software for searching and library building; and the use of libraries in areas such as metabolomics, food science, clinical proteomics, and environmental analysis. By the end of the workshop, participants will have a comprehensive understanding of how MS libraries can enhance their data analysis and the wide variety of software tools that can support this process.

Panelists: Michael MacCoss (University of Washington), Stephen Stein (NIST), Lloyd Sumner (University of Missouri), Arpana Vaniya (UC Davis), Mingxun Wang (UC Riverside).

**08 Ion traps as reaction vessels**  
**Ion Trap MS Interest Group**  
**Presiding:** Dalton Snyder, Lucas Szalwinski  
**Room 332**

Ion traps are remarkably versatile analytical devices. They are capable of a wide range of capabilities that other analyzers can only dream of, from ion isolation to mass analysis and a full suite of MS/MS experiments. But that’s not all! Ion traps can also serve as clean, selective, fast, and efficient reaction vessels for squeezing every ounce of chemical and structural information out of analytes. This year’s Ion Trap MS workshop will focus on the ion trap’s ability to serve as a vessel for conducting ion/ion, ion/molecule, ion/photon, and fragmentation reactions. A diverse selection of speakers from academia and industry will give lightning talks on reactions of all sorts. These talks will then be followed by a panel discussion with audience Q & A.
09 Career Opportunities for Chinese Students and Scholars

Presiding: Junmin Peng, Shuguang Ma
General Assembly A

With the rapid development of mass spectrometry technologies and the increasing applications to academic research, medicine, industry, and regulatory agencies, a growing number of mass spectrometrist including thousands of Chinese students and scholars are trained. The workshop for Career Development Opportunities for Chinese Students and Scholars aims to provide career perspectives to students and scholars to learn the career paths at different career stages. We will invite four speakers from academia, clinic, industry, and regulatory agencies to share their experiences for career development. We will also assemble a group of discussion panelists to answer questions from the audience. We believe the workshop is beneficial to both students and scholars of all ASMS members and potential employers. The workshop will provide opportunities for students and scholars to prepare for their career development during and after mass spectrometry training and help them to set up career goals in the field of mass spectrometry.

10 Making Top-Down Mass Spectrometry Easier to Develop and Apply: Ways to Work Together and How Everyone Can Contribute

Top-Down Proteomics Interest Group
Presiding: Yuri van der Burgt, Mowie Zhou
General Assembly B

Top-down mass spectrometry (TDMS) provides unique and complementary information at the intact protein level that is commonly masked when using bottom-up proteomic methods. Nevertheless, the community has experienced various challenges in adopting TDMS strategies due to a lack of a “one size fits all” solution. The difficulty is exacerbated by many options for sample preparation protocols, instrument parameters, and data analysis software, especially when dealing with complex samples. After the feedback from the 2022 workshop, the Consortium for Top-down Proteomics (CTDP) has established an Early Career Researcher (ECR) committee to help identify opportunities and plan activities to address many of these challenges as a community.

In this workshop, we will first have ECR representatives: 1) present planned near-term activities about more expertise sharing, including experimental protocols; 2) discuss the vision for the newly opened CTDP LinkedIn group for barrier-free communication; 3) discuss an initiative to create “golden datasets” for software development with inputs from the community; 4) solicit ideas for further improvements and new activities. This will be followed by an update about the CTDP initiative on an interlab study of capillary electrophoresis from Alexander Ivanov, Liangliang Sun, and Kevin Jooss. Last, we will host an open panel discussion for the audience to ask questions and suggest ideas.

Lastly, we will invite two newcomers to the field to discuss future TDMS applications with the audience, with the goal of inspiring new ideas and collaborations.

11 New Aspects in the Development and Implementation of Multi-Attribute Method (MAM)

Biotherapeutics Interest Group
Presiding: Da Ren, Andrew Mahan
General Assembly C

The advances of new indication and therapeutic modalities in the pharmaceutical industry drives the development of new analytical methods that provide enhanced content in a more efficient manner. In the past of decade, liquid chromatography (LC)-mass spectrometry (MS)-based Multi-Attribute Method (MAM) has successfully demonstrated its capability in replacing traditional chromatographic, electrophoretic, and binding assays for monitoring both product and process quality attributes (Rogers R. et al., AAPS J, 2017, Ren D., Trends Biotechnol. 2020).

As we enter a new decade of technology and method development, MAM’s utility is expanding. Recent advances in mass spectrometry instrumentation have provided novel opportunities in reforming the original MAM. The industry-wide MAM Consortium inspires method development and diversity for new MAM approaches that are fitting into different application in biopharma R&D schemes. New approaches to MAM are emerging, e.g. fully automatic sample preparation, MAM for cell and gene therapies, compact MS for MAM in QC, and new data acquiring approaches. The biotherapeutic interest group workshop offers a forum for members to share and discuss those new aspects in the development and implementation of MAM.

12 Data quality in the core lab: Preventing, catching, reporting and sometimes even fixing! suboptimal “bad data” in a omics core facility aka the “Bad data Workshop”

Analytical Lab Managers Interest Group
Presiding: Brett Phinney, Uri Keshet, Dave Quilici
Room 340AB

Bad samples, bad data? Data quality in the omics core lab is a challenging task because of the large-scale and untargeted nature of omics experiments, and the variety of instruments and assays that a core lab is expected to provide. Some of the causes for bad data are Sub optimal sample prep , miss behaving LC’s, and Mass spectrometers on the verge of blowing up. While there are ways to minimize bad data, it still happens, and it happens more than we like. Come to the workshop and share tips and strategies for preventing and, if necessary, dealing with bad data in both proteomics and metabolomics core facilities. After a few brief examples from our speakers, audience members will be given a shoulder to cry on or asked to share their strategies for dealing with BAD DATA.

13 Emerging Techniques for Rapid Fabrication in MS Laboratories

Independent

Presiding: John F. Cahill, Vilmos Kertesz
Room 351ABDE

The use of additive and subtractive manufacturing, as well as open-source electronic prototyping platforms, has become increasingly prevalent in scientific research, including in the field of MS. These technologies allow for rapid prototyping of components and devices, which can greatly enhance the efficiency of the research process. In the workshop series, participants will share their experiences with designing and fabricating custom components. We will also discuss the use of open-source
### EVENING WORKSHOP DESCRIPTIONS

All evening workshops are 5:45 – 7:00 pm. There are light refreshments in the foyers, 5:30-5:45 pm.

<table>
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<th>MONDAY WORKSHOPS, 5:45 -7:00 PM</th>
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<td><strong>14 Cannabis &amp; Hemp Science: The Importance of Mass Spectrometry</strong></td>
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<tr>
<td><em>Independent</em></td>
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<td>Presiding: Jordan Witkop</td>
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<td>Room 351CF</td>
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The global legalization of cannabis and hemp-derived medicine and consumer products has paved the way for advances in cannabis science from the accurate detection of active cannabinoids and harmful, trace contaminants to more informative strain typing, advanced breeding programs and clinical research. **GOALS:** Deliver key opinion leader panel discussions on novel applications of cannabis and hemp in the medical arena as well as future directions. Foster discussions regarding the applications of mass spectrometry to cannabis and hemp science and research. Encourage expanded use of mass spectrometry in cannabis/hemp applications by sharing information and discussing emerging growth areas.

Panelists:
- Brett Ginsburg, PhD (START Center Genetic Research Professorship Department of Psychiatry, The University of Texas Health Science Center at San Antonio) “Using Mass Spec to evaluate recreational and medical cannabinoid use in clinical samples.”
- Russell W. Jessup, PhD (Associate Professor of Perennial Grass & Industrial Hemp Breeding Department of Soil and Crop Sciences, Texas A&M University) “Developing high-throughput & low-cost chemotyping tools”
- Matt Vergne, PhD (Associate Professor, Dept of Pharmaceutical Science, Lipscomb University) “Development of a cannabinoid testing method using blood plasma collection cards and LC-MS/MS”

**15 Mind the (Translation) Gap**

**Clinical Chemistry Interest Group**

Presiding: Brian Rappold

Room 360ABDE

The ASMS annual meeting is replete with novel technologies, new biomarkers and evolving means to assess diseases in patients. However, the path to utilize these innovations in the clinical environment is not a common point of discussion. This workshop will discuss the framework of translating an innovation into reality with a panel of experts in diagnostic medicine, including representatives from manufacturers of FDA-approved materials and assays, venture capital/biotech investment and international reference labs. A discussion of the regulatory and financial environment will take place with a “Shark Tank”-like approach; imaginary proposals will be offered to the panel to launch a conversation about bridging the gap from a discovery to a deployment in a diagnostic laboratory.

**16 Exposome research: overcoming challenges to deliver answers**

**Exposomics Interest Group**

Presiding: Benedikt Warth, Ruth Marfil-Vega, Silvia Balbo

Room 360CF

The workshop will inform and discuss the latest developments in the expanding field of exposome research. An overview of the latest technological developments and global initiatives will be presented. The discussion will focus on the tools, infrastructure, and support necessary to continue successful exposomics research. This includes comprehensive mass spectrometric and bioinformatic workflows. Researchers from renowned labs working in the area will be present to share their views on current shortcomings (infrastructure, standardization, harmonization, chemical coverage, sensitivity issues) but also share their vision of how full-scale exposure assessment can be successfully established. Future directions of exposomics will be discussed in light of a massive push coming from both, US-based and European initiatives leading the way toward innovative research in the arena of environmental health and public and personalized prevention.

**17 Using Casanovo for de novo peptide sequencing**

**Independent**

Presiding: Melih Yilmaz, William Noble, Will Fondrie

Room 361ABDE

Casanovo is a new de novo peptide sequencing method that uses a deep learning model trained on massive data to achieve very high prediction accuracy. The software is implemented in Python and is available open source with an easy installation procedure. The goal of this hands-on workshop is to train users to install the software, run Casanovo using a pre-trained trypsin or non-enzymatic model, and interpret and visualize the results. We will also show you how to fine-tune the model with data from your own lab to make Casanovo work well for you. Attendees may wish to bring their own laptops to follow along with the demos. The workshop will close with a discussion of the pros and cons of de novo sequencing, with the aim of eliciting feedback for improving the utility of Casanovo and other similar tools for the user community.
The proposed FT-MS interest group workshop will focus on applying open and reproducible workflows to analyze FT-MS data. It will build on the designation of 2023 as the Year of Open Science by the White House Office of Science and Technology Policy. While the general subjects of open science and FAIR data will be mentioned, the workshop’s primary focus will be practical methods that researchers can use to ensure that the analysis of data collected using FT-MS instruments can be effectively shared and reproduced by other researchers. This will include using computational workflows implemented in open-source programming languages such as Python and R, workflow languages, containerization technologies, metadata capture and standards, and other existing and emerging methods. The exact content of the workshop will be at the discretion of the speakers, who will have expertise in software and workflow development for FT-MS data analysis.

The workshop will consist of a 15-minute introduction given by the co-chairs, followed by three 10-minute talks/demonstrations given by the recruited speakers on a specific aspect or example of reproducible analysis of FT-MS data. In the final 30 minutes, questions will be taken from the audience.

The overall goals are to:
1. Provide researchers with experience in computer programming and practical advice in making their data analyses open and reproducible.
2. Communicate to researchers without computer programming skills the value gained from implementing reproducible data analysis practices.
3. Promote the use of these practices in the FT-MS community.

The human radiolabeled adsorption-distribution-metabolism-excretion (ADME) study provides a quantitative and comprehensive overall picture of the disposition of a drug and is required for new drug approval. The accelerator mass spectrometry (AMS), which enables microtracer and microdosing studies, to ultrasensitively quantify radiolabeled compounds in biological matrices, offers various strategic advantages in drug development. Advanced AMS technology allows administration of 100-fold to 1000-fold lower amounts of carbon-14, which significantly reduces radiation burden to human volunteers. With microtracer hADME studies, the safety of trial participants is greatly improved as well as the need for a GMP grade drug substance can be eliminated. This is especially critical in vulnerable populations, such as pediatric or pregnant subjects, which further reenforce the need to keep radiation burden to a minimal level. AMS further facilitates innovative approaches for study designs to allow dosing by alternative dose routes. Administration of drug via routes such as ocular and dermal can be introduced with the sensitivity of AMS. With the AMS-enabled ADME study, we can have data on a complete metabolic profile in circulation and excreta earlier than the currently well-established timeline (before end of Phase II). Overall, the drug development timeline can be accelerated with the AMS-enabled ADME study, and a complete understanding of drug disposition can be achieved earlier. This workshop will bring together established researchers from the pharma industry and research institution to discuss current utility and future opportunities of the AMS technology in drug development.

The concept of the Individual Development Plan (IDP) is employed frequently in industrial settings to help employees construct a definitive plan for achieving career goals; however, IDP can be used in any work setting. In 2003, the Federation of American Societies for Experimental Biology (FASEB) proposed an IDP framework for postdoctoral fellows; subsequent polling of postdocs who developed an IDP reported it helpful to self-assess their abilities and skills, and identify which skills they would need for career advancement. Borrowing this framework, we will provide an overview of developing an IDP: 1) self-evaluation of skills, interests, and values, 2) use the self-assessment as a guide to evaluate and explore career opportunities (including alternative options), 3) setting specific goals for the aspired-to career path, including discussion with mentors, and 4) putting the IDP into place. We hope the workshop will either lead to the formulation of individual IDP or will refresh thoughts to those with existing IDPs. Although geared toward young mass spectrometrists, members from any stage of their career are welcome.

Many ASMS members and conference participants are supported by the National Institutes of Health and 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. The session will also provide an opportunity to inquire about the latest NIH and NSF initiatives and priorities. 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.

This workshop will discuss the common practices to “break the ice” in data simplification and interpretation. Most ASMS conference attendees deal with large datasets that require processing, sorting,
filtering, and representation. Is there a rulebook for approaching these tables? The answer is no. However, we will discuss some of the most used and accepted workflows for interpreting -omics datasets and how best to approach data representation. We will focus on both understanding the quality of MS-data output and reducing the complexity of biological data extracted. At the end of this session, we expect attendees to have acquired tips and tricks to minimize the activation barrier facing -omics data interpretation.

We will present some of the most commonly used and freely available software to interpret proteomic data and display data graphically. We will focus on how to analyze proteomes, including their protein post-translational modification (PTM), without needing a driving hypothesis. Furthermore, we will introduce the repositories used to match newly generated data with pre-existing knowledge on gene/protein/PTM biodiversity and how to cross-validate novel findings with what is reported in the literature. Finally, we will open a roundtable discussion of the most common issues and bottlenecks in data interpretation. We will welcome different perspectives, ideas, and practices in unbiased hypothesis generation using -omics datasets. Ultimately, our overall goal is to encourage non-experts in bioinformatics to explore user-friendly resources for MS data analysis.

06 Recognizing the “A” in DEIA: Effective Ways to Improve Accessibility for Mass Spectrometrist

Membership, Diversity, and Inclusion Committee
Presiding: ASMS Membership, Diversity, and Inclusion Committee Members
Ballroom B

Accommodations for persons with disabilities are rarely implemented with a “one-size fits all approach” as disabilities can be multi-faceted, ranging in severity, vary in impact based on the setting, and be classified as visible or non-visible in nature. Accessibility barriers, especially those experienced in a laboratory or workplace environment, can stifle knowledge exchanges, limit collaboration and participation, or reduce a scientist’s quality of life. It is therefore important to promote a work culture where every member is appreciated, respected, and given the tools to succeed. Dialogue is the first step in recognizing the needs of persons with disabilities and formulating effective accommodation ideas.

The ASMS Membership, Diversity, and Inclusion (MDI) committee will host the first ASMS workshop on accessibility. To address the needs of visible and non-visible disabilities, the workshop program will be divided into 3 segments that highlight physical, sensory, and cognitive disabilities. The workshop format will feature a panel composed of students, post-docs, faculty, and staff that will speak to the unique issues experienced by persons with disabilities as well as evidence-based solutions that have been implemented to make laboratories and work environments more accessible.

07 Data Independent Acquisition: After the Acquisition

Data Independent Acquisition Interest Group
Presiding: Lindsay Pino, Lukas Reiter
Ballroom C

Data independent acquisition (DIA) has drawn the interest of (proteo)omics researchers thanks to its high levels of reproducibility, capacity for large sample sizes, and the completeness of quantitative data. As academia and industry strives towards scaling workflows to hundreds or thousands of samples, derived from single cells, cell line screens, or large clinical cohorts, the boundaries of throughput and proteome depth are rapidly increasing, requiring advances in liquid chromatography-mass spectrometry systems and bioinformatics to support the scope of experimentation.

In this workshop, we invite experts in the field to discuss topics of importance and debate amongst DIA users. We explore both fads and trends that are emerging as DIA opens proteomics to larger and larger data, with a focus on what happens after acquisition, from preliminary data processing to data storage to formatting and data interpretation and dissemination. This includes the use of deep learning to better process DIA on the level of spectra but also on the level of interpreting large scale sample cohorts. Further, we are going to discuss how the next 10 years of DIA may look like or what users would like to see developed in the next 10 years. Along these lines, we’ll revisit some of the topics from previous DIA workshops to compare the direction the field seemed to be going to where things ended up going. For example, the prediction last year was that “more peptide/protein detections” would be this year’s great breakthrough, stemming from increased use of AI/ML in data analysis. We will also explore new applications for DIA, or the lack of new applications, to evaluate where DIA is being most heavily used versus applications that are still challenging for DIA approaches.

08 FAIR Data Sharing Principles and Barriers: the New NIH Data Management and Sharing (DMS) Policy

Metabolomics Interest Group
Presiding: Tytus Mak, Thomas Horvath, Maryam Goudarzi
Room 332
As of January 2023, all National Institutes of Health (NIH) funded investigators are required to abide by the new NIH Data Management and Sharing Policy (DMS). This policy requires new proposals to include a data management plan, and experimental data generated using NIH funds to be Findable, Accessible, Interoperable, and Reproducible, or FAIR. FAIR data sharing is integral to spur research reproducibility, promote data reuse, and accelerate research. The meeting will open with a few opening remarks regarding the theme of the meeting, a short introduction for each of the speakers, and a short Slido poll regarding the challenges facing the community and suggestions for the ASMS 2024 meeting topic (5-10 mins). The first speaker will be Dr. Reed Shabman, Program Officer at NIH-NIAID (or another NIH representative), who will comment on the implementation of the new DMS policy (15 mins). Then, a short presentation (15 mins) on the advantages, obstacles, and solutions of FAIR Data Sharing in scientific research will be presented by Dr. Laura Hughes (Scripps Research). Then, attendees will be asked to form small groups to discuss the obstacles and potential solutions for complying with the DMS policy in their respective laboratory environments (20 mins). The balance of the time will be spent discussing the findings discussed in each of the small group interactions (~15-20 mins).

09 Kahoot Trivial LCMS (and other topics)

LCMS & Related Topics Interest Group
Presiding: James Dodds, Jack Ryan, Karen Butler
General Assembly A
For the past couple of years we’ve been hosting a phone based trivia evening where attendees can login to a free app (Kahoot) and play along with trivia questions against their friends for
enjoyment and the top 3 players get prizes (usually stuffed animals like microbes and such).

Our attendance last year was something like 80 people, not sure how that stacks up to the other workshops. Maybe it was Monday/ Tuesday night, can’t recall.

10 Lipidomics: What does International Lipidomics Society offer to the lipidomic community?
Lipids & Lipidomics Interest Group
Presiding: Michal Holcapek, Jeffrey McDonald
General Assembly B

The lipidomics community is growing, and many newcomers are joining or at least using the lipidomics data in their research. However, there are not yet standardized methods for lipidomic analyses and data reporting, which may sometimes lead to confusion. The International Lipidomics Society (ILS) was established in 2019 with the goal of fostering the cooperation of lipidomic researchers and harmonizing methodologies, nomenclature, data reporting, and organization of ring trials. This lipidomics workshop has two main objectives. First, we would like to introduce the key activities of the ILS, such as the harmonization of lipidomics workflows with the help of minimum reporting standards, the updated shorthand lipid nomenclature, and the organization of ring trials. Second, we would like to initiate a discussion with the attendees to get a feeling of what the lipidomics community would expect from ILS and where ILS still has room for improvement. This discussion can also be regarded as an incentive for the lipidomics community to get involved in ILS and actively shape the future of the research field of lipidomics.

Workshop schedule (75 min)
- M. Holcapek – Introduction & CLIG human plasma lipidome trial (15 min)
- A. Gassiot – Ceramide and bile acids ring trials (15 min)
- J. McDonald – Minimum reporting checklist (15 min)
- Discussion (30 min) - What else can we do for lipidomic community? Suggestions and ideas on how we should do together a better job for the lipidomic community.

11 Native MS: new approaches to enable discovery in academia and industry
Native Mass Spectrometry Interest Group
Presiding: Justin Benesch, Kristine Parson, Art Laganowsky
General Assembly C

Native MS is recognized as a cutting-edge approach in the molecular characterization of protein targets and therapeutics, and their interactions. It can provide information on assembly stoichiometry, structural integrity, ligand and drug binding, all with unrivalled mass resolution and accuracy. As research targets in academia and industry become more challenging, there is an increasing need to push the limits of native MS in terms of the samples it can address, the ease in which it does so, and how it can integrate with orthogonal technologies.

We are witnessing a continuing growth in native MS and associated methodologies. Exciting developments have been made in the ability to deliver samples of greater inherent complexity, and from “dirty” sources, as well as big steps forward in online delivery and throughput. At the same time, there is continued effort at the interfaces with other MS-based or structural biology methods.

This workshop will highlight the cutting edge of native MS technology development, focusing on disseminating the newest approaches in the field that are breaking down barriers for examining previously intractable complex samples. This workshop, in an informal style, will therefore demystify the state-of-the-art, and be valuable both for newcomers to the individual topics as well as those already proficient in the native MS field.

The native MS workshop has long supported collaboration and knowledge transfer between academia and industry. We are assembling a diverse panel of experts from both theatres; they will each deliver short presentations, and (together with the attendees) participate in an open discussion facilitated by the workshop organisers.

12 New fragmentation methods as seen through the lens of radical ion chemistry
Fundamentals Interest Group
Presiding: Yury Tsybin, Alexander Makarov
Room 340AB

Rapid advances in the resolution and sensitivity of mass spectrometry instrumentation over the last decade have fueled the steady performance enhancement of the arsenal of diverse fragmentation methods. In addition, novel and old ion activation and dissociation reaction ideas have been probed experimentally to further increase the MS/MS capabilities. The most notable recent advances relate to the broader use of higher-energy electrons in, e.g., EID (or EIEIO?) for singly charged small molecule analysis and the combination of multiple fragmentation methods for better characterization of macromolecular complexes.

The dramatic expansion of available data raises the question of whether the established understanding of underlying gas phase ion activation and dissociation chemistry needs any revision - or whether we are already well equipped with our existing models. This interactive workshop will involve speakers from diverse research areas united by the passion for gas phase radical (and non-radical) ion chemistry and its use to advance the frontiers of analytical science.

They all probably would endorse (and suggest their versions of) the poem composed on the radical ion chemistry theme by ChatGPT:

*Radical ions, charged and free,*  
*They’re torn apart with a rush,*  
*Their masses revealed,*  
*In the hands of the expert,*  
*Unlocking the mysteries,*  
*With a radical push,*  
*Of the world’s great histories.*

13 Non-target analysis (NTA): Modern tools for unknown analysis
Environmental Applications Interest Group
Presiding: Ahmed Hamid, Kevin Tucker
Room 351ABDE

Environmental pollutants cause adverse health effects in humans and ecosystems. Due to rapid industrialization and urbanization, many pollutants have entered the environment, including pharmaceutical compounds, illicit drugs, pesticides, and personal
care products. In addition, various per/polyfluoroalkyl substances (PFAS) have been found in many sources such as water, air, fish, soil, food, and food packaging, etc. Interestingly, PFAS degrade very slowly in the environment, which makes them one of the most important research topics for non-target environmental analysis. Liquid chromatography-mass spectrometry (LC-MS) and gas chromatography-mass spectrometry (GC-MS) have been used to analyze many pollutants in the environment. Many investigators reported that structural determination of ions can be achieved by high-resolution-MS, ion mobility spectrometry (IMS), and artificial intelligence. For example, one of the artificial intelligence tools is FluoroMatch, which is helpful for automated non-target analysis of PFAS. This workshop will discuss advances and challenges in the analysis of contaminants in the environment by non-target analysis, presented by several scientists in short overviews. This will be followed by a panel discussion led by researchers with relevant experience, along with active engagement of the audience. The goal is to share current experiences and knowledge about different instrumentation platforms for non-target analysis of pollutants in the environment to stimulate further thinking and perspectives among researchers, as well as new artificial intelligence software packages, development of libraries of contaminants, sample preparation, and the benefits of 4D workflows, such as LC-IM-MS/MS.

14 Trans-Proteomic Pipeline: Recent Advances and Future Directions

Presiding: David Shteynberg, Michael Hoopmann
Room 351CF

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 their challenges in proteomic data analysis and help drive directions in software approaches through needs of the community. The topics for discussion will be focused on the new functionalities in the upcoming TPP version 6.3.0 release, including:

- Overview of the Cloud enabled TPP
- Cleavable crosslinker data analysis with Ving
- Integrating open searching into your usual workflow
- Mining for rare PTMs in your data

Each topic will be introduced with a brief summary of features and ideas. Then feedback and discussion by the workshop participants will be promoted.

15 Imaging MS: Isomer Differentiation in Biological Imaging

Presiding: Ingela Lanekoff, Boone Prentice
Room 360ABDE

The differentiation of chemical isomers in mass spectrometry imaging can provide important information on biological processes. However, there are a number of limitations and challenges associated with separating and identifying isomers in conventional biological imaging workflows. A growing number of creative approaches and impressive methods have been reported recently, revealing new levels of chemical detail that provide novel insights into cellular biochemistry. Yet, the almost infinite number of isomeric compounds in biological systems suggests that additional efforts and tools are still required by the community. This workshop aims to discuss the current state of the field and the importance of defining the analyte with isomeric structural resolution. We also seek to highlight promising methods and paths forward that will increase the number of isomers that can be separated in mass spectrometry imaging.

This workshop will be presented in two parts. First, several speakers will briefly describe their methodologies, including the pros and cons, for isomer differentiation in biological imaging. Second, the speakers will serve as a panel for a general discussion with the audience on the challenges that exist within the field, and identify opportunities and strategies for the future. The audience is encouraged to come prepared with questions and ideas.

16 Mass Spectrometry Support for Extractables and Leachables and Biocompatibility testing

Presiding: Gyorgy Vas, Kate Comstock
Room 360CF

Aspects of mass spectrometry support for extractables and leachables for pharmaceuticals and biocompatibility testing for medical devices will be discussed. Discussion will be focused on component identification and the required data support for component identification in the regulated environment. Another discussion topic would be non-targeted testing for biocompatibility, and leachables assessment.

17 Mass Spectral Tools to Enhance Characterization and Identification of Forensic Evidence

Presiding: Ruth Smith, J. Tyler Davidson
Room 361ABDE

Mass spectrometry is routinely used in forensic science for the characterization and identification of multiple different evidence types, ranging from seized drugs, to explosives, ignitable liquids, trace evidence, and even biological samples. Although GC-MS is perhaps the most widely used analytical technique, an increasing number of laboratories are implementing LC-MS/MS and DART-MS systems to enhance workflow and improve sensitivity. Given the continued complexity of forensic evidence submissions, even with these newer techniques, innovative approaches to mass spectral data analysis and data interpretation are needed. This workshop will include a discussion of current challenges in forensic evidence analysis along with an overview of most mass spectral tools developed by the National Institute of Standards and Technology (NIST). The panel will include forensic science practitioners who will discuss challenges within their area of expertise. Representatives from NIST will present various software tools that are freely available (e.g., AMDIS, MS Interpreter) and discuss ways that these tools can be employed to address the identified challenges. After the formal presentations, the moderators will facilitate an open-forum discussion in which workshop participants are encouraged to bring their own challenges for discussion.
01 High throughput screening mass spectrometry - current status and future landscape
Pharmaceuticals Interest Group
Presiding: Kiran Iyer, Jeremy Manheim
Room 310A
High throughput screening (HTS) systems provide the opportunity to measure several hundred thousand samples a day and is therefore in high demand in the pharmaceutical industry. Coupled to a sensitive and specific technique such as mass spectrometry (MS), HTS-MS systems are employed in several stages of the drug discovery process for applications that include, but not limited to, biomarker discovery, disease monitoring, targeted metabolomics, and the development of new chemical entities. While there are several established MS platforms available for HTS, there are often constraints in trying to balance the throughput and the need for specialized equipment and custom-built software for data analysis. Some common HTS-MS platforms include the RapidFire-MS, multiplexed LC-MS/MS systems, Acoustic systems coupled to MS, MALDI-MS, and the more recently emerging HTS-DESI-MS systems.

This workshop aims to present:
1. The status on the use of HTS-MS systems for pharmaceutical analysis
2. Current developments, instrumentation, limitations and constraints with HTS-MS systems
3. Future outlook

The workshops aims to gather several presenters from instrumentation and pharmaceutical companies. Order of the presentations will be: 1) opening remarks from the presiders covering Topic 1, 2) two presentations from instrument companies (Bruker, Sciex) 3) two presentations from scientists in the pharmaceutical industry, and 4) closing remarks by the presiders. The audience for the workshop will be the industry community, researchers in academia, and analytical contract laboratories. Appropriate time will be designated to encourage participation and idea exchange with the audience. An expected outcome is to trigger the interest in the industry to embrace HTS-MS and for instrument companies to showcase exciting developments within this space.

02 Late-Night Lightning Lectures! Independent
Presiding: Emily Sekera
Room 310BC
This workshop will provide poster presenters a chance to present a 90-second lightning talk consisting of one slide maximum. This activity is intended to help challenge presenters to put their knowledge-translation skills to the test and gain experience presenting at a podium. It is our hope that the lightning talk will help speakers to garner interest in their posters during the week. Speakers will be chosen before the conference that cover a wide range of topics within ASMS. After the announcement of oral and poster presenters and confirmation of the workshop, we will send out a survey to aid in finding scientists interested in presenting. Preference will be given to speakers in labs who do not have an oral presentation at ASMS Houston 2023. Time permitting and level of interest, we will either conclude with a 15-minute open forum to allow audience members to give feedback to presenters and ask questions.

03 Utilizing GC/MS Technologies and Associated Software Tools to Address Challenging Applications in the Flavor, Fragrance and Foodstuffs Laboratory
Flavors, Fragrance, and Foodstuff (FF) Interest Group
Presiding: Joe Binkley, Liz Humston-Fulmer
Room 320A
There are many challenging questions that a flavor, fragrance or food laboratory may be tasked to answer. These applications can include developing new products, deforming competitive products, creating effective quality control methodologies, or identifying off odors and flavors, among many others. Addressing these challenges generally requires both hardware and software solutions. Due to the nature of many of the molecules responsible for a product’s flavor and fragrance profile, GC/MS is frequently the hardware tool of choice. Once samples are analyzed, gleaning useful information from the rich GC-MS data is the next analytical challenge. Software tools that automate data processing and compile analyse information from the various samples can facilitate data review and improve efficiency for analytical scientists in this application field.

The goal of this workshop is to enhance attendees’ knowledge about software tools which are available to make their day-to-day tasks easier and more efficient. Some of the software attributes which will be demonstrated during this workshop will include automated peak finding/identification, comparison strategies, and strategies for processing and comparing groups of samples. These demonstrations will serve as a starting point for a group discussion intended to engage and benefit attendees.

The workshop format will consist of two parts: 1) Panelists will provide brief examples and demonstrations of software tools which were used to effectively extract information from analytical data to solve real world problems in their laboratories. 2) Interactive discussion among attendees and panelists moderated by the interest group coordinators, including engagement with attendees by interactive, smartphone-based polling.

04 Biomarkers Development: How Mass Spectrometry Is Changing the Field
Regulated Bioanalysis Interest Group
Presiding: Wenkui Li, Jian Wang
Room 320BC
A biomarker or biological marker is considered a measurable indicator of a certain biological state or disease related condition. Biomarkers are often evaluated qualitatively or quantitatively using blood, urine or tissues to examine normal biological processes, pathogenic processes, or pharmacologic responses to a therapeutic intervention. LC-MS is a powerful analytical tool for the analysis of various biomarkers including small molecule and large molecule biomarkers. This workshop is to be featured by presentations covering LC-MS biomarker analysis-When? How? Why? hybrid LC-MS for protein biomarker quantitation, use of a universal surrogate matrix assay for biomarker analysis, and quantitative target occupancy analysis using immunoadfinity capture 2D-LC/MS/MS, etc.

This workshop will develop future discussions and consensus on LC-MS biomarker analysis in support of regulated studies, including topics on sample preparation, mass spectrometric methods and data processing. Experts in the field will share their experience in this highly interactive workshop.
Should we focus in the future on more accurate scattering models have changed significantly from those in the condensed phase? Molecular descriptor-based approaches, and molecular dynamics “frozen-structure” scattering models, Machine Learning/first-principles approaches. We aim to invite a panel of speakers that are working on different approaches, such as conventional “frozen-structure” scattering models, Machine Learning/molecular descriptor-based approaches, and molecular dynamics approaches. Example topics of discussion include: When might it be useful to understand the structures of gas-phase ions, if they have changed significantly from those in the condensed phase? Should we focus in the future on more accurate scattering models or on improving predictive capabilities of molecular descriptors? How can these approaches learn from each other?

06 MS Career Options: How to Kick Start Your Career Young Mass Spectrometrists Interest Group Presiding: Christopher Pulliam, Ryan Bain Ballroom B Description: The Young Mass Spectrometrists workshop focuses on a panel discussion where representatives of various careers paths discuss their journey to their current position and answer questions regarding their current and past experiences. Through this discussion mass spectrometrists at the undergrad, graduate, or postdoctoral stage of their career learn information or strategies that will help them navigate the next steps in their career. This panel typically comprises representatives from a wide swath including academia, biotech/pharma, start-up companies, government, and non-traditional career paths to provide a comprehensive view of career opportunities for young researchers who have mass spectrometry skills.

07 Ambient Ionization in Application Fields: What is Required, Desired, and Provided? Ambient Sampling & Ionization Interest Group Presiding: Chris Gill, Roshan Javanshad, Jacob Jordan Ballroom C Ambient ionization mass spectrometry has been a durable topic at ASMS since 2006 (“Direct Ionization Techniques”). Since the first workshop in 2019, it has been a great platform for attendees to discuss innovations and issues in instrumentation, sampling, ionization, and related applications, as well as the underlying scientific mechanisms. In recent years (2021, 22), this workshop had 50 and 86 attendees from academia, industry, and government. At the first workshop in 2019, concerns and interest in the field were polled from some 200 attendees. The workshops in the following years have responded to the interests of our community, with foci of “reproducibility, 2020”, “quantitation, 2021”, and “molecular coverage, 2022”.

This year, the workshop will highlight the applications of ambient ionization while continuing our discussion of these figure of merit (FoM) topics. The versatility of ambient ionization methods makes mass spectrometry approaches more accessible in a wide range of areas including forensics, security, environmental analysis, manufacturing, imaging, and clinical/patient-of-care diagnostics. Each application has a set of different desired and required FoMs for analytical methods. Besides exhibiting the state of the art in these areas via lightning talks, the workshop will survey these FoMs in relevant applications. Attendees will put stickers on a prepared poster (like in 2019) to indicate the desired FoMs (sensitivity, accuracy, molecular, etc.) in their application/areas. Expert panelists will lead a Q&A-style discussion that covers challenging aspects, recent breakthroughs, and potential research directions in our research community.

08 Target Protein Degradation and MS-based Proteomics Independent Presiding: Pankaj Dwivedi Room 3332 Target Protein Degradation (TPD) research field is evolving rapidly. Given proteins are the functional unit of the cell, it is very promising to target “bad” proteins in the cell with respect to finding a potential therapeutic avenue for certain disease. Proteomics has always been instrumental in understanding of the normal and disease biology. This workshop is dedicated to understanding/active discussion regarding the opportunities and challenges associated to MS-based proteomics for TPD.

09 What are the future needs of photoionization mass spectrometry for complex mixture analysis? Photoionization MS Presiding: Christopher Rüger General Assembly A Photoionization schemes for mass spectrometry, either by laser or discharge lamps, have been widely examined and deployed for almost every application area and field of science. Fundamentals on the reaction mechanisms for atmospheric pressure photoionization (APPI) have been described in the early 2000s. Different manufacturers developed and launched APPI sources commercially, and various research groups published on specific geometries and designs. However, APPI development has been largely halted, and APLI has fallen into a niche without major commercialization. Consequently, this workshop aims to address the future needs for APPI development and potential application areas in complex mixture characterization from the fields of environmental and material sciences as well as energy transition. Questions are raised for: What are the light sources utilized in the mass spectrometry market for photoionization? What novel light sources are available and might be handy in mass spectrometry, such as innovative laser concepts, e.g., OPO? What are photoionization’s unique chemical application fields and benefits, and how can this be combined with established ESI/APCI workflows? The workshop will feature different short presentations to initiate a discussion atmosphere.
**10 Houston, We Have a Microbiome Problem (...and how the Metaproteomics Initiative aims to solve it!)**

*Independent*

Presiding: Pratik Jagtap, Robert Hettich, Timothy Griffin, Tim Van Den Bossche

**General Assembly B**

Mass spectrometry-based metaproteomics research has experienced rapid growth due to its ability to help characterize complex microbial communities and is likely to become a central approach for understanding how microbiomes function. Despite its value, metaproteomics offers analytical and bioinformatic challenges beyond those encountered in traditional, single-organism MS-base proteomics. As a solution, the Metaproteomics Initiative (www.metaproteomics.org) is a global initiative that promotes the dissemination of metaproteomics fundamentals, analytical and bioinformatic advancements, and microbiome applications. Members of the Initiative will present the updates on two recent CAMPI (Critical Assessment of Metaproteome Investigation) benchmark studies on sample preparation and functional annotations, and future projects that will be designed to propel this field forward. The members will also provide highlights from the 5th International Metaproteomics Symposium (Avignon, France), which was held in April 2023.

The workshop will invite a panel of leading metaproteomics experts who will participate in a discussion that covers the status of metaproteomics, research needs, and growth opportunities. The panel will also interact with the audience and address discussion points on how the initiative will help in gaining deeper insights into microbiome dynamics. The workshop will also describe the Initiative along with information on how interested researchers can join, participate, and contribute to its growth.

**11 Hispanics and Latinx in Mass Spectrometry**

*Independent*

Presiding: Benjamin Garcia, Livia Eberlin, Francisco Fernandez Lima

**General Assembly C**

This workshop proposal looks to organize the first official meeting of the newly forming Hispanics and Latinx in Mass Spectrometry outside interest group. Since 2003, Hispanics/Latinx have been one of the largest growing minority groups in the United States population. Nevertheless, this has not been reflected in our ASMS community membership of scientists. According to the ASMS demographic data, Hispanics/Latinx only comprise ~3% of the scientist membership, well under the U.S. population average. In order to continue to support and grow this important group, several Hispanic/Latinx scientists have come together to begin to form a new outside interest group. It is our hope that by becoming more visible and active at ASMS Conferences and beyond, we can encourage the younger Hispanic/Latinx scientists to become more involved in the mass spectrometry field. Specifically for this workshop at the ASMS Conference, we plan to have an event where we will showcase the research that Hispanic/Latinx scientists are currently engaging in, making sure to highlight the younger members of our society. It is hoped that in addition to the cutting-edge research, the speakers will also discuss their personal journeys that got them to this point in their careers. Additionally, we’d like to spend some time to have an open panel discussion to give the opportunity to our audience to ask questions, and also to solicit ideas and feedback on how this new outside interest group can be more effective to organize, outreach and grow. It is anticipated that this workshop will be the first event catalyst to encourage and support the Hispanic/Latinx members of ASMS. This workshop is open to anyone who identifies as Hispanic/Latinx in any way, and also to members who have trainees/co-workers from these groups as well (Allies).

**12 Polymeric materials: tackling hydrocarbon-based polymers**

*Polymeric Materials Interest Group*

Presiding: Thierry Fouquet, Anthony Gies

**Room 340AB**

Following a brief introduction on the interest group business (application for Sanibel/Asiomyar conference, informal meetings), we will start out discussing the analysis of hydrocarbon polymers with one presentation from a member (10-15 min). The presentation will include a brief overview of existing MS techniques for the microstructure analysis of styrenic and olefinic polymers and cover the current limitations / possible solutions to explore. Attendees are invited to ask questions throughout the presentation. The main part of the workshop will then take the form of a live session of data processing using commercial and free programs for the exploration of complex MS and MS/MS data. The hosts (one or both organizers, at least one more invited presenter) will provide examples to show the advantages of advanced data analysis approaches. Attendees are encouraged to share their own datafiles in advance - or during the workshop to spice up the demonstration - to help drive the interactivity. Such a live demonstration (at least 40 min) will be the first of its kind for our interest group and will undoubtedly trigger fruitful discussions among members. It is envisioned that the flow of ideas will enable the development of new data analysis tools or pinpoint the need to modify preexisting software solutions. The final discussion (typically 15 minutes) will be focused on the potential use of ion mobility to complement MS for the detailed characterization of these highly complex polymeric materials (tentative topic), and/or any topic attendees may wish to tackle, e.g. via the presentation of a single slide of their results/ideas.

**13 ProteomicsML: An online educational platform for machine learning in proteomics**

*Independent*

Presiding: Juan Antonio Vizzaino

**Room 351ABDE**

Open data science practices in proteomics have been largely driven by the efforts of the Proteomics Standards Initiative (PSI, http://www.psidev.info) and the ProteomeXchange Consortium of proteomics resources (http://www.proteomexchange.org). Both are two highly collaborative community initiatives that are open to the contribution and ideas from everyone. Since 2002, the mission of the PSI is the development and promotion of open data standards and related software in the proteomics field. Some recent and ongoing projects are focused on the development of a standard format for spectral libraries (mzSpecLib), the standard notation ProForma 2.0 for peptidoforms and proteoforms and the Universal Spectrum Identifiers, apart from updates in other widely adopted formats such as mzML and mzIdentML. 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,
Remote sampling of biological fluids relies on volumes that are much smaller roughly defined as less than 1 ml and typically is in the range of 50-300 μL needed on average during collection. This microsample can be either liquid (wet) or a dried in a matrix such as paper. Newborn screening has used the dried microsample for more than 50 years as part of its sample collection format from newborns. The analysis of these DBS includes many classical clinical chemistry methods as well as mass spectrometry (specifically tandem MS).

The are many issues facing microsampling in terms of precision and accuracy of such small volumes whether they are wet or dry. For mass spec, an inherently selective and accurate measurement device, precision is important as well as detection limits, limits of quantification etc. Further automation of sampling handling, interpretation are all issues that are important, many of which were identified in newborn screening. Microsampling has numerous advantages but also challenges that are being addressed.

This interest group will be focused on best practice for microsampling from isotope dilution MS, standardization, recovery from the matrix, analyte stability, suitability for analysis. It is a rapidly evolving field for which mass spec is a key player.

We will briefly highlight current trends in the increasing re-use of public proteomics datasets. As a key recent output of open science practices in the field, we will highlight the ProteomicsML platform (https://proteomicsml.org/). ProteomicsML provides ready-made datasets for machine learning models accompanied by tutorials on how to work with even the most complex data types. The resource is set up to evolve together with the field, and we welcome everyone to contribute to the project by adding new datasets and accompanying notebooks.

**14 Art, Museums, and Archaeology Independent**
Presiding: G. Asher Newsome, Paul A. Haynes
Room 351CF

The study of artworks, archaeological specimens, and other cultural heritage objects by mass spectrometry requires the adaptation of previously developed techniques, as well as the development of new approaches. Analytical methods used in biomedicine, industrial and natural product research, and forensics must be carefully tailored to be successfully applied in diverse fields such as anthropology, archaeology, natural history, art history, paleontology, and more. This multidisciplinary workshop will feature lightning talks selected from ASMS poster abstracts - students and fellows are encouraged to volunteer in advance by contacting the organizers. Lightning talks will be followed by audience Q&A with a panel of academic, government, and private institution scientists to discuss areas of interest in the field. This will provide a great opportunity to exchange detailed information about essential methodology which is often excluded from published literature. Science and science-adjacent topics may include: ethics and permissions involved in analyzing culturally sensitive samples; the risk of damage to objects as a result of analysis; sample-limited preparation and recovery approaches for rare and precious analytes; considerations for historical and contemporary sample contamination; the significance of preservation and prediction of material degradation; discerning the importance of chemicals identified from an analyte removed from context; employment, funding, and fellowship opportunities; and many more.

**15 Remote Sample Collection and Microsampling is Driving New Mass Spectrometry Analytical Solutions Independent**
Presiding: Donald Chace, Timothy Garrett
Room 360ABDE

Large volumes of blood, urine and other biological fluids (1mL or more) are becoming more obsolete and impractical in clinical chemistry practice with the exception of the inpatient environment (hospital). There is a shift in demand for sampling outside of the hospital or clinic because of concerns regarding access, rise in telemedicine, and the desire for direct to patient solutions. The covid pandemic likely accelerated this sea change in biological fluid sampling.
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

Consult online planner or mobile app for detailed program.
### Poster Presentation Schedule

**Odd-numbered posters present**
- **10:30 am - 11:30 am PLUS 12:30 – 2:30 pm**
- **10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm**

**Even-numbered posters present**
- **10:30 am - 11:30 am PLUS 12:30 – 2:30 pm**
- **10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm**

###摆脱Poster Overview

#### **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**

  - Ambient Ionization: Applications I 
    - 001-020
  - Antibodies & Antibody Drug Conjugates II 
    - 021-046
  - Biomarkers: Quantitative Analysis III 
    - 047-069
  - Cancer Research III 
    - 071-096
  - Carbohydrates 
    - 097-115
  - Data-Independent Acquisition I 
    - 116-135
  - Drug Discovery/DMPK/ADME 
    - 136-152
  - Drug and Metabolite Analysis 
    - 153-174
  - Environmental: General II 
    - 175-197
  - Extractables & Leachables 
    - 199-204
  - Forensics 
    - 205-231
  - Fundamentals: Formation and Structures of Big Ions 
    - 232-233
  - Fundamentals: Ion Spectroscopy 
    - 234-241
  - Fundamentals: Ionic Clusters, Nanomaterials, and Catalysis 
    - 242-244
  - Fundamentals: Ionization 
    - 245-257
  - GC/MS: Instrumentation and Applications 
    - 258-280
  - H/D Exchange: Hardware, Software and Methodology 
    - 281-297
  - High Mass Accuracy/High Performance MS: Applications and Instrumentation 
    - 298-321
  - Imaging MS: Disease Markers 
    - 322-334
  - Imaging MS: Pharmaceuticals, Metabolites, Lipids, and Glycans I 
    - 335-355
  - Industry: Trace Analysis, Quality Control, and Automation 
    - 356-371
  - Informatics: General, SRM, and DIA 
    - 372-380
  - Informatics: Multimics Integration 
    - 381-396
  - Instrumentation: New Concepts 
    - 397-406
  - Instrumentation: New Developments in Ion Detection 
    - 407-408
  - Instrumentation: New Developments in Ionization and Sampling 
    - 409-432
  - Ion Mobility: Applications I 
    - 433-451
  - Ion Mobility: Fundamentals 
    - 452-460
  - Ion Mobility: Structure 
    - 461-482
  - LC/MS: General 
    - 483-510
  - Lipids: ID and Structural Analysis 
    - 511-542
  - Lipids: Targeted and Quantitative Analysis 
    - 543-568
  - Metabolomics: Untargeted Metabolite Profiling I 
    - 569-594
  - Neurodegenerative Disease Research I 
    - 595-617
  - Proteomics: Quantitative III 
    - 618-638
  - Single Cell MS I 
    - 639-661
  - Small Molecules: Qualitative and Quantitative Analysis I 
    - 662-681
  - Stable Isotope Labeling 
    - 682-695
  - Systems Biology 
    - 696-711
  - Viruses and Virus-Like Particles 
    - 712-730

#### **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*

- **At 2:30 pm**

  - Ambient Ionization: Applications II 
    - 001-018
  - Antidoping, Cannabis, and Opioid Detection 
    - 019-025
  - Data-Independent Acquisition II 
    - 026-046
  - Education: Teaching MS and Teaching with MS 
    - 047-052
  - Elemental Analysis 
    - 053-054
  - Energy: Petroleum, Biofuels, and Algae 
    - 055-064
  - Environmental: General III 
    - 065-089
  - Environmental: Pharmaceuticals and Pesticides 
    - 090-101
  - Exosomics 
    - 102-121
  - Food Safety & Chemistry: Foodomics, Allergens, Bacteria, Foods, and Supplements II 
    - 122-147
  - Fundamentals: Ion Activation/Dissociation 
    - 148-159
  - Fundamentals: Ion Structure/Energetics 
    - 160-170
  - Glycomics 
    - 171-191
  - H/D Exchange: Protein Structure/Function 
    - 192-227
  - High Throughput MS II 
    - 228-253
  - Imaging MS: Instrumentation 
    - 254-267
  - Imaging MS: Pharmaceuticals, Metabolites, Lipids, and Glycans II 
    - 268-303
  - Imaging: Spatially-Resolved Omics II 
    - 304-322
  - Informatics: Metabolomics and Lipidomics 
    - 323-356
  - Informatics: Peptide ID and Quantification 
    - 357-379
  - Ion Mobility: Applications II 
    - 380-401
  - Isotope Labeling and Fluxomics Applications 
    - 402-410
  - LC/MS: Sample Preparation II 
    - 411-432
  - Lipids: Profile Analysis 
    - 433-455
  - Metabolomics: General 
    - 456-490
  - Metabolomics: Identification of Unknown Metabolites 
    - 491-500
  - Metabolomics: Untargeted Metabolite Profiling II 
    - 501-528
  - Neurodegenerative Disease Research II 
    - 529-552
  - Nucleic Acids and Oligonucleotides II 
    - 553-581
  - Peptides: Identification and Fragmentation Mechanisms 
    - 582-591
  - Peptides: PTM Identification 
    - 592-620
  - Process Development MS 
    - 621-625
  - Proteins: Complexes/Non-covalent Interactions 
    - 626-655
  - Proteomics: New Approaches 
    - 656-688
  - Single Cell MS II 
    - 689-713
  - Small Molecules: Qualitative and Quantitative Analysis II 
    - 714-735
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

Art, Archaeology & Paleontology.......................001-009
Biomarkers: Discovery I ......................................010-035
Biomarkers: Quantitative Analysis I ..................036-060
Biomolecular Structure Analysis:
  Chemical Crosslinking and Covalent Labeling .......061-079
  Cancer Research I ......................................080-106
  Clinical Analysis I .....................................107-131
  Covalent Labeling and Chemical Crosslinking I ....132-150
  Disease Biomarkers ....................................151-171
Drug Discovery: Qualitative and Quantitative Analysis I ........172-191
Epigenetic Modifications .....................................192-201
Food Safety: General ....................................202-230
Fundamentals: Ion Molecule, Ion/Ion, Ion/Electron Interactions ....231-248
  Fundamentals: Native MS ................................249-268
  Glycoproteins I .....................................269-293
  High Throughput MS I .................................294-316
 Imaging MS: Computational Methods, Software, and Analysis ........317-335
 Imaging MS: Method Development I ..................336-364
 Informatics: Algorithms and Statistical Advances ....365-392
 Instrumentation: General ..................................393-411
 Ion Mobility: FAIMS/DMS ................................412-420
 LC/MS: Sample Preparation I ........................421-438
 Lipids: General .........................................439-466
 MALDI: Applications .....................................467-479
 MALDI: Innovation in Instrumentation and Sample Preparation ....480-492
 Metabolomics: Clinical Applications ................493-504
 Metabolomics: Sample Preparation ....................505-511
 Microorganisms and the Microbiome .................512-543
 Nanoscale and Microfluidic Separations and MS ....544-551
 Peptidomics ..................................................552-569
 Phosphopeptides and phosphoproteins ................570-588
 Plant Biology and Biotechnology ....................589-602
 Protein Therapeutics: Structural Characterization ..603-630
 Proteins: Conformation Analysis and Structural Biology ........631-662
 Proteins: PTMs I ........................................663-687
 Proteomics: Infectious Diseases ..........................688-701
 Proteomics: Intact Proteins and Top Down Analysis 1702-721
 Proteomics: Quantitative I .............................722-741

MP 001 Developing a molecular approach to the species identification of plant-based fibres in ancient Egyptian textiles using mass spectrometry; Dylan H Mulliari1; Michelle F Whittord1; Ronika K Power1; Paul A Haynes1; Macquarie University, Sydney, Australia

MP 002 Metabolomics on osteoarchaeological material allows the discovery of biomarkers related to the consumption of tobacco in ancient British populations; Diego Armando Badillo-Sanchez1; Maria Serrano Ruber1; Anna M. Davies-Barrett1; Donald J. L. Jones1; Sarah A. Inskip1; University of Leicester, Leicester, United Kingdom

MP 003 Sex determination of four two-million-year-old Paranthropus robustus fossil teeth from South Africa by mass spectrometry; Claire Koening1; Palesa Petunia Madupe1; Ioannis Patramanis1; Patrick L. Rüther1; Nomawethu Hlazo2; Meaghan Mackie3,4,5; Lauren Schroeder4; Alberto John Taurozzi1; Clément Zanolli6; Fernando Racimo7; Jesper Velgaard Olsen7; Rebecca Rogers Ackermann8; Enrico Cappellini9;10; University of Copenhagen, Copenhagen, Denmark; 2University College Dublin, Belfield, Ireland; 3University of Toronto, Toronto, ON; 4University de Bordeaux, Bordeaux, France

MP 004 MALDI MS, ATR/FTIR & Raman Imaging - a Comprehensive Toolbox to Assess Environmental Damage in Cultural Parchment Objects; Antonia Melissa1; 2Manfred Schreiner1; 3Martina Martens1; 4,5,10Malissa Deschmann1; 6TU Wien, Vienna, Austria; 2Academy of Fine Arts Vienna, Vienna, Austria

MP 005 Insights into patterns and pathways of protein degradation: A case study with β-lactoglobulin; Bharath Nair1; Meaghan Mackie2; Tina Ravnsborg3; Samantha Presslee4; Kirsty Penkman5; Jesper Velgaard Olsen7; Ole Jensen1; Carsten Wiuf1; Matthew Collins1,2; 1University of Copenhagen, Copenhagen, Denmark; 2University College Dublin, Belfield, Ireland; 3University of Southern Denmark, Odense, Denmark; 4University of York, Helsington, United Kingdom; 5University of Cambridge, Cambridge, United Kingdom

MP 006 New perspectives in archival textile science; a unique workflow for the double characterization of dyes and proteins from extremely degraded textiles; Patrícia de Souza Leite1; 2Gabrielle Favero1; Roberta Curini1; 2Gwénaléïve M. Kavič1; 2Timothy P. Cleland2; Caroline Solazzo3; 4Sapienza University of Rome, Rome, Italy; 5Smithsonian Museum Conservation Institute, Suitland, MD

MP 007 Chromatography-free analysis of pigments by high resolution mass spectrometry with direct sample introduction; Sam Putnam1; 2Rachel Deschmann2; 3Wiiliam L. Fatigante1; 4Nobuiko Shibayama1; 2Maria Goretti Mielies Alonso1; 3Bruker Scientific, LLC, Billerca, MA; 5The Metropolitan Museum of Art, New York City, NY

MP 008 Comparing intramineral proteins from the eggshells of ratite birds, crocodiles and a dinosaur eggshell fossil; Connor E. Gould1; Rocio Elejalde Cadena2; Alan Friedman3; Abel Moreno4; Troy D. Wood1; 1Department of Chemistry, University at Buffalo, Buffalo, NY; 2Instituto de Química, Universidad Nacional Autónoma de Mexico, Ciudad de México, Mexico; 3Department of Materials Design and Innovation, School of Engineering and Applied Sciences, University at Buffalo, Buffalo, NY

MP 009 Collagen Remains in Palaeotherium Bone from the Isle of Wight (UK); Joseph Hubbard1; Steven Robinson2; Ardern Hulme-Beaman3; Martin Munt1; Krzysztof Pawlak2; 1Department of Electrical Engineering & Electronics, University of Liverpool, Liverpool, United Kingdom; 2Materials Innovation Factory, University of Liverpool, Liverpool, United Kingdom; 3University of Liverpool, Liverpool, United Kingdom; 4Dinosaur Isle Museum, Sandown, United Kingdom

MP 001 The First Profile of Steroid Hormones in Human Aqueous Humor is Generated from the LC MS/MS Approach; Tiansheng Chou1,2; Xiaosheng Huang3; Jun
**MONDAY POSTERS**

**MP 011 Direct measurement of Plasma Phosphatidylinositol and Polyphosphoinositols in Lung Cancer Patients Using UHPLC/MS/MS**

Hai Bu1; Kenneth D. Roth2; Eli Lilly and Company, Indianapolis, IN

**MP 012 Structural proteomic profiling of cerebrospinal fluids to reveal novel conformational biomarkers for Alzheimer’s disease**

Bin Wang1; Xiaofang Zhong1; Lauren Fields1; Haiyan Lu1; Zexin Zhu1; Lingjun Li1; UW-Madison, Madison, WI

**MP 013 High salt diet damaged blood vessel and induced hypertension is elucidated by vascular bed systematic profiling**

Siu Kwan Sze1; Brock University, St Catharines, ON

**MP 014 High-performance metabolic fingerprints of aqueous humor for retinoblastoma monitoring**

Wanshan Liu1; Kun Qian2; Shanghai Jiao Tong University, Shanghai, China

**MP 015 Proteomics Analysis of Rheumatoid Arthritis Patients sera Identified a Multi-Biomarker Panel for Predicting Anti-TNF Response**

Ara Cho1; Jinsung Ahn2; Andrew Kim1; Eugene C. Yi1; Department of Molecular Medicine and Biopharmaceutical Sciences, Graduate School of Convergence Science and Technology and College of Medicine or College of Pharmacy, Seoul National University, Seoul, South Korea

**MP 016 Tear metabolic fingerprinting identifies glaucoma**

Jiao Wu1; Kun Qian2; Med-X Research Institute, SJTU, Shanghai, China; Shanghai Jiao Tong University, Shanghai, China

**MP 017 Metabolomic Profiling of Cancer Biomarkers from Methanol Extracts from Pathology Specimens using LC-MS/MS**

Alexandra M. Izydorczak1; Wilfrido D. Mojica1; Troy D. Wood2; SUNY at Buffalo, Buffalo, NY

**MP 018 Contribution of the microRNAs to a metabolomic signature predictive of risk for pancreatic cancer**

Johannes Fahrmann1; Ehsan Iraizoz2; Jody Vykoukal2; Ranran Wu3; Jennifer B Dennison3; James P Long2; Anirban Maitra2; Kim-Anh Do2; Samir Hanash3; University of Texas, MD Anderson, Houston, TX; UTMEDACC, Houston, TX

**MP 019 Novel LC-MS Strategies to Enable Discovery and Quantification of Glutam Inmunogenic Peptides and Their Deamidated Forms in Human Urine**

Jie Pu1; Qingsong Shen1; Chao Xue1; Timothy Sikorski2; Thomas Angel1; Zhuo Chen2; John T Meh1; Huaping Tang2; Jun Qu3; 1University at Buffalo, Buffalo, NY; 2GSK, Collegeville, PA; 3New York State Center of Excellence in Bioinformatics & Life Sciences, Buffalo, NY

**MP 020 Study of the cholesterol biosynthesis pathway perturbation in demyelination/remyelination of cuprizone mice using GCMS and proteomics**

Xiaoping L Hronowski1; Rongfang Gu1; Kayla Sourcey1; Benbo Gao1; Zhaofu Shao1; Ru Wei1; Biogen, Cambridge, MA

**MP 021 Biomarker discovery pipeline with chemical isotope labeling LC-MS method**

Wayne Chang1; Rui Qin1; Shuang Zhao1; Liang Li1,2; 1The Metabolomics Innovation Centre (TMIC), Edmonton, Alberta; 2University of Alberta, Edmonton, AB

**MP 022 Depleted or non-depleted serum, establishing a best practice approach for monitoring peptide biomarkers using DIA methodologies**

Alison Porter1; Abigail Burrows Franco1; Cecily Petemen1; Scott D Wood2; Scott T Peterson1; Stanley1; 1University of Kentucky, Lexington, KY; 2Thermo Fisher Scientific, San Jose, CA

**MP 023 Biomarker discovery in human plasma samples from patients suffering from myalgic encephalomyelitis and post-viral fatigue using mass spectrometry-based quantitative proteomics**

Ganna Shevchenko1; Anastasiya Ushenkina1; Jonas Bergquist1; 1Department of Chemistry - Biomedical Center, Analytical Chemistry and Neurochemistry, Uppsala University, Uppsala, Sweden; 2The ME/CFS Research Centre, Uppsala University, Uppsala, Sweden

**MP 024 DIA-MS-based proteomics for discovery of protein biomarker signature from >100 cancer plasma samples**

Yi-Jun Chen1; Kuen-Tyng Lin1; Yi-Jing Hsiao2; Goo-Chen Chang3; Jin-Shiang Chen2; Sung-Liang Yu2; Yu-Ju Chen3; 1Institute of Chemistry, Academia Sinica, Taipei, Taiwan; 2Department of Clinical Laboratory Sciences and Medical Biotechnology, College of Medicine, National Taiwan University, Taipei, Taiwan; 3Institute of Medicine of Chung Shan Medical University, Taichung City, Taiwan; 4Department of Surgical Oncology, National Taiwan University Cancer Center, Taichung, Taiwan

**MP 025 Development of a Biomarker Discovery Pipeline for High-Grade Serous Carcinoma using Biofluid Extracellular Vesicles and Data-Independent Acquisition**

Tyler T. Cooper1,2; Lynne M Postovit1; Gilles A Lajoie1; 1Queen’s University, Kingston, ON; 2Western University, London, ON

**MP 026 In silico Approach for Monitoring of Gangliosides Structural Diversity in Fungal Cell Factories by LC-MS/MS**

Javier Fernando Montero-Bullón1; Javier Martín-González2; Gloria Muñoz-Fernández3; Alberto Jiménez1; Jose Luis Revuelta Doval1; 1University of Salamanca, Salamanca, Spain

**MP 027 Sample preparation using dried blood devices enables quantification of 3900 proteins from whole blood and biomarker identification in lung cancer**

Sung Chiu1; Sangio Bio, Sydney, Australia; 2Insight Stats, Sydney, Australia

**MP 028 Proteomic evaluation of sex differences in the plasma of non-human primates exposed to ionizing radiation for biomarker discovery**

Christina Williams1; Mehar Widemaertian1; Mark Patel1; A. Kaval1; 1University of Maryland, School of Pharmacy, Baltimore, MD

**MP 029 LC-MS based translational pharmacoproteomics allows the discovery of drug-perturbed liquid biomarkers across species bridging preclinical and clinical biomarker decision-making strategies**

Andreas David Brummer1; Anouk Oldenburg1; Larissa Pfister1; Daniel Veyel1; Eva Grieser1; Wolfgang Ber1; Patrycia Schlingloff1; Julian Schmidberger1; Mark Haenle1; Wolfgang Kratzer1; Heike Neubauer1; Markus Werner1; Tom Brettschneider1; 1Boehringer Ingelheim Pharma, Biberach, Germany; 2Department of internal medicine I, University Hospital Ulm, Ulm, Germany

**MP 030 Development of red blood cells and plasma-based diagnostic lipid biomarker panel for Parkinson’s disease**

Fathima Shaima Muhammednaz1; Anne M Roberts1; Ankit Jain1; Malcolm Horne2; Stephan Klatt2; Blaine Roberts1; 1Emory School of Medicine, Emory University, Atlanta, GA; 2CSIRO Health and Biosecurity, Herston, Australia; 3Institute for Vascular Signaling, University of Frankfurt-Goethe University, Germany

**MP 031 Unbiased Biomarker Discovery for IBD Target Validation and Patient Stratification**

Mostafa J Khan1; Faizan Zubair1; Chris Deboever1; Paul Harris1; 1Takeda Pharmaceuticals, San Diego, CA

**MP 032 Exploration towards the novel biomarkers of human cystic echinococcosis based on coupling of LC-MS/MS and immunossay**

Qingmin Zhang1; Xi Gao2; San A1; Sang Hua1; Wangmu Danzeng1; Scott T Peterson2; 1Beijing Genomics Institute, shenzhen, China; 2College of Life Sciences, University of Chinese Academy of Sciences, Beijing, China
Development of proteomic biomarker panel for Cervical Cancer from Indian population; Amrita Mukherjee1; Sanjeeda Srivastava1; IIIT Bombay, Mumbai, India

A Comprehensive Strategy for Building and Evaluating Plasma Proteomics DDA Derived Spectral Libraries with ZENO-TOF 7600; Yi (jimmy) Zeng1; Hao Qian1; Ruby Karimjee1; Joon-Yong Lee1; Mark Marişpin1; Jessica Chan1; Megan Mora1; Benjamin Ta1; Ehdieh Khaledian1; Chi-Hung Lin1; Robert Zawada1; Philip Ma1; Bruce Wilcox1; PrognomiQ Inc, San Mateo, CA

Optimization of a multi-omic workflow for biomarker discovery in a medaka fish model of chronic low dose ionizing radiation exposure; Sydney Bedillon1; Michael Tiemeyer1; Franklin E. Leach III1; University of Georgia, Athens, GA

Quantitative reagent-free bioanalysis of proteins in humanized mouse models: Enrichment and Normalization Strategies; Jingjing Deng1; Eugene Ciccomaro1; Petia Shipkova1; BMS, Princeton, NJ

Liquid chromatography-tandem mass spectrometry reveals association of acute myocardial infarction risk with the dynamic balance between trimethylamine-N-oxide, betaine, and choline; Sam Li1; Shan Huang1,2,3; Si Ying Lim1; Sock Hwee Tan1; Mark Chan1; Wuzhong Nai2; National University of Singapore, Singapore, Singapore; Zhejiang University, Hangzhou, China

Development and Validation of the Measurement of Cotinine and Hydroxycotinine in Serum: An Automated Sample Preparation and new LC/MS/MS Method; Danielle L. Sowle1; Tiffany H Seyler1; Madeline L Weaver1; Lanqing Wang1; CDC, Atlanta, Georgia

Deep Proteomic Profiling of the Serum Proteome Across the Murine Lifespan; Amit K Dev1; Simonetta Camandola1; Nathan L Price1; Siam Investigators1; Rafael de Cabo1; Nathan Basty1; National Institute on Aging, NIH, Baltimore, MD

A path from discovery to targeted proteomics approach for the verification and validation of tissue-derived biomarkers in coronary artery diseases; Chi D. L. Nguyen1; Jonathan Bul1; Zachary Dwight1; Jesse G. Meyer2; Austin L. Seal1; Annie Moradlan1; Stephen A. Whelan1; Mitra Mesali1; Sarah J. Parker1; DKM1; Herrington3; Susan Mockus1; Jennifer E. Van Eyk1; 1Precision Biomarker Laboratories, Cedars-Sinai Medical Center, Beverly Hills, CA; 2Heart Institute & Advanced Clinical Biosystems Research Institute, Los Angeles, CA; 3Department of Cardiovascular Medicine, Wake Forest University, Winston-Salem, NC

A Rapid Method for Simultaneous Quantification of Monoamines in Rat Brain in a Tetramethane-Induced Model of Depression; Lilia Magomedova1; Sophie R Pan1; Julia Izhakova1; Monica Ortiz1; Guy A Higgins2; Leo B Silienks3; Ines De Lannoy1; 1Transpharmation Canada Ltd, Mississauga, ON; 2Transpharmation Canada Ltd, Fergus, Ontario

A targeted workflow for investigating the tear proteome of patient with Sjögren’s syndrome by LC-MS/MS; Maggy Lepine1; Marie-Claude Robert1, 2, 3; Lekha Sleno1, 3, 4; 1University of Quebec in Montreal, Montreal, QC, Canada; 2Hospital Research Center of the University of Montreal, Ophthalmology department, Montreal, QC; 3CEMOC-FC, Centre d’Excellence de Recherche sur les Maladies Ophthalmo-Neuro-Fondation Courtois, Montreal, QC

Direct Determination of 4-Beta-Hydroxycholesterol without Derivatization in Human Plasma by LC-ACPI-MS/MS; Jingguo Hou1; Zhu Xiaodong1; Bian Alicia1; Perry Fan1; Andrew Cunningham1;1Worldwide Clinical Trials, Austin, TX

Exploring protein expression across multiple experiments using Mass Dynamics; Anna Quaglieri1; Aaron Triantafyllides1; Bradley Green1; Mark Rococo Condina1; Paula Burton Ngov1; Giuseppe Infusini1; Andrew Ian Webb1, 2, 3; 1Mass Dynamics, Melbourne, Australia; 2The Walter and Eliza Hall Institute, Melbourne, Australia; 3Department of Medical Biology, University of Melbourne, Melbourne, Australia

Minimum Required Dilution, Matrix Effect and Parallelism Evaluation in Regulated LC-MS Assay for Endogenous Biomarker; Moumny Yuan1; Kumar Shah1; Guoyan Xu1; William R. Mylott Jr.1; PPD, part of Thermo Fisher Scientific, Richmond, VA

Novel LC-MS-PRM method for simultaneous protein quantification using a synaptic and lysosomal panel assay; Johanna Nilsson1; Johan Gohbom1; Gunnar Brinkmalm1; Henrik Zetterberg1, 2, 3; 4, 5; Kai Bjennow1; Ann Brinkmalm1; 1Institute of Neuroscience and Physiology, Department of Psychiatry and Neurochemistry, University of Gothenburg, Mölndal, Sweden; 2UK Dementia Research Institute at University College London, London, United Kingdom; 3Department of Neurodegenerative Disease, UCL Institute of Neurology, London, United Kingdom;4Hong Kong Center for Neurodegenerative Diseases, Hong Kong, China

Quantitative Targeted Proteomics of Mouse Plasma Protein Biomarkers by using Nano LC coupled to Triple Quadrupole Mass Spectrometer; Xi Qiu1; Thomas Walker2; Claudia Gaither1, 4; Robert Popp1; Christoph H. Borchers1; John Sausen1; 1Agilent Technologies, Wilmington, DE; 2Agilent Technologies, Lexington, MA; 3MRM Proteinome Inc, Montclaire, ONC; 4Agilent Technologies Inc, Montreal, QC; McGill University, Montreal, Québec; 1Agilent Technologies, Inc, Santa Clara, California

Reduced Ion Suppression in an Automated Extraction of Vitamins B1 and B6 from Whole Blood for LCMS Analysis; Kyle Dukes1; Biotage, Charlotte, NC

Analysis of Frataxin Proteoforms in Human Heart with Pig Heart Surrogate Matrix to Monitor Gene Therapy of Friedrich’s Ataxia; Teerapat Rojsajjakul1; Clementina Mesaro1; Ian Alexander Blair1; 1University of Pennsylvania, Perelman School of Medicine, Philadelphia, PA

Comparison of Some Derivatives for the Quantitative Analysis of Short-Chain Fatty Acids (SCFA) by LC/MS/MS; Anna M. Caldwell1; John M. Halket1; Ana Rodriguez-Matose1;2King’s College London, London, United Kingdom

Development of a Comprehensive Quantification Assay for Fast Plasma Protein Screening Using a Novel Triple Quadrupole LC/MS; Linteng Wu1; Guanlan Li1; Patrick Batoon1; 1Agilent Technologies, Santa Clara, CA

Development of a Quantitative Biomarker Assay for Marmoset Metabolism; Robin Gov1; 2, 3, 4; Amila Kapoor1; 1University of Wisconsin-Madison, Madison, WI; 2Wisconsin National Primate Research Center, Madison, WISCONSIN

Extensive thiol profiling for assessment of intracellular redox status in cultured cells by HPLC-MS/MS; Jiandong Wu1; Anna Chernyatynskaya1; Annalise Pfaff1; Huai Kou1; Nan Cen1; Nuran Ercal1; Honglan Shi1; Hu Yang1; 1Missouri University of Science and Technology, Rolla, MO

Fast determination of plasma catecholamines and metanephrines by solid phase-extraction and liquid chromatography–tandem mass spectrometry applied to clinical assay; Thibaut Duval1; Aziz Kinard1; Laura Akbal1; Guillaume Chaplain1; Olivier Deschamps1; 1Shimadzu France, Noisiel, France; 2Cerba, Saint-Ouen-l’aumône, France; 3Biotage, Uppsala, Sweden

Investigation of deep proteomic and peptidomic signatures of urine specimen from chronic kidney disease and bladder cancer for disease prediction; Roland Bruderer1; Dominic Hoch1; Luca Raess1; Marco Tognetti1; Claudia Moresi1; Yuehan Feng1; Lukas Reiter1; 1Biogносys AG, Schlieren, Switzerland; 2Thermo Fisher Scientific, Reinach, Switzerland

Mass spectrometry approaches for the quantification of Neurofilament-light in cerebrospinal fluid: towards a reference method; Salome Coppen1; Jerome Vialaret2; Sylvain Lehmann2; Christophe Hirtz2; Christopher Hopley1;
MP 057  Nanoparticles as alternative affinity reagents for developing targeted mass spectrometric assays of low-abundance biomarkers: Shans S. Kelly1; Tai-Tu Lin1; Matthew J. Gaffney1; Wei-Jun Qian1; 1Pacific Northwest National Laboratory, Richland, WA

MP 058  promor: An R package for label-free proteomics analysis and building machine learning models with candidate proteins: Chathurani Ranathunge1; Sagar S Patel1; Lubna Pink1; Vanessa C. Correll1; Shumin Chen1; O. John Semmes1; Robert K Armstrong1; C. Donald Combs1; Julius O Nyalwi1; 1Eastern Virginia Medical School, Norfolk, VA; 2Medarry Medical College, Nashville, TN

MP 059  Quantitation of Gait-1P by LC-MS/MS to evaluate GALT activity after AAV Treatment: Allison N Schorzman1; Jennifer Franks1; Jeremy Rouse2; Kirsten Romero3; Eric Yearley1; David Scott1; Michael Guerrero1; Clayton Beard1; 1BridgeBio Gene Therapy, Raleigh, NC; 2BelGene, Cambridge, MA

MP 060  The Urinary Post-translational Modification Landscape and Applications in Clear Cell Renal Cell Carcinoma Biomarker Discovery: Daniel J Geisler1; Nazli Ezgi Ozkan-Kocak1; Gamze Nur Yapiç1; Murat Can Kiremit1; Nurhan Ozlu1; 1Koc University, Sariyer, Turkey

MP 061  Utilizing structural mass spectrometry to probe the dynamics of the progerin-associated receptor transcription complex: Matthew D Mann1,2; Min Wang3; Anna Malovannaya1; Raj Kumar1; Dean P Edwards3; Patrick R Griffin1,2; 1Skaggs Graduate School of Chemical and Biological Sciences, The Scripps Research Institute, Jupiter, FL; 2The Herbert Wertheim UF Scripps Institute for Biomedical Innovation & Technology, Jupiter, FL; 3Baylor College of Medicine, Houston, TX; 4Touro College of Pharmacy, New York, NY

MP 062  Development of whole blood HR-HRPF for structural pharmacology of protein pharmaceuticals: Darrienne M Martin1; University of Mississippi, University, MS

MP 063  Conformational dynamics of a Van-activated GLP-1 receptor-Gs complex revealed by cross-linking mass spectrometry and integrative structure modeling: Shijia Yuan1; Lisha Xia1; Chenxi Wang1; Liping Sun1; Wenqing Shui1; 1ShanghaiTech University, Shanghai, China

MP 064  Evaluation of viral and allergenic protein complexes by dual cleavable crosslinking technology (DUCCT): Akash Talukder1; Frhu Ashima1; Zacharias1; Saiful M. Chowdhury1; 1University of Texas at Arlington, Arlington, TX

MP 065  Expanding the protein crosslinking tool kits by developing a tyrosine reactive crosslinker: Adoway O. Zacharias1; Saiful M. Chowdhury1; 1University of Texas at Arlington, Arlington, TX; 2University of Texas at Arlington, Arlington, TX

MP 066  Characterization of Protein-Protein Interactions by Quantitative Cross-linking Mass Spectrometry in Alzheimer’s Disease: Zexin Zhu1; Bin Wang1; Xiaofang Zhong1; Lingjun Li1,2; 1University of Wisconsin-Madison, School of Pharmacy, Madison, WI; 2University of Wisconsin-Madison, Department of Chemistry, Madison, WI

MP 067  Structural interactomic profiling of the synapse by cross-linking mass spectrometry: Ke Wang1; Cong Wang1; Ying Zhu1; Fan Liu1; 1Leibniz-Forschungsinstitut für Molekulare Pharmakologie im Forschungsverbund Berlin e.V. (FMP), Berlin, Germany

MP 068  Mapping the multiple DNA contacts made by the neuronal regulatory protein MeCP2 using protein oxidative footprinting: Yan Sun1; Sergei Khrapunov1; Subray Hegde1; Simonie Siddle1; Michael Brenowitz1; 1Albert Einstein College of Medicine, Bronx, NY

MP 069  FOX Photolysis System-Generated Carbene Footprinting of Peptides: Lyle W Tobin1; Sandeep K. Misra2; Joshua S. Sharp2; 1University of Mississippi, University; 2University of Mississippi, University, MS

MP 070  Structural mass spectrometry justification of AlphaFold generated PsbS structure on the elongated stromal loop region: Manjula Mummadisetti1; Yanchun Lin1; Masakazu Iwai1,2; Krishna K Niyogi1,2; Michael L Gross2; Hailun Liu5; 1Boaiglytx, Raleigh, NC; 2Department of Chemistry, Washington University in St. Louis, St. Louis, MO; 3Department of Plant and Microbiology, University of California, Berkeley, Berkeley, CA; 4Molecular Biophysics and Integrated Imaging Division, Lawrence Berkeley National Laboratory, Berkeley, CA; 5Department of Biology, Washington University in St. Louis, St. Louis, MO

MP 071  RNA-protein crosslinking mass spectrometry - quantification of crosslinking sites: Luisa Mathilde Welp1,2; Aleksander Chernev1; Tim Sachsenberg3,4; Monika Raabe1; Arslan Siraj1,4; Aditi Sharma1; Bernard Delanghe1; Rosa Viner1; Oliver Kohlbacher1; Henning Ural1; 1Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany; 2Institute for Clinical Chemistry, University Medical Center Göttingen, Göttingen, Germany; 3Applied Bioinformatics, Department for Computer Science, University of Tübingen, Sand 14, 72076, Tübingen, Germany; 4Institute of Bioinformatics and Medical Informatics, University of Tübingen, Tübingen, Germany; 5Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; 6ThermoFisher Scientific, San Jose, California

MP 072  Exploring an alternative cysteine-reactive chemistry to enable proteome-wide PPI analysis by cross-linking mass spectrometry: Fenglong Jiao1; Leah J Salituro1; Clinton Yu1; Craig B. Gutierrez1; Scott D. Rychnovsky1; Lan Huang1; 1Department of Physiology and Biophysics, University of California, Irvine, IRVINE, CA; 2Department of Chemistry, University of California, Irvine, Irvine, Irvine, CA

MP 073  Improved Methods for Residue-Level Mass Spectrometry Data Acquisition and High-Resolution Hydroxyl Radical Protein Footprinting (HRPF) Data Interpretation: Zhi Cheng1; Emily Chea1; Jiana Duan1; Sandeep K. Misra1; Scott Weinberger1; Joshua S. Sharp1,2; 1GenNext Technology, Half Moon Bay, CA; 2University of Mississippi, University, MS

MP 074  Mass Spectrometric Footprinting of Protein Adsorption and Desorption at Chromatographic Interfaces: Kimber N. Focke1; Brian T. Cooper1; 1UNC Charlotte, Charlotte, NC

MP 075  Mass spectrometry-based footprinting methods characterize the interaction between human cytochrome P450 enzymes and their redox partner cytochrome P450 reductins: Adwo O. Zacharias1; Sarah Burris-Hidayat1; Emily E. Scott1; Michael L. Gross1; 1Washington University in St.Louis, Saint Louis, MO; 2University of Michigan, Ann Arbor, MI

MP 076  AZURIN: A MODEL METALLOPROTEIN TO STUDY AN OXIDOMERIZATION PROCESS: Roman Tuzhlikin1; Vladimir Ondruska1; Jiri Hudecek1; Miroslav Sule1; 1Department of Plant and Microbiology, Charles University, Prague, Czech Republic

MP 077  Crosslinking-MS Captures Transient Interactions within Phase Separated Viral Replication Factories: Nicole D. Wagner1; Austin B. Moyle1,2; Chao Wu1; Gayu K. Amarasinghe3; Daisy W Leung1; Michael L Gross1; 1Washington University in St. Louis, St. Louis, MO; 2AbbVie Inc., North Chicago, IL; 3Washington University School of Medicine, St. Louis, MO

MP 078  Kinase phosphoprobining for profiling protein conformational changes: Asato Maeda1; Kosuke Ogata1; Naoyuki Sugiyama1; Yasushi Ishihama1,2; 1Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, Japan; 2National Institutes of Biomedical Innovation, Ibaraki, Japan

MP 079  Characterization of Varroa destructor proteins targeted by new acaricides: Osei Boakye Fordwou1; Leonard
Towards a global phosphoproteomic map of chemotherapy-specific signaling responses; William Comstock1; Ethan J Sanford2; Yiseo Rho2; Marcus Sustamante Smolka1; "Cornell University, Ithaca, NY

Comprehensive proteome analysis of few neutrophils exposed to melanoma cells of various aggressiveness; Susmita Ghosh1; Zülaif Cibiri; Laxminkanth Kollipara; Matthias Gunzer1; 2; Albert Sickmann1; "Leibniz Institute for Analytical Sciences - ISAS, Dortmund, Germany; 1; University of Duisburg-Essen, Essen, Germany; 2; Leibniz Institute for Analytical Sciences - ISAS, Dortmund, Germany

Identification of Putative Early-Stage Ovarian Cancer Biomarkers Using Bottom-Up Proteomics from Patient Derived Tampons; Gordon T Luu1; Chang Ge2; Yisha Tang2; Andrew K Godwin1; 2; Judith Su2; Laura M Sanchez1; "University of California Santa Cruz, Santa Cruz, CA; 1; University of Kansas Medical Center, Kansas City, KS; 2; University of Arizona, Tucson, AZ; 3; University of Kansas Cancer Center, Kansas City, KS; 4; University of Arizona, Tucson, AZ

Photobleaching and photoproducts analyses of the photosensitizers, protoporphyrin IX and protoporphyrin IX dimethyl ester, for photodynamic diagnosis/therapy of cancers; Soojin Oh Orbon2; Hisanao Hazama1; Katsuyoshi Masuda1,2; Kunio Awazu1,3,4; "Graduate School of Engineering, Osaka University, Suita, Japan; 2; Graduate School of Medicine, Kyoto University, Kyoto, Japan; 3; Global Center for Medical Engineering and Informatics, Osaka University, Suita, Japan

Quantitative analysis of extracellular matrix-enriched fresh tissues and formalin-fixed paraffin-embedded tissues reveals distinct protein signatures of lung cancers; Samah Shah1; Deng Pan2; Joanna Bons3; Jacob P. Rose1; Rosemary Bai4; Chira Chen-Tanylko2; Xinhong Wang2; Veena Sangwan2; Sophie Camilleri-Broét3; Philippe Gascard2; Lorenzo Ferri4; Thea D Tisty2; Birgit Schilling1; "Buck Institute for Research on Aging, Novato, CA; 1; Department of Pathology, University of California, San Francisco, CA; 2; Division of Thoracic and Upper Gastrointestinal Surgery, Montreal General Hospital, McGill University Health Centre, Montreal, QC; 3; Department of Pathology, McGill University, Montreal, QC

Establishing proteome divergence between high-grade serous ovarian tumors and their patient-derived xenograft experimental models; Joonhyun Ryu1; Mihir Shetty1; Boris Winterhoff1,2,3; Timothy K. Statt3,4; Stefani N. Thomas2,5; "Microbiology, Immunology, and Cancer Biology Program, University of Minnesota, Minneapolis, MN; 2; Department of Laboratory Medicine and Pathology, University of Minnesota, Minneapolis, MN; 3; Department of Obstetrics, Gynecology and Women's Health University of Minnesota, Minneapolis, MN; 4; Masonic Cancer Center, University of Minnesota, Minneapolis, MN

Quantification of Cross-Tissue Extracellular Matrix Alterations Associated with Malignancy in Human Chronic Inflammation-Associated Cancers using an Optimized Data-Independent Acquisition Workflow; Joanna Bons1; Deng Pan2; Samah Shah1; Rosemary Bai3; Chira Chen-Tanylko2; Nathan Basisty1; Amy O'Broin1; Jacob P. Rose3; Veena Sangwan2; Sophie Camilleri-Broét3; Philippe Gascard2; Lorenzo Ferri4; Thea D. Tisty2; Birgit Schilling1; "Buck Institute for Research on Aging, Novato, CA; 1; Department of Pathology, University of California, San Francisco, CA; 2; Division of Thoracic and Upper Gastrointestinal Surgery, Montreal General Hospital, McGill University Health Centre, Montreal, QC; 3; Department of Pathology, University of California, San Francisco, CA; 4; Division of Thoracic and Upper Gastrointestinal Surgery, Montreal General Hospital, McGill University Health Centre, Montreal, QC

Intra- and Inter-Patient Tumor Proteome Heterogeneity in Metastatic Lung Cancer; Sudhir Putty Reddy1; Hilal Ozakinci2; Lamees Saeed3; Bin Fang4; Victoria Izumi5; Joseph Johnson1; Brooke Smedley1; Eric Welsh2; Steven Eschrich1; Eric Haura1; Theresa Boyle1; John M Koomen1; "H. Lee Moffitt Cancer Center, Tampa, FL

Surfaceome Enrichment Strategies for Discovery of Immunotherapy Targets in Multiple Myeloma; Bin Fang1; Eric Welsh2; Umasangtongkul Sure-Attha1; Mark Meads3; Meghan Menges1; Alugubelli Raghuandan Reddy1; Frederic Locke2; Ken Shain3; John M Koomen1; Ciara L Freeman1; "H. Lee Moffitt Cancer Center, Tampa, FL

Spatially resolved multi-omic imaging of glioblastoma multiforme to examine hypoxic signatures; Caroline Pollard1; Rory T Steven2; Alina Finch1; Laura Porto3; Victoria Wykes2; Colin Watts2; Sabrina Naylor-Jones3; Jack McMurray2; Andrew Filer4; Daniel A Tennant2; Josephine Bunch2; National Physical Laboratory, Teddington, United Kingdom; 1; National Physical Laboratory, Teddington, United Kingdom; 2; Institute of Cancer and Genomic Science, University of Birmingham, Birmingham, United Kingdom; 3; Institute of Inflammation and Ageing, University of Birmingham, Birmingham, United Kingdom; 4; Institute of Metabolism and Systems Research, University of Birmingham, Birmingham, United Kingdom

PSA proteomics between cancer tissues and blood among 20 prostate cancer patients for early diagnosis; Wonnyeon Cho1; Miseon Jeong1; "WONKWANG UNIVERSITY, Iksan, South Korea

Comparative Analysis of Tumours, Their Metastases and Derived Primary Cell Lines by Rapid Evaporative and Desorption Electrospray Ionization Mass Spectrometry; Adrienn Molnár1,2; Gabriel Stefan Horkovics-Kovats1,2; Nóra Kucsma3; Richard Schäffer1; Zsuzsanna Szegő1; Attila Egr1; Gitta Schlosser2; Gergely Szakács3,4; Bálint András Dek3; Juliá Balog4; "Waters Research Center, Budapest, Hungary; 1; ELTE Eötvös Loránd University, Budapest, Hungary; 2; ELK-H Research Centre for Natural Sciences, Institute of Enzymology, Budapest, Hungary; 3; Center for Cancer Research, Medical University of Vienna, Vienna, Austria; 4; Department of Pathology, Forensic and Insurance Medicine, Semmelweis University, Budapest, Hungary

Advancing precision medicine in colorectal cancer using ambient ionization mass spectrometry and high-throughput personalised in vitro metabolomics; Stefania Maneta-Stavrakaki1; Annalisa Lorenzato2; Daniel Simon2; Yuchen Xiang1; Mariangela Russo2; Andrew Campbell3; Owen Sansom4; Alberto Bardelli5; Zoltan Takats2; "Imperial College London, London, United Kingdom; 1; University of Turin, Turin, Italy; 2; Beatson Institute for Cancer Research, Glasgow, United Kingdom; 3; University of Birmingham, Birmingham, United Kingdom; 4; University of Birmingham, Birmingham, United Kingdom; 5; University of Birmingham, Birmingham, United Kingdom

TMT Proteomics and Phosphoproteomics identifies LIN28A and STAT3 synergistically confer Chronic Myeloid Leukemia Resistance; Owen J.H. Hovey1; Mallory I Frederick2; Jenica H Kakadia3; Tingting Wu4; Courtney Voss5; Ilka U Heinemann1; Shawn S.C. Li6; "University of Western Ontario, London, ON, Canada; 1; University of Western Ontario, London, ON, Canada

Prolyl Isomerase Pin1 is involved in regulating PML-RARα in APL; Nina Guest1; Anna L. Sadowski1; "Purdue University, West Lafayette, Indiana

Extensive Three-Dimensional Intratumor Proteome Heterogeneity Revealed by Multiregion Sampling in Uterine Serous Tumor Specimens; Allison L Hunt1; 2; Nicholas W. Bateman1; 2; Waleed Barakat1; 2; Sasha Ch, Makohon-Moore1; 2; Scott E. Land2; 3; Brian L. Hood2,3; 4; "Kitty A. Conrads2,3,4; Ming Zhou2,3; Jeremy Loffredo2,3,4; Kattin N. Wilson2,3,4; Tracy J. Lititz3,4; Neil T. Phippen3; Emanuel F. Petricoin5; Uma N. Rao2,3,4; G. Larry Maxwell1

Extended Abstracts

MONDAY POSTERS
MP 097 Using substrate trapping to identify HDAC6 interactors in the setting of BRCA1/2wildtype high-grade serous ovarian cancer: Jelena M. Duda & Stefani N. Thomas; 1University of Minnesota, Minneapolis, MN

MP 098 Mass spectrometry imaging combined with orthogonal techniques identifies therapeutic vulnerabilities in the pediatric brain tumor, embryonal tumor with multilayered rosettes; Kelly C O'Neill; Evangelos Liapis; Annapurna Pamreddy; Allison Maas; Derek Hanson; Claire Louise Cartier; 1Hackett Meridian Center for Discovery & Innovation, Nutley, NJ

MP 099 Proteomic Characterization of the Tumor Microenvironment in Patients with Oral Squamous Cell Carcinoma; Allison L Hunt1, 2; Tamara Abulez1, 3, 4; Kelly A. Conrads1, 3, 4; Kattin N. Wilson1, 3, 4; Brian L. Hood1, 3, 4; Nicholas W. Battern1, 3, 4; Jaeli Ahn1; Julius Benicky1, 3, 4; Thomas P. Conrads1, 3, 4, 5; Radoslav Goldman1, 3, 4, 5, women's Health Integrated Research Center, Gynecologic Cancer Research, University of Toronto, Toronto, ON; 6Department of Obstetrics and Gynecology, Uniformed Services University and Walter Reed National Medical Center, Bethesda, Maryland; 7Women's Health Integrated Research Center, Gynecologic Cancer Research, Uniformed Services University and Walter Reed National Medical Center, Bethesda, Virginia; 8Center for Applied Proteomics and Molecular Medicine, George Mason University, Manassas, Virginia

MP 100 Metabolomic profiling of patient-matched primary and recurrent glioblastoma reveals dynamic metabolic reprogramming through therapy; Olivia Taverniti1, 2; William D. Gwynne1, 2; Andrew T. Quidel1; William T. Zadrow1; Shekla K. Singh1; J. Rafael Montenegro-Burke1; 1Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, ON; 2Center for Discovery in Cancer Research, McMaster University, Hamilton, ON

MP 101 Investigating the Role of Proteins in Regulating Breast Density in Premenopausal Breast Cancer Patients: Minsoc Son1; Antonia Zamacona Calderon1; Adetunji Toriola2; Young Ah Goo1; 1MTAC, MGI, Washington University School of Medicine in Saint Louis, St. Louis, MO; 2Washington University School of Medicine, St. Louis, MO

MP 102 Alterations in glutamate to glutamine ratios detected by DESI and MSPen allow diagnosis and molecular subtyping of breast cancer; Keishah E. Libenberg1; Erin Craig2; Meredith L Spradlin1; Michael F Keating1; Robert Tibshirani2; Livisa S. Eberlin1; 1Baylor College of Medicine, Houston, TX; 2Stanford University, CA

MP 103 Therapeutic targeting of lipid saturation in recurrent MYC-amplified medulloblastoma.; William D. Gwynne1; Jeremy K Chan1; Stefan Custers2; Andrew T Quidel1; Chitra Venugopala3; Sheila K. Singh1; J. Rafael Montenegro-Burke1; 1Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, ON; 2Center for Discovery in Cancer Research, McMaster University, Hamilton, ON

MP 104 Enhanced glucose oxidation in Birt-Hogg-Dubé syndrome renal tumors revealed by Ion-Chromatography coupled with Ultra-High-Resolution Mass Spectrometry based Stable-Isotope-Resolved Metabolomics; Ye Yang1; Daniel R. Crooks1; Laura S. Eberlin1; 1Department of Toxicology and Cancer Biology, Markey Cancer Center, University of Kentucky, Lexington, Kentucky

MP 105 Molecular correlates for head and neck squamous cell carcinoma engraftment are associated with patient outcomes. Matthew Waas1; Christina Karamboula; Laurie Alles1; 2; Thomas Kislinger1; 1, 2Princess Margaret Cancer Centre, Toronto, ON, 1University of Toronto, Toronto, ON; 2Princess Margaret Cancer Centre, University Health Network, Toronto, ON

MP 106 Characterization of Metabolic Heterogeneity in Pediatric Hepatoblastoma; Trevor M. Godfrey1; Andres F. Espinoza1; 2; Sarah E. Woodfield1; 2Sanjeev A. Vasudevan1, 2; Livisa S. Eberlin1; 2Baylor College of Medicine, Houston, TX; 2Texas Children's Hospital, Houston, TX

MP 107 Preoperative Classification of Thyroid Nodules by DESI-MS Imaging of Fine Needle Aspiration Biopsies; Rachel J. Dehoog1; Ahmed Al-Fartosi1; Neda Zarrin-Khameneh1; Rongrong Huang1; Livisa S. Eberlin1; James Sulibb1; 2Baylor College of Medicine, Houston, TX

MP 108 Application of Magnetic Beads in Automated Sample Preparation for Simultaneous Detection of Angiotensin I and Steroids in Plasma by LC-MS/MS; Pengyu Liu1; Xiaofen Yuan1; WeiJia Wu1; Huafen Liu1; 2Calibra Diagnostics, Hangzhou, China

MP 109 Classifying membranous nephropathy by mass spectrometry; Aaron J Storey1; Samar Hassen1; Christian Herzog1; John M Arthur1; Rick D Edmondson1; Tiffany N Caza1; Chris P Larsen1; 1University of Arkansas for Medical Sciences, Little Rock, AR; 2Arkana Laboratories, Little Rock, AR

MP 110 Mass Spectrometry Imaging Guided Spatial Proteomics for Stratification of Patient with Glioblastoma and Identification of Prognosis Markers; Marie Duhamel1; Maxence Wisztorski1; Isabelle Fourrier1; Michel Salzet1; 1PRISM Inserm U1192 - University of Lille, Villeneuve D’Ascq Cedex, France

MP 111 Gas Chromatography Rapid Automation and Quantitative Procedure for the Measurement of Hydrogen Cyanide in Whole Blood; Paul Brito-Vargas1; James Lapaieme1; Elizabeth Bair1; Ona Adair1; Nicolas Epie1; 1South Carolina Public Health Laboratory, Columbia, SC

MP 112 Finger-Sticking Good: Clinical Fatty Acids GC-MS Analysis from a Dried Microsample; Meghan Bradley1; Matthew L. Crawford1; Christopher M. Shuford1; Russell P. Grant1; 1LabCorp, Burlington, NC

MP 113 Adapting the MassSpec Pen for Non-destructive Screening of Oral Premalignancies (OPMDs) to Identify Oral Premalignant Cells (OPCCs): Charles A. Wolfe1; Michael F. Keating1; Gabrielle Wolter2; Erich M. Sturgis2; Carlos Chone4; Livisa S. Eberlin1; 1Department of Surgery, Baylor College of Medicine, Houston, TX; 4Ben Taub General Hospital, Houston, TX
MP 114  Multiplexed targeted assay for detection of sphenoglycolipids: Seul Kee Byeong1; Kimyo Raymond2; Devin Oglesbee3; Matthew Schultz1; Dietrich Matern1; Akhilesh Pandey4; 1Mayo Clinic, Rochester, MN

MP 115  Microprobe-Capture In-Emitter Elution Coupled with Mass Spectrometry for Structural Elucidation and Clinical Testing of β2-Transferrin; Ruben Y Luo1,2; Christopher Pfaffroth1; Samuel Yang1; Kevin Hoang1; Priscilla SW Yeung2; James Zehnder1; Run-Zhang Shi2; 1Stanford University, Palo Alto, CA; 2Stanford Health Care, Palo Alto, CA

MP 116  Development of 3D Microfluidic Paper-based Analytical devices (μPADs) with Mass Spectrometric Signal Amplification for diagnosis of Malaria in clinical setting; Ayesha Seth1; Abraham Kgabe Badu-Tawiah1; 1The Ohio State University, Department of Chemistry and Biochemistry, Columbus, OH

MP 117  Determination of 18 Steroid Hormones in Human Serum Using Rapid Protein Precipitation Method in Coupled With Liquid Chromatography-Tandem Mass Spectromet; Dan Liu1; Fengmei Hu2; Chao Huang2; Xianglong Zhao4; Shanghai AB SCIEX, Shanghai, China; 1China AB SCIEX, Shanghai, China

MP 118  Therapeutic Drug Monitoring (TDM) of 26 medications in urine samples of hypertensive patients using LC-MS/MS for medication adherence; Yi Ting Tan1; Troy Puar1; Daryl Hee1; 1Changi General Hospital, Singapore, Singapore

MP 119  Acyclcarbinilines in Dried Blood Spots (DBS) Samples by FIA-MS/MS: Convenient use of Single Stable Isotope Labeled Internal Standards CRM Mix; Arun Babu Kumar1; Laurens Lytwak1; Laura Min Xuan Chai1; Ming-Hsun Wu1; Kuen-Yuan Chen1; Cheng-Chih Hsu2; 1National Taiwan University, Taipei, Taiwan; 2National Taiwan University Hospital, Taipei, Taiwan

MP 120  Rapid Diagnosis of Cytologically Indeterminate Thyroid Fine-Needle Aspiration Biopsies using Paper Spray Ionization Miniature Mass Spectrometry; Jia Ying Yu1; Laura Min Xuan Chai1; Ming-Hsun Wu1; Kuen-Yuan Chen1; Cheng-Chih Hsu2; 1National Taiwan University, Taipei, Taiwan; 2National Taiwan University Hospital, Taipei, Taiwan

MP 121  Generic Methods for Simultaneous Analysis of Four Direct Oral Anticoagulants in Human Plasma and Urine by UPLC-Tandem Mass Spectrometry; Xin Zheng1; Xinge Cui1; 1Peking Union Medical College Hospital, Beijing, China

MP 122  Quantification of therapeutic proteins with a focus on TDM; Albert Sickmann1; Rob Dahlmann2,3; Phil Carbow4,5; Roman Sakson1,6; Yvonne Reinders1; 1Leibniz-Institut für Analytische Wissenschaften - e.V., Dortmund, Germany; 2Leibniz-Institut für Analytische Wissenschaften - ISAS e.V., Dortmund 44139, Germany, Dortmund, Germany; 3University of Applied Science, Hamm-Lopstad, Hamm, Germany; 4MilliporeSigma, Round Rock, TX; 5MilliporeSigma, Round Rock, TX

MP 123  Predicting Septic Shock in Emergency Patients with Serum Metabolic Profiles and Machine Learning; Yu Heng1; Li-Hua Lf2; Ting-Hao Ku3; Yi-Tzu Lee3; Cheng-Chih Hsu1; 1Department of chemistry, National Taiwan University, Taipei, Taiwan; 2Department of Pathology and Laboratory Medicine, Taipei Veterans General Hospital, Taipei, Taiwan; 3Department of Emergency Medicine, Taipei Veterans General Hospital, Taipei, Taiwan; 4Faculty of Medicine, School of Medicine, National Yang-Ming University, Taipei, Taiwan

MP 124  Simultaneous Quantitation of Renin Activity, Aldosterone and Angiotensin II in Human Plasma Using Rapid Prot; Fengmei Hu1; Dan Liu2; Chao Huang2; Xianglong Zhao4; 1Shanghai AB SCIEX Analytical Instrument Trading Co., Ltd., Shanghai, China; 2Shanghai AB SCIEX Analytical Instrument Trading Co., Ltd., Shanghai, China

MP 125  Efficient Extraction of Proteins from Desiccated Blood followed by On-Bead Trypsinization - An Efficient Alternative to Plasma-based LC-MS Analysis; Debadeep Bhattacharyya1; Patrick McCarthy1; Heidi Giese1; Martina Werner1; Eugene Daviso1; Sameer Vasantagadkar1; Ulrich Thomann1; 1Covaris, Lexington, MA

MP 126  Advancing Clinical (Auto)antibody Analysis: Fc-Proteoform Profiling of IgG Allotypes in Rheumatoid Arthritis; Constantin Blobchi1; Christoph Gostlotten1; Eva Maria Stork1; Rainer Schröter1; Peter A. van Veelen2; Hans Ulrich Scherer2; Rene E. M. Toses2; Manfred Wuhrer1; Elena Dominguez-Vega1; 1Center for Proteomics and Metabolomics, Leiden University Medical Center, Leiden, Netherlands; 2Department of Rheumatology, Leiden University Medical Center, Leiden, Netherlands

MP 127  Development of direct mass spectrometry platform for shotgun metabolomics analyses of whole blood samples for malaria diagnosis; Riley Ferguson1; Abraham Kgabe Badu-Tawiah1; 1The Ohio State University, Columbus, OH

MP 130  Clinical applications utilizing in-pipet dispersive SPE prior to LC-MS/MS; Yong Chen1; Hugh Cramer2; M James Ross1; Gabriel Duguezel1; MilliporeSigma, Bellefonte, PA; 1Millipore Sigma, Bellefonte, PA; 2University of Maryland School of Pharmacy, Baltimore, MD

MP 131  Determination of nine neurotransmitters in plasma by HPLC-ESI-MS/MS; Ruichen Liu1; Xuzhe Pei1; Chao Huang2; Xianglong Zhao2; Lihui Guo1; 1SCIEX, Beijing, China

MP 132  High-throughput profiling of reactive cytokines and lysis by automated proteomics workflow; Zixiang Fang1; Taylor P Ma1; Hanna G Budayeva1; 1Genentech, Inc., South San Francisco, CA

MP 133  Fast and Sensitive Analysis of FPOP data using MSFragger and FragPipe; Carolina Rojas Ramirez1; Daniel A. Polasky1,2; Patrick Battoon3; 1Cesar Gozzo1,2; 2University of Michigan, Ann Arbor, MI

MP 134  Comparing Common Biophysical Methods to Evaluate MS-based Footprinting-Induced Perturbation of Protein High Order Structure (HOS); Wesley J. Wagner1; Austin B. Moyie1,2; Nicole D. Wagner1; Michael L. Gross2; 1Washington University in St. Louis, St. Louis, MO; 2AbbVie Inc., North Chicago, IL

MP 135  Single Sequence Identification of Probe-Modified Peptides by TrypIC-terminal Clipping of Tryptic Peptides; Cleodette Punzalan1; Mariel Ciores1; Connor Jewell1; Xudong Yao1; 1University of Connecticut, Storrs, CT

MP 136  Building fully controlled interactomes and tools to advance protein interaction identification by cross-linking mass spectrometry; Milan Avila Clasen1; Max Ruwolt2; Louise Ulrich Kurt1; Fabio Cesar Gozzo2; Paulo Costa Carvalho3; Diogo Borges Lima4; Fan Liu5; 1Laboratory for Structural and Computational Proteomics, Carlos Chagas Institute, Fiocruz, Curitiba, Brazil; 2Department of Structural Biology, Leibniz-Forschungsinstitut für Molekulare Pharmakologie (FMP), Berlin, Germany; 3Dalton Mass Spectrometry Laboratory, University of Campinas, Campinas, Brazil

1University of Texas at Austin, Austin, TX; 2Department of Otolaryngology, Baylor College of Medicine, Houston, Texas; 3Department of Otolaryngology, University of Campinas, Campinas, Brazil
MONDAY POSTERS

MP 137  Developing LC-MS workflows for cross-link identification from low sample amounts; Abigail H Lewis; Siang-Wun Siao; Tomas Koudelka; Julia Kraegenbring; Rosa Viner; Ilaria Piazza; Fan Liu; Leibniz-Forschungsinstitut für Molekulare Pharmakologie, Berlin, Germany; Max Delbrück Center for Molecular Medicine in the Helmholtz Association, Berlin Institute for Medical Systems Biology, Berlin, Germany; "Thermo Fisher Scientific, Bremen, Germany; "Thermo Fisher Scientific, San Jose, CA

MP 138  New insight into SARS-CoV-2 interactions with host cells using in vivo Crosslinking Mass Spectrometry; Martial Rey; Florence GUILVÉ-BENNASSINE; Karen Druart; Olivier Schwartz; Julia Chamot-Rooke; "Mass Spectrometry for Biology Unit, Université Paris Cité, Institut Pasteur, CNRS, UAR 2024, Paris, France; "Virus and Immunity Unit, Institut Pasteur, Université Paris Cité, CNRS UMR3569, Paris, France

MP 139  Comparison of Protein Footprinting Approaches for Epitope Mapping of TFalpha39 (nuclear receptor ligand); Samantha J Knott; Daniel Benjamin; Richard Y-C Huang; James Dowell; Ekaterina G. Deyanova; Tahmid Hassan; Robert Langish; Yun Wang; Faraz Choudhury; "Immuno Scientific Inc., Madison, WI; "Bristol Myers Squibb, Princeton, NJ; "Janssen Pharmaceuticals, Spring House, PA

MP 140  Probing Antibody-Host Proteome Interactions via Intracellular Cross-linking; Bradley Hart; Yi He; Lauren M Kraft; Michael Pottash; Chris Sauer; Elsa Gorre; Andrew Mahan; Thomas Kelly; Hirsh Nanda; Rosa Viner; Harsha Gunawardena; "Thermo Fisher Scientific, San Jose, CA; "JOHNSON AND JOHNSON, Spring House, PA

MP 141  Application of FoxWare® Software for Resolving Isomeric Heterogeneity and Retention Time Drift in Oxidized Peptides from Hydroxy Radical Protein Footprinting; Jiana Duan; Robert Egan; Calyx Liu; Tyler Fletcher; Emily Chea; Sandeep K. Misra; Joshua Sharp; Scot Weinberger; "GenNext Technology, Half Moon Bay, CA; "University of Mississippi, University, MS

MP 142  Large scale identification of cross-linked peptides from bovine exosomes using a multiplexed hypochromatography approach; Yiran Ma; Noor H. Naseeb; Adam J Anthony; Andrew D. Couse; Jonathan C. Trinidad; David E. Clemmer; "Indiana University, Bloomington, IN

MP 143  Benchmarking MS2- and MS3-based acquisition strategies for XL-MS using a developmental ProteinProspector/Touchstone pipeline; Clinton Yu; Mike Trinka; Peter Baker; Robert Chaikley; A Burlingame; Lan Huang; "University of California, Irvine, Irvine, CA; "University of California San Francisco, San Francisco, CA

MP 144  An atlas of reactive and functional chromatin-associated cysteines in cancer; Daniele Caranzani; Brian McEllin; Erin Broderick; Tonibelle Gatbonton-Schwager; Yang Gao; Julia E. Robbins; Andrea I. Gutierrez; Carolyn Allen; J. Sebastian Paez; William E Fondrie; Lindsay K Pino; Alexander J Federation; "Talus Bioscience, Seattle, WA

MP 145  Mapping of the Interaction Site of a Novel Fungal Lectin to a Peptidoglycan from Listeria innocua; Sandeep K. Misra; Sushil S. Mishra; Nika Janez; Robert J. Doeksen; Jerica Sabol; Joshua S. Sharp; "University of Mississippi, University, MS; "Jozef Stefan Institute, Jamova cesta 39, Slovenia

MP 146  Identifying the culprits of novel proteolytic activity in secreted proteins of B. subtilis using N-terminal covalent labeling; Matthew Davison; Charles Dann; Jonathan C. Trinidad; James Reilly; "Indiana University, Bloomington, IN; "Indiana University Bloomington, Bloomington, Indiana; "Indiana University Bloomington, Bloomington, IN

MP 147  Visualization of transient DOT1A-nucleosome interactions in solution by X-ray protein footprinting; Janna Kiesel; Victoria S Frisbie; Mark R Chance; Hideharu Hashimoto; Erik W Deabler; "Case Western Reserve University, Cleveland, OH; "Thomas Jefferson University, Philadelphia, PA

MP 148  Applying Machine Learning Tools to Analyze Crosslinking and TMT Mass Spectrometry Datasets; Zhuhui Wen; Yan Zhang; Yan Hao; Laurence Flores; "Stowers Institute for Medical Research, Kansas City, MO

MP 149  Protein structure and higher order assembly in Vaccinia virus by combination of XLMS with deep learning protein structure methods; Michael Wun Siao; Calyx Liu; Yi He; Joshua Sharp; "McGill University, Montreal, QC; "Biomedical and Life Sciences, University of Montreal, Montreal, QC; "McGill University, Montreal, QC; "Bristol Myers Squibb, Princeton, NJ; "ThermoFisher Scientific, San Francisco, CA

MP 150  Enrichable covalent labeling for efficient global, temporal, in situ profiling of protein structural changes in living cells; Chengzhi Cai; Guoting Qin; Shara Duong; John Mansour; "University of Mississippi, University, MS; "Buck Laboratory, University of Cincinnati, Cincinnati, OH; "Indiana University Bloomington, Bloomington, IN

MP 151  Mass spectrometry analysis of IgA N-glycans for biomarker discovery: Application in a pilot study to discriminate patients with ankylosing spondylitis; Hui-Ling Chiang; Ming-Chi Lu; Ning-Sheng Lai; Chien-Hsu Tung; Kuang-Yung Huang; Bao-Bao Hsu; Chih-Chia Yu; Yi-Ling Lin; "Division of Pathology, St. John's Health Center, New York, NY; "Division of Rheumatology, Dalin Tzu Chi Hospital, Buddhist Tzu Chi Medical Foundation, Dalain, Taiwan; "Department of Medical Research, Dalin Tzu Chi Hospital, Buddhist Tzu Chi Medical Foundation, Dalain, Taiwan; "Department of Biotechnology, National Formosa University, Taiwan

MP 152  Multi-Omic molecular characterisation of pre-invasive breast ductal carcinoma using tumor micro arrays identifies putative biomarkers and readily druggable targets; Georgia Mitsa; Liiva Florianova; Josiane Lefleur; Adriana Aguilar-Mahecha; Mark Basik; Gerald Batist; 1, 2, 4, 8; Christoph H Borchers; 1, 2, 4, 8; "Division of Experimental Medicine, McGill University, Montreal, QC; "Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; "Department of Pathology, McGill University, Montreal, QC; "Department of Pathology, McGill University, Montreal, QC; "Department of Medicine, McGill University, Montreal, QC; "Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; "Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; "Department of Oncology and Surgery, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; "Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; "Department of Oncology, McGill University, Montreal, QC; "Department of Oncology, McGill University, Montreal, QC; "Department of Oncology, McGill University, Montreal, QC; "Department of Oncology and Pathology, Segal Cancer Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC

MP 153  A comparative investigation of plasma proteome profiling with state-of-the-art mass spectrometry and affinity-based assays; Noor H. Naseeb; Roland Bruderer; Jakob Vowinckel; Karel Novy; Kristina Beeler; Raphael Heilig; Sebastian Müller; Lukas Reiher; Yuehan Feng; Biognosys AG, Schlieren, Switzerland

MP 154  Development of an MS-based multimarker glycomics test for earlier detection of pancreatic cancer among high risk individuals and treatment monitoring; Yuni Van Der Burg; Derk C.F. Klatte; Iris J.M. Levin; Bert A. Borsing; Wilma E. Mesker; Djuna L. Cahen; Gwenny M. Fuhler; Marco J. Bruno; Monique E. Van Leerdam; "Leiden University Medical Center, Leiden, The Netherlands; "Erasmus Medical Center Rotterdam, Rotterdam, The Netherlands; "Erasmus Medical Center Rotterdam, Rotterdam, The Netherlands

MP 155  3-Dimensional Primary Human Chondrocyte Pellets and Cellular Alterations during Osteoarthritis and Senescence; Jacob P. Rose; Sandip Patil; Joanna Bons; Charles A. Schurman; Christina D. King; Samah
Shah1, Judith Campisi1,2; Tamara Alliston3,4; Birgit Schilling3; 1Buck Institute for Research on Aging, Novato, CA; 2Lawrence Berkeley Laboratory, University of California, Berkeley, CA; 3University of California San Francisco, Department of Orthopaedic Surgery, San Francisco, CA; 4UC Berkeley/UCSF Graduate Program in Bioengineering, Berkeley, CA

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Explore protein glycosylation as non-invasive biomarker for chronic liver diseases; Mark M. Kushnir1; Carmen Dunbar1; Yanhong Wu2; Yifei Yang3; IARUP Laboratories, Salt Lake City, UT; 4Mayo Clinic, Rochester, MN

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Combined serum proteome profile of Alzheimer’s disease; Jiayi Zhang1; Huali Shen1; 1Fudan University, Shanghai, China

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LC-MS/MS based absolute quantitation of hemoglobin subunits from DBS reveals novel biomarkers for a-thalassemia; Zhe Ren1; Guoying Zhang1; Jianhong Chen2; Weining Zhao3; Guixue Hou4; Zeyan Zhong5; Jialong Li6; Yuhua Ye7; Xiangmin Xu8; 1BGI Genomics, China; 2IISc, Bangalore, India; 3BGI, Shenzhen, China; 4BGI Genomics, Shenzhen, China; 5BGI Shenzhen, Shenzhen, China; 6Department of Medical Genetics, School of Basic Medical Sciences, Southern Medical University, Guangzhou, China; 7Department of Medical Genetics and Prenatal Diagnosis, Huizhou First Maternal and Child Health Care Hospital, Huizhou, China; 8College of Pharmacy, Shenzhen Technology University, Shenzhen, China; 9Innoveda Research Center for Diagnosis and Therapy of Thalassemias, Nanfang Hospital, Southern Medical University, Guangzhou, China

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Metabolite profiling applied to biomarker discovery in pancreatic cancer using high resolution LC-MS/MS; Alan Barnes1; Emily G Armitage2; Neil Loftus3; Eloï Correa4; Lynne Howells5; Sén Takeda6; Wen Chung7; 1Shimadzu Corporation, Manchester, United Kingdom; 2Liverpool John Moores University, Liverpool, United Kingdom; 3Institute for Precision Health, The University of Leicester, Leicester, United Kingdom; 4Department of Anatomy, Teikyo University School of Medicine, Tokyo, Japan; 5Leicester HPB Unit, Glenfield Hospital, Leicester, United Kingdom

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High-content imaging and mass spectrometry-based drug screening platform to study stress-induced tau aggregation; Jie Xue1; Long Cheng2; 1Benoit Fatou1; 2Mukesh Kumar1; 3Kathrin Wenger1; 4Arthur Viode1; 5Hanno Steen1; 6Juditte Steen1; 7Boston Children’s Hospital, Boston, MA; 8Harvard Medical School, Boston, MA

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Molecular characterization of inverse agonists targeting PPARG in bladder cancer using structural and quantitative proteomics; Kuang-Ting Kuo1; 2Ruben D. Garcia-Ordonez2; Bibi Bdiri3; Theodore Kamenecka4; Patrick R. Griffin5; 1The Scripps Research, Jupiter, FL; 2Skaggs Graduate School of Chemical and Biological Sciences, The Scripps Research Institute, Jupiter, FL; 3The Herbert Wertheim UF Scripps Institute for Biomedical Innovation & Technology, Jupiter, FL

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Head-to-tail automation of covalent fragment screening and hit characterization by mass spectrometry for rapid lead discovery; Jing Xue; Alexandra Frommelt; Robert Blake; Alexis Rohou; Melinda Mulvihill; Ke Sherry Li; Genentech, South San Francisco, CA

Covalent inhibitor screening of cellular protein targets using mass spectrometry for hit identification in living cells; Sherry Ke Li; Ryan Conrad; Ryan Raisner; Brett Babin; Jing Xue; Melinda Mulvihill; Genentech, South San Francisco, CA

The Limited-Profile Analysis Method in Drug Development: Powerful workflow to identify drug targets and evaluate drug specificity; Fabio Sabino; Jaruscha Pecnik; Roland Bruderer; Lukas Reiter; Biognosys AG, Schlieren, Switzerland

Development and validation of an LC-MS/MS method for quantifying ociclofungin in rabbit plasma; Andrew Cotrell; Ryan Conroy; Jamie Leit Smith; Texas A&M University, College Station, TX; Sano Chemicals, College Station, Texas

Multiplexed CETSA MS as a tool for lead optimization; Tuomas A Tolvanen; Jennifer A Amrhein; Thomas Hanke; Tomas Friman; Alexey Chernobrovkin; Stefan Knapp; Michael Sundström; Daniel Martinez Molina; Pelago Bioscience AB, Solna, Sweden; University of Rheumatology, Department of Medicine Solna, Karolinska University Hospital and Karolinska Institut, Solna, Sweden; Institute of Pharmaceutical Chemistry, Goethe-University Frankfurt, Biozentrum, Frankfurt am Main, Germany

Measuring protein thermal stability and phosphorylation changes to capture early cellular responses to small molecule drugs; Alexey Chernobrovkin; Daniel Martinez Molina; Pelago Bioscience AB, Solna, Sweden

Point-of-care quantification of immunosuppressive drugs in blood by fast microextraction and miniature mass spectrometry analysis; Yikun Liu; Jinling Lu; Wenpeng Zhang; Zheng Ouyang; Tsinghua University, Beijing, China

The Target Engagement Atlas - Mapping cell biology through small molecule perturbations; Alexey Chernobrovkin; Tomas Friman; Erin Gilson; Bolette Bossen; Tuomas A Tolvanen; Daniel Martinez Molina; Pelago Bioscience AB, Solna, Sweden

Identification of Functionally Relevant and Druggable Protein Targets of Colorectal Cancer Chemoresistance using Protein Folding Stability Profiling; Baji Quan; Morgan A. Bailey; John Mantyh; Hsu S. Hsu; Michael C. Fitzgerald; Duke University, Durham, NC; Duke University Medical Center, Durham, NC

Development and Optimization of an LC-MS/MS Method for CD73 Endogenous Biomarkers of Adenosine-5'-Monophosphate, Adenosine and Inosine; Ashley Davie; Remeng Liu; Yiding Hu; Ting Wang; Yurong La; Gilead Sciences, Foster City, CA

Mass Spectrometry Analysis with Cellular Thermal Shift Assay to Assess Senolytic Pathways in Senescent Monocytes; Delaney Rutherford; Reema Banjarie; Quinn Strassheim; Amit K Dey; Dimitrios Tsitsipatis; Anjana Ram; Ruin Moaddel; Myriam Gorospe; Nathan Basisty; National Institute of Aging, Bethesda, MD

Validation of an Automated Process for the Determination of Covalent Modifier Potency: Kinac/KI of the Btk/Ibrutinib Model System; William A Lamarr; Somayeh Talebzadeh; Jim Breunig; Lars Hansen; Brian Healey; PureHoney Technologies, Inc., Billerica, MA; Beantown Biotech LLC, Billerica, MA; Revolution Biosciences LLC, Norwell, MA

Characterization of Hyaluronic Acid-Based Hydrogel Drug Delivery Systems via Online Multimodal Liquid Chromatography-Mass Spectrometry; Brady W Drennan; Kevin A. Schug; Sam H. Yang; University of Texas at Arlington, Arlington, TX; Genentech Inc., South San Francisco, CA

Implementing antibody-free strategies for protein quantitation in monkey liver tissues using liquid chromatography coupled with mass spectrometry; Yifan Shi; Sheng-Ping Wang; Lifeng Wang; Fritz Kramer; Wenying Jian; Janssen Research & Development, Spring House, PA

Rapid rank ordering of binding affinities of pools of test compounds against an RNA target with Affinity Selection Mass Spectrometry; Somayeh Talebzadeh; Zane Thistleford; William J. Oztal; PureHoney Technologies, Billerica, MA

The Neuropeptide Neuroparin-A Regulates Caretaking Behavior in Leafcutter Ants; Michael Gilbert; Karl Glastad; Maxx Fioriti Fioriti; Tierney Gannon; Matan Sorek; Lindsay Pino; Shelley Berger; Benjamin A Garcia; University of Pennsylvania, Philadelphia, PA; Telus Biocentury, Seattle, WA; Washington University School of Medicine, St. Louis, MO

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Comprehensive interactome profiling of replication stress response and centromere instability by proximity labeling and affinity purification-mass spectrometry; Alexander S. Lee; Matthew A. Mattamana; Justin E. Bodner; Renu Goel; Daniel R. Foltz; Neil L. Kelleher; Department of Biochemistry and Molecular Genetics, Northwestern University Feinberg School of Medicine, Chicago, IL; Simpson Querrey Institute for Epigenetics, Northwestern University, Chicago, IL; Chemistry of Life Processes Institute, Northwestern University, Evanston, IL; The Proteomics Center of Excellence, Northwestern University, Chicago, IL; Department of Chemistry and Molecular Biosciences, Northwestern University, Evanston, IL

METTL3 Promotes Histone H3K9 Acetylation through Recruitment of Histone Acetyltransferase 1 to Chromatin; Yen-Yu Yang; Xiaomei He; Jun Yuan; Chengjie Ma; Yinsheng Wang; University of California Riverside, Riverside, CA

Quantification of linker histone H1 proteomes in naive versus germinal center B cells using capillary electrophoresis-top-down mass spectrometry; Ashley Ives; Antonin Papin; Alexey A. Soshnev; Kevin Jooss; Navid AYon; Matt Robey; Ethan Cesaran; Ari M. Melnick; Rafael Melani; Neil L. Kelleher; Northwestern University, Evanston, IL; Department of Pathology and Laboratory Medicine, Weill Cornell Medical College, New York, New York; Department of Neuroscience & M ans Developmental and Regenerative Biology, University of Texas at San Antonio, San Antonio, Texas; Proteinaceous, Evanston, Illinois; Department of Medicine, Weill Cornell Medicine, New York, New York

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MP 199  Scoring Post-translational Modification Crosstalk from Histone Posttranslational Data; Karl Fali Poncha1; Nicolas L. Young1, 2, 3; Verna and Marrs McLean Department of Biochemistry and Molecular Biology, Baylor College of Medicine, Houston, TX; 2 Department of Molecular and Cellular Biology, Baylor College of Medicine, Houston, TX; 3 Center for Precision Environmental Health, Baylor College of Medicine, Houston, TX

MP 200  Histone Post-translational Modification Mapping of Aplysia californica Ganglia after Juvenile Exposure to Hypoxia using LC-TIMS-PASEF-ToF MS/MS; Cassandra N. Fuller1; Javier A. Rodriguez-Casariego2, 3, 4; Lilian Valadares Tose1; Jose M. Eirin-Lopez5; Lynne A. Fieber5; Francisco A. Fernandez-Lima5; 1 Department of Chemistry and Biochemistry, Florida International University, Miami, FL; 2 Department of Biological Science, Florida International University, Miami, FL; 3 Department of Marine Biology and Ecology, Rosenstiel School, University of Miami, Miami, FL; 4 Neurosciences Institute, University of Puerto Rico, San Juan, PR

MP 201  Quantitative Top-Down Analysis of H3.3K36M Oncohistone Proteoforms and Post-Translational Modifications; Alyssa T. Paparellia1; Karl Poncha1; Pratim Chowdhury1; Ruhee Derry1; Cheryl Lyn Walker1; Nicolas L. Young1; 1 Baylor College of Medicine, Houston, Texas

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MP 208  Simultaneous Determination of Neonicotinoids, Parabens, and Bisphenols in Canned Food Products by a Simplified QuEChERS and ID- UPLC-MS/MS; Heim-Chang Chen1; Zou-Xiao Huang2; Jung-Wei Chang3; Po-Chin Huang4, 5, 6; 1 Department of Chemistry, Tunghai University, Taichung City, Taiwan; 2 Institute of Food Safety and Health, College of Public Health, National Taiwan University, Taipei, Taiwan; 3 Institute of Environmental and Occupational Health Sciences, School of Medicine, National Yang Ming Chiao Tung University, Taipei, Taiwan; 4 National Institute of Environmental Health Sciences, National Health Research Institutes, Miaoli, Taiwan; 5 Research Center for Environmental Medicine, Kaohsiung Medical University, Kaohsiung, Taiwan; 6 Department of Medical Research, China Medical University Hospital, China Medical University, Taichung City, Taiwan

MP 209  Determination of nitrofuran metabolite residues in shrimp by LC-MS/MS; Dan Lu1; Qiang Li2; Hongyuan Hao3; Taohong Huang4; 1 Shimadzu (China) Co., LTD, Wuhan, China; 2 Shimadzu Corporation, Kyoto, Japan; 3 Shimadzu (China) Co., LTD, Shanghai, China; 4 Shimadzu (China) Co., LTD, Shanghai, China

MP 210  Analysis of Antibiotics and Veterinary Drugs in Animal Feeds and Animal Tissues by QSight LC-MS/MS; Jingcun Wu1; Feng Qin1; 1 PerkinElmer Inc., Woodbridge, ON

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MP 212  Analysis of Veterinary Drugs in Chicken Tenders using the Quadrupole Time-of-Flight Mass Spectrometer; Yukito Ito1, 2; Jun Watanabe1, 2; Junko Iida1, 2; 1 SHIMADZU Corporation, Kyoto, Japan; 2 Osaka University Shimadzu Omics Innovation Research Laboratories, Suita, Japan

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MP 215  Standard-Free Absolute Quantitation of Cyclic Imines using Tademon Mass Spectral Matching and LC/HR-MS; Nari Seo1, 2; Hee Young Jo3; 1 Hanyang University, Seoul, Korea; 2 Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, South Korea; 3 Asia-Pacific Glycoscience Research Site, Daejeon, South Korea

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MP 217  Automated sample preparation using CTC PAL3 to analyze >570 pesticides in orange by the combination of LC/MS/MS using Tadem Mass Spectr

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Gas-Phase Schiff Base Formation via PAMAM Dendrimer Molecular Containers: Sarah Nsiah; Scott A McMuckley; Purdue University, West Lafayette, IN; 2Purdue University, WEST LAFAYETTE, IN

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Acidity of Organic Compounds and Small Peptides in Solution and in the Gas-Phase: Kim Harvey; Mandy Brinkmann; Michael Browne; Erica Meng; Raj Patel; Jianhua Ren; 1University of the Pacific, Stockton, CA; 2University of The Pacific, Stockton, CA

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Selective, gas-phase decarboxylation of formic acid catalyzed by polyoxoanions: Howard Z. Ma; Allan J. Canty; Richard A. J. O’hair; 1University of Melbourne, Parkville, Australia; 2University of Tasmania, Hobart, Australia

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Computational modelling of reaction intermediates in gas-phase charge inversion ion/ion reactions: Yingchan Guo; Jonathan T. Specker; Ramon Alain Miranda-Quintana; Boone M. Prentice; 1Department of Chemistry, University of Florida, Gainesville, FL

**MP 245**
Manipulation of gas-phase charge inversion ion/ion reaction reagents for kinetic and thermodynamic control over phospholipid identification in imaging mass spectrometry: Jonathan T. Specker; Boone M. Prentice; 1University of Florida Department of Chemistry, GAINESVILLE, FL

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Studies of Negative Electron Transfer Dissociation Reagents: Keaton L Mertz; Katie Kothlow; Michael S. Westphal; John E.P. Syka; Joshua J. Coon; 1University of Wisconsin-Madison, Department of Chemistry, Madison, WI; 2University of Wisconsin-Madison, Madison, WI; 3Thermo Fisher Scientific, San Jose, California

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Fragmentation Patterns of Peptides Containing a Basic Residue: Ashleigh Ramos1; Yadwinder Singh Mani1; Jianhua Rens1; University of the Pacific, Stockton, CA; 2University of Leipzig, Leipzig, Germany

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Structural elucidation of the 20S Proteasome using native ultraviolet photodissociation mass spectrometry: Jada N. Walker1; Amit Kumar Singh Gautam2; Andreas Matouschk3; 1Jennifer S. Brodbelt1; Department of Chemistry, The University of Texas at Austin, Austin, TX; 2University of Leipzig, Leipzig, Germany

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Improved Signal Processing for Orbitrap Charge Detection Mass Spectrometry: Michael Goodwin1; Kyle Patrick Bowen1; Dmitry Grinfeld1; Ping Yi2; Michael Senko1;1 Thermo Fisher Scientific, San Jose, CA

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Fluorinated ethylamines as ESI-friendly neutral pH buffers for native mass spectrometry: Brad Davis1; Algirdas Velyvis1; Siavash Vahidi1; 1University of Guelph, Guelph, ON

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Towards understanding the effect of isoelectric point on the gas-phase stability of proteins in native MS: Alexis N. Edwards1; Michael S. Cordes2; Elysia S. Gallagher3; 1 Baylor University, Waco, TX; 2University of Michigan, Madison, WI; 3Baylor University, Waco, TX

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Native ESI MS for Deep Characterization of Target Engagement and Molecular Mode of Action: Xinong Feng1; Wenli Hu2; Jayasankar Jasti1; Timothy Foley1; DaYddy Owen2; Matthew D Troutman3;2 Pfizer, Groton, CT; 3Pfizer Inc., Groton, CT

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Are Native Conformations of Proteins Protected Throughout Laser Ablation?: Neda Feizi Gilandeh1; Blessing Chisom Egbejiogu2; 1University of The Pacific, Stockton, CA; 2University of the Pacific, Stockton, CA

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Size-Exclusion Chromatography-Assisted Native Mass Spectrometry Coupled with In-Source Denaturation Facilitates Characterization of Biologics for Drug Discovery: Xiao Guo1; Dongdong Wang1; 1Takeda Pharmaceuticals, Cambridge, MA

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In-depth characterization of monoclonal antibody variants with native mass spectrometry: Jun Dai1; Chengjie Ji2; 1NovaBioAssays, Woburn, MA; 2Goethe University Frankfurt, Frankfurt am Main, Germany

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The University of Texas at Austin, Austin, TX; 2University of Leipzig, Leipzig, Germany

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Exploring Nonannular Belt of Membrane Proteins Using a Mass Spectrometry/mass spectrometry Program, CSIRO, Clayton, Australia; 2Drug Delivery, Disposition and Dynamics, Monash Institute of Pharmaceutical Sciences, Monash University, Parkville, Australia; 3ARC Centre for Fragment-Based Design, Monash Institute of Pharmaceutical Sciences, Monash University, Parkville, Australia; 4Biological Group, Biomedical Manufacturing Program, CSIRO, Clayton, Australia; 2Drug Delivery, Disposition and Dynamics, Monash Institute of Pharmaceutical Sciences, Monash University, Parkville, Australia

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Two Nonannular Belt of Membrane Proteins Using Canada; 2Drug Delivery, Disposition and Dynamics, Monash Institute of Pharmaceutical Sciences, Monash University, Parkville, Australia; 3ARC Centre for Fragment-Based Design, Monash Institute of Pharmaceutical Sciences, Monash University, Parkville, Australia; 4Biological Group, Biomedical Manufacturing Program, CSIRO, Clayton, Australia; 2Drug Delivery, Disposition and Dynamics, Monash Institute of Pharmaceutical Sciences, Monash University, Parkville, Australia

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Native MS for gas-phase metallochemistry of amyloid B: Sarah Brandon1; Tanja Habeck1; Frederik Lemytte1; 1TU Darmstadt, Darmstadt, Germany

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Charge State Distributions of Proteins in Femto-Capillary ESI with Different pH: Tenghao Wang1; Huishan Li1; Nicholas Allen1; Ian T Ferraro1; Anyin Li2; 1University of New Hampshire, Durham, NH; 2University of Wisconsin-Madison, Madison, WI

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Improving Ion Activation on a 1.5 m Fourier Transform Ion Mobility (FT-IM) Orbitrap using a Segmented Quadrupole Ion Trap: Kacie Evans1; Robert Schrader2; Carter Lantz2; David H. Russell3; 1Texas A&M University, College Station, TX; 2Texas A&M University, College Station, TX; 3Texas A&M University, College Station, TX

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Quantitative Analysis of noncovalent Interactions via LILIB-MS: Jonathan Schulte1; Nina Morgner1; Phoebe Young1; 1Goethe University Frankfurt, Frankfurt am Main, Germany

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Matrix-Landing Mass Spectrometry for Electron Microscopy Imaging of Native Protein Complexes: Austin Z. Salm1; Kornel W. Wysocki1; Timothy Grant1; Michael S. Westphall1; Joshua J. Coon2; 1University of Wisconsin-Madison, Madison, WI

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CDMSAnalysisof Intact 19S, 20S, 26S, and 30S Proteasomes: Evidence for Higher-Order 20S Assemblies at low pH: Adam J Anthony1; Amit K. S. Gautam2; Lohra M. Miller1; Anya G. Hardwick1; Anu Sharma2; Subhadip Ghatak2; Andreas Matouschk2; Martin F. Jarrold3; David E. Clemmer3; 1Indiana University, Bloomington, IN; 2Department of Molecular Biosciences, Austin, TX; 3Indiana Center for Regenerative Medicine and Engineering, Department of Surgery, Indianapolis, IN

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An Evaluation of Ion Mobility-Collision Induced Unfolding (IM-CIU) Methods Leveraging Cyclic Ion Mobility Separation for the Evaluation of Protein Dynamics: Addison E. Bergman1; Devin M. Makey1; Ryan Schroeder1; Brandon T. Ruotolo1; 1University of Michigan, Ann Arbor, MI

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A Mass Spectrometry-Based Chemical and Enzymatic Method to Comprehensively Analyze Protein O-
Xinyue Liu1; Joao A. Paula1; Steven P. Gyg1; Qing Yu1;  
1Department of Cell Biology, Harvard Medical School, Boston, MA;  
2Department of Genome Sciences, University of Washington, Seattle, WA

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Developing a Semi-Automated Sample Preparation Method for the Enrichment of Biotinylated Proteins:  
Noah Smerdjo1; Ashley Frankenfield1; Haorong Li1; Jiawei Ni1; Ling Hao1;  
1Department of Chemistry, George Washington University, Washington, DC

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Screening Clones for Monoclonal Antibody Production Using Droplet Microfluidics Interfaced to Electrospray Ionization Mass Spectrometry:  
Cara I D'Amico1; Gillian E. Robbins2; iris Po2; Chao Fang2; Thomas R. Slaney1; Li Tao3; Gabi Trenml1; Brandon T. Ruotolo2; Robert T. Kennedy2;  
1Bristol Myers Squibb, Summit, NJ;  
2University of Michigan, Ann Arbor, MI;  
3Bristol Myers Squibb, New Brunswick, NJ

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RTMS: An R Toolkit for Extracting, Analyzing, and Visualizing High-Throughput MALDI Mass Spectrometry Data:  
Yamuna Rajarama1; Nathan Nelson1; Nathaniel R. Twarog1; John Bowling2; Brandon Young3; Anang A Shelat1; Zoran Rankovich1;  
1St. Jude Children's Hospital, Memphis, TN

MP 301  
High-throughput Late-stage Synthesis of Complex Bioactive Molecules by Desorption Electrospray Ionization Mass Spectrometry (DESI-MS):  
Kai-Hung Huang1; Nicolas M. Morato1; Veronica Feng1; Eric Dziekonski2; R. Graham Cooks1;  
1The University of Tokyo, Tokyo, Japan;  
2Research Science Institute, Ewing, NJ

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Multiplex analysis of bile acids using isobaric labeling with triple quadrupole mass spectrometry:  
Suzumi M Tokuoka1; Yoshiya Oda1;  
1The University of Tokyo, Tokyo, Japan

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High-throughput and low-volume analysis of native and intact protein mixtures with LAPI-MALDI MS:  
Bob Challen1; Mike Morris1; Rainer Cramer1;  
1University of Reading, Reading, United Kingdom;  
2Waters Corporation, Milwaukue, United Kingdom

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Fast Quantification of essential amino acids in plasma using LDTD-MS/MS:  
Francis Briere1; Jacques Corbeil2;  
1Centre Nutris, INAF, Universite Laval, Quebec, QC;  
2CHU de Quebec, Universite Laval, Quebec, QC

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Introducing ion mobility spectrometry for rapid LC-MS:  
Validation and its application to large scale human blood sample sets:  
Yoshiiro Kita1; Suzumi M Tokuoka1; Giorges Isaac1; Lee A Gethings1; Robert S Plumb1; Yoshiya Oda1;  
1The University of Tokyo, Tokyo, Japan

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Simultaneous Multi-Omics by Direct Infusion Mass Spectrometry (SMAD-MS):  
Yuming Jiang1; Jesse Meyer2;  
1ceders-sina medical center, Los Angeles, CA;  
2Cedars-Sinai Medical Center, Los Angeles, CA

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Snapshots of the Membrane: A high-throughput proteomic screen capturing membrane proteins in their native environment for structural and functional studies:  
Caroline Brown1; Snehasi Ghosh1; Yansheng Liu1; Moitrayee Bhattacharyya1; Kallol Gupta1;  
1Nanobiology Institute, Yale University, West Haven, Connecticut;  
2Yale School of Medicine, Department of Cell Biology, New Haven, CT;  
3Vale School of Medicine, Department of Pharmacology, New Haven, CT;  
4Cancer Biology Institute, West Haven, CT

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Incorporating Ferrimagnetic Beads to High Through Affinity Selection Mass Spectrometry:  
Jonathan Shrimp1; Nate Hoxie1; John Janiszewski1; Colin Kelly1; Matthew Hall1; Sam Michael1; Meghan Verma1; Anton Simeonov1;  
1University of Kansas, Laboratory, Heidelberg, Germany;  
2EMBL, Heidelberg, Germany;  
3Molecular Medicine Partnership Unit, Heidelberg, Germany;  
4Bio Studio, Bioinnovation Institute, Copenhagen, Denmark

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All-in-One Design and Analysis of Quantitative Studies for High Throughput Experiments:  
Richard Lee1; Nikki Dare1; Nikolay Malashchenko1; Karl Demmuns1;  
1ACD/Labs, Toronto, ON

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Fully-integrated, high-throughput, dual-stream microflow LC-MS/MS for in vitro screening bioanalysis:  
Jamie R Kirsch1; Jillian Racich1; Daria Vemikovskyava1;  
1Brendon Kapinos1; Anthony Carlo1; Wayne Lootsma1;  
2Steve Ailey1;  
3Pfizer Inc., Groton, CT;  
4Sound Analytics, Niantic, CT

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Ultra-fast Online SPE Applicable to a Wide Range of Compounds with Various Hydrophobicity for High-throughput Analysis using Multiplexed 4-channel 2D-LC-MS/MS:  
Eishi Imoto1; Toshiya Matsubara1;  
1Shimadzu Scientific Instruments, Columbia, MD

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Ultra-High-Throughput Compound Quality Control with Acoustic Emission Mass Spectrometry:  
Chang Liu1; Alandra Quinn2; Gordan1;  
1UCSF;  
2UCSD

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A Real-time Informatics Platform Enables Screening of Biologics during High-Throughput Expression:  
Xiaorong Zhai1; Behnam Keshavarz1; Sidharth Mohan1; Bo Zhao1;  
2Elsa Gorre2; Jing Li1; Andrew Mahan1;  
3Irish Nanda1; Marshall Bern1; Harsha Gunawardena1;  
4Protein Metric Inc., Cupertino, CA;  
5JOHNSON AND JOHNSON, Spring House, PA

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Coupling online buffer exchange with automated data processing for screening designed protein complexes by native mass spectrometry:  
William Resager1; Marius M Kostelic2; Vicki H Wysocki2; Marshall Bern1;  
3Protein Metrics, LLC, Cupertino, CA;  
4Ohio State University, Columbus, OH

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Rapid Identification of Changes in Small Molecules in MALDI-MSI Data:  
Yijing Wang1; David Hua1; Heather Desaire2; Amanda B Humphrey1;  
1The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH;  
2University of Kansas, Department of Chemistry, Lawrence, KS

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METASPACE-ML: A machine-learning approach for annotating metabolites and lipids in imaging mass spectrometry data:  
Bishoy W Abdelmalak1; Lachlan Stuart1;  
2Mads Ekeland1; Sergi Mamedov1; Lucas Maciel Vieira1;  
3Theodore Alexandrow1, 3, 4, 5;  
4Structural and Computational Biology Unit, European Molecular Biology Laboratory, Heidelberg, Germany;  
5EMBL, Heidelberg, Germany;  
6Metabolomics Core Facility, Heidelberg, Germany;  
7Molecular Medicine Partnership Unit, Heidelberg, Germany;  
8Bio Studio, Bioinnovation Institute, Copenhagen, Denmark

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Ion-to-image (I2I) – a new application for unique and rapid processing of mass spectrometry imaging data:  
Johan Liljala1; Kyle D. Duncan1; Ingela Lanekef1;  
2Upsala University, uppsala, Sweden;  
3Vancouver Island University, Nanaimo, BC;  
4Upsala University, Uppsala, Sweden

iFAMS Imagier: A Streamlined Gabor Deconvolution Workflow for MALDI Spectrometry Imaging, Protein Localization, and Heatmap Cross-Comparison:  
Lily E Miller1; Andrew K Swansiger1; Manxi Yang2; Julia Laskin3;  
James S Prell1, 2, 3;  
1University of Oregon, Eugene, OR;  
2Cold Spring Harbor Laboratory;  
3Cold Spring Harbor Laboratory
MP 332 Low-Rank Modeling with Sparse and Dense Residuals Enables Advanced Dimensionality Reduction for Imaging Mass Spectrometry Measurements of Human Eye Tissue: Roger A. R. Moens1; Lukasz G Migas2; David Anderson3; Christine A. Curcio4; Richard M Caprioli1,2,4,6,7; Kevin Scheyvey4; Jeffrey M Spraggins4,5,8; Raf Van De Plass1,5,4,8; Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; 2Department of Biochemistry, Vanderbilt University, Nashville, TN; 3Department of Ophthalmology and Visual Sciences, University of Alabama at Birmingham, Birmingham, AL; 4Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; 5Department of Chemistry, Vanderbilt University, Nashville, TN; 6Department of Medicine, Vanderbilt University, Nashville, TN; 7Department of Pharmacology, Vanderbilt University, Nashville, TN; 8Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN

MP 333 Enhancing Spatial Resolution in Tandem Mass Spectrometry Ion/Ion Reaction Imaging Experiments through Image Fusion using Convolutional Neural Networks: Xizheng (colin) Diao1; Zhongling Liang1; Yingchan Guo2; Boone M. Prentice1; 1University of Florida, Gainesville, FL

MP 334 A multi-modal image fusion workflow incorporating MALDI imaging mass spectrometry and microscopy for the study of small pharmaceutical compounds: Zhongling Liang1; Abhisheak Sharma2; Christopher R. McCurdy2; Boone M. Prentice1; 1University of Florida Department of Chemistry, GAINESVILLE, FL; 2College of Pharmacy, University of Florida, Gainesville, FL

MP 335 From Spectra to Molecules in Spatial Metabolomics: Data processing and metabolite annotation of AP-SMALDI-Orbitrap data using METASPACE: Dominic Dreischub2; Carolin M Morawietz2; Theodore Alexandrov2; Bernhard Spengler1,2; Kerstin Strupa1; 1TransMIT GmbH, Giessen, Germany; 2Institute of Inorganic and Analytical Chemistry, Justus Liebig University Giessen, Germany; 3European Molecular Biology Laboratory, Heidelberg, Germany; 4Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany

MP 336 A data interpretation workflow for the analysis of peptides from complex atmospheric pressure MALDI mass spectrometry histochemistry (MSHC) imaging datasets: Nivedita Bhattacharya1,2,3; Kenneth Verheggen1; Konstantin O. Nagornov1; Yuriy O. Tsybin1; Peter D. Verhaert1; 1MassTech, Columbia, MD; 2ProteoFormX, Beerse, Belgium; 3Barefeet Analytics Private Limited, Pune, India; 4SpectraTune, Olney, UK; 5AstraZeneca, Cambridge, United Kingdom; 6Imperial College, London, London, United Kingdom

MP 337 Are biological mass spectrometry imaging (MSI) studies sufficiently powered? Measurement and characterisation of uncertainty in mass spectrometry imaging experiments: Alexander Dexter1; Felicia Wirtz1; Rory Thomas Steen1; Caroline Pollard1; Lily Ellis1; Gibbings1; Stephanie Ling1; Richard J A Goodwin1; Simon T Barry1; Josephine Bunch1; 1National Physical Laboratory, Teddington, United Kingdom; 2AstraZeneca, Cambridge, United Kingdom; 3Imperial College, London, London, United Kingdom

MP 338 Innovative Software Solutions for Measuring Analyte Delocalization in MALDI Imaging: Cole C Johnson1; Dalton R Brown1; Caitlin M. Tressler1; Nathan Riemann1; Jason Fan1; Kristine Glunde2; 1Johns Hopkins School of Medicine, Baltimore, MD

MP 339 Pixel-to-pixel metabolite ratio imaging as a novel tool to advance pathway analysis in MALDI MS Imaging studies: Joshua L Fischer1; Ethan Yang1; Dawson Miller2; Steven S Gross3; Guiyi Ling1; 1Brucker Scientific, LLC, Billerica, MA; 2Weill Cornell Medicine, New York, NY; 3Cornell University Medical College, New York, NY
Advances in MALDI imaging of tryptic peptides: improved spatial resolution in mammalian tissue and first results for plant proteins; Andreas Roeppl¹; Bastian Jahres¹; Oliver Wittek²; ¹Bioanalytical Sciences and Food Analysis, University of Bayreuth, Bayreuth, Germany

Systematic optimization of the DESI-MS imaging workflow to enhance detection of endogenous small molecule metabolites; Meredith Spradlin¹,²; Livia S. Eberlin¹; ¹The University of Texas at Austin, Austin, TX; ²Baylor College of Medicine, Houston, TX

Measuring spatial resolution of different Mass Spectrometry Imaging modalities; Martin Metodiev¹,²; Rony Thomas Stevent¹; Angeliki Christakopoulou¹; Zoltan Takats³,⁴; Josephine Bunch³,⁴; INPL, Teddington, United Kingdom; ²Imperial College, London, London, United Kingdom; ³National Physical Laboratory, Teddington, United Kingdom; ⁴Rosalind Franklin Institute, Harwell, Didcot, United Kingdom

Spatialtemporal study of carbon metabolism in developing maize embryos with in vivo 13C labeling; Pubudu Niwan Perera Hapuarachchige¹; Young Jin Lee¹; ¹Towa State University, Ames, IA

Commercial ZnO NP matrix optimization for small molecule detection in rat brain by Matrix-Assisted Laser Desorption Ionization Mass Spectrometry Imaging; Juan Pablo Galindo¹; Natalie Merola¹; Kristina Juric¹; Steven R. Lavolette¹; Ken K.-C. Yeung¹; ¹Western University, London, ON

Novel reactive mass tags for the sensitive detection of steroidal ketones by MALDI MSI; Rachel S. Pryce¹; Nassim Maarouf¹; Ayyoub Selka¹; Dominique Trudel¹; Fred Saad¹; Karina Gasbarrino²; Stella S. Daskalopoulou³; William D. Lubell¹; Pierre Chaurand¹; ¹University of Montreal, Montreal, QC; ²McGill University, Montreal, Quebec

Characteristics of a new caged matrix with high vacuum stability for MALDI mass spectrometry imaging; Qiuyin Zhou¹; Stefano Rizzo²; Janina Oetjen³; Annabelle Fülop¹; Miriam Ritter¹; Hartmut Gilland¹; ¹Carsten Hopf¹,²,³; ²CeMOS - Center for Mass Spectrometry and Optical Spectroscopy, Mannheim, Germany; ³Sinnis Fine Chemicals GbR, New York City, Germany; ⁴Bruker Daltonics GmbH & Co. KG, Bremen, Germany; ⁵Bruker Bioanalytik GmbH, Bremen, Germany; ⁶Mannheim Center for Translational Neuroscience (MCTN), Medical Faculty Mannheim, Heidelberg University, Mannheim, Germany

Evaluation of a new poly-N-acetyllactosamine endo-β-galactosidase as a multi-enzyme N-glycan MALDI imaging mass spectrometry tissue workflows; Richard D Drake¹; Minyong Chen¹; Grace Grimley¹; Christopher H Taron¹; ¹Medical University of South Carolina, Charleston, SC; ²New England Biolabs, Inc., Ipswich, MA

Multi-Site Assessment of the MALDI HiPLEX-IHC Miralyx System; Kyle A Vanderheugd¹; Emily R. Sekera¹; Gargey B. Yagnik¹; Mark J. Lim¹; Kenneth J. Rothschild¹; Katherine A. Stump¹; Amandla B. Hammon¹; Erin H. Seeley¹; Elizabeth K. Neumann¹; ¹University of California, Davis, Davis, CA; ²The Ohio State University-Comprehensive Cancer Center, Columbus, OH; ³AmberGen, Inc., Billerica, MA; ⁴Bruker Scientific, LLC, Billerica, MA; ⁵University of Texas at Austin, Austin, TX; ⁶University of California Davis, Davis, CA

Unsupervised co-registration of hematoxylin and eosin (H&E) stained microscopy images and mass spectrometry images (MSI) with feature filtering; Sai Srikanth Lakkimsetty¹; Andreas Weber¹; Kylie Ariel Bemis¹; Melanie Christine Föll¹; Olga Vittek¹; ¹Northeastern University, Boston, MA; ²University of Freiburg, Freiburg, Germany

Accurate Quantitative Mass Spectrometry Imaging via Aziridine-based Isobaric Tags Reveals Temporal and Spatial Changes of Isomeric Lipids in Medulloblastoma
Mice; Xiaxin Feng; Milagros Suarez2; Dallas Freitas; Tingyuan Yang; Xi Chen; Shuli Tang; Yuhang Yang; Xiaonian Li; Yun Huang; Yuchen Du; Yin Yan; 'Department of Chemistry, Texas A&M University, College Station, TX; 'Ann & Robert H. Lurie Children’s Hospital of Chicago, Chicago, IL; Robert H. Lurie Comprehensive Cancer Center, Feinberg School of Medicine, Chicago, IL; Center for Epigenetics & Disease Prevention, Texas A&M Institute of Biosciences and Technology, Houston, TX

MP 362 On-Tissue Derivatization for enhanced Carbohydrates and Steroids detection in Bombus Impatiens Bee via MALDI mass spectrometry; Nilay Saha; Andrew Goodenough; Taylor Hackett; Franco Basile; University of Wyoming, Laramie, WY

MP 363 Optimization of embedding media for MALDI-mass spectrometry imaging of frozen tissue; Ching-Yuan Yang; Yatata Shii; Yuan Liu; Lingjun Li; Department of Chemistry, University of Wisconsin-Madison, Madison, WI; School of Pharmacy, University of Wisconsin-Madison, Madison, WI

MP 364 Spatial single-cell multilomics using dual cluster ion beams secondary ion mass spectrometry (SIMS) imaging reveals 3D multilevel heterogeneities in liver; Hua Tian; University of Pittsburgh, Pittsburgh, PA

MP 365 Unified and standardized mass spectrometry data processing in Python using spectrum_ultis; Wout Bittremieux;Lie Levitsky; Maleo Pilz; Timo Sachsenberg; Florian Huber; Mingxun Wang; Pieter C Dorrestein; University of Antwerp, Antwerpen, Belgium; Moscow institute of physics and technology, Moscow, Russia; University of Tübingen, Tübingen, Germany; Hochschule Düsseldorf, Düsseldorf, Germany; University of California Riverside, Riverside, CA; University of California San Diego, San Diego, CA

MP 366 Improved identification of isomers using the High Dimensional Consensus Mass Spectral similarity algorithm; Deborah F McGlynn; Jason Evelth; Nirina Rabe Andriamiharavo; Anthony Kearsley; National Institute for Standards and Technology, Gaithersburg, MD; Brown University, Providence, RI

MP 367 Novel DNN-powered quadruplet isolation profile analysis algorithm for improved speed, measurement robustness, and quality control; Adrian Schütz; Amelie Peterson; Bastian Reitemeier; Bernd Hagendorf; Thermo Fisher Scientific, Bremen, Germany

MP 368 High-throughput plasma proteomics to identify diabetes associated protein biomarkers and pQTLs; Harendra Guturu; Guhan Venkataraman; Amir Alavi; Ryan Benner; Khris.Proppe; Northwestern University, Chicago, IL; National Institute of Diabetes and Digestive and Kidney Diseases, Bethesda, MD; National Institute of Biomedical Imaging and Bioengineering, NIH, Bethesda, MD

MP 369 Crema: an open-source Python tool for target-decoy false discovery rate estimation; Andy Lin; Donovan See; Uri Reich; William E Fordrie; William Stafford; Pacific Northwest National Laboratory, Seattle, WA; University of Washington, Seattle, WA; University of Sydney, Sydney, Australia; Talus Bioscience, Seattle, WA

MP 370 An automated computational pipeline for retention time alignment across LC systems; Ian Reath; Scott Trinkle; Ryan P Marchand; Chris Preston; Ian Morris; Richard Chapman; Paul Fitch; Waters Corporation, Newcastle upon Tyne, United Kingdom; Waters Corporation, Milford, MA

MP 371 Statistical analysis of tandem mass spectra; Felix Servant; Alexandre Giuliani; Laurent Nahon; Synchrotron SOLEIL, L'Orme des Merisiers, Départementale 128, 91190 Saint-Aubin, France, Saint-Aubin, France; INRAE, UAR1008, Transform Department, Rue de la Géraudière, BP 71627, 44316 Nantes, France, Nantes, France

MP 372 Relative Probabilities of Library Search: A Comprehensive analysis of NIST/EPA/NIH EI and Tandem Libraries; Adva Baratz; Stephen E Stein; Israel Institute for Biological Research, Ness-Ziona, Israel; NIST, Gaithersburg, MD

MP 373 Enhancing compound identification workflows with a novel library manager software application; Elizabeth Alvare; Emma E Rennie; James P Pyke; Tristan Chutka; Andrew McEachran; Agilent Technologies, Santa Clara, CA

MP 374 Sin.R: A SAINT-like AP-MS protein-interaction score implemented in R; Manor Askenazi; Beatrix Ueberheide; Jackeline Ponce; Biomedical Hosting LLC, Arlington, MA; NYU Langone Health, New York, NY

MP 375 MetaprobeDec: a novel algorithm to appraise the quantitative composition of a microbiome based upon metaproteome; Jiahua Mu; Hongkai Xu; Yuxing Zhang; Yamei Deng; Da Qi; Siqi Liu; College of Life Sciences, University of Chinese Academy of Sciences, Beijing, China; Center of Proteomic Analysis, BGI Life Science Research Institute, Shenzhen, China

MP 376 How well did you peak that ion? Finn but with PeptidePrisoner!; Luis Mendoza; Michael R. Hoopmann; Eric W. Deutsch; Robert L. Moritz; Institute For Systems Biology, Seattle, WA; Institute for Systems Biology, Seattle, WA

MP 377 SARS-CoV-2 Spike Protein Post Translational Modification Landscape and its Impact on ProteinStructure and Function using MetaPep; Shaojun Tang; Hong Kong Center for Neurodegenerative Diseases, Hong Kong, China

MP 378 Optimal transport-based LC-MS alignment algorithm; Stanislaw Jan Grodzki; Justyna Paulina Krol; Michael Piotr Startek; Anna Barbara Gambin; Faculty of Mathematics, Informatics, and Mechanics, University of Warsaw, Warsaw, Poland; Institute for Immunology, University Medical Center of the Johannes-Gutenberg University Mainz, Mainz, Germany

MP 379 Tripler for Data Independent Acquisition Data; Patrick Truong; Matthew The; Lukas Kall; Royal Institute of Technology, Stockholm, Sweden; Technical University of Munich, Freising, Germany

MP 380 Estimating relative quantities of analytes using computational optimal transport; Michal A. Ciach; Barbara Domżal; Michal Piotr Startek; Grzegorz Skoraczyński; Dirk Valkenborg; Blażej Miasojedow; Anna Barbara Gambin; Faculty of Mathematics, Informatics, and Mechanics, University of Warsaw, Warsaw, Poland; Hasselt University - DSI, Hasselt, Belgium; Institute for Immunology, University Medical Center of the Johannes-Gutenberg University Mainz, Mainz, Germany

MP 381 MassLite: An Integrated Python Platform for Single Cell Mass Spectrometry Data Pretreatment; Zhu Zou; Zhibo Yang; Department of Chemistry and Biochemistry, University of Oklahoma, Norman, OK

MP 382 Spectrum Averaging Algorithms for Increasing Mass Accuracy and Signal-To-Noise for Poorly Resolved and Low Abundance Peaks in Top-Down Proteomics; Nicholas E. Bollis; Austin V. Carr; Claire Boos; Lloyd M Smith; University of Wisconsin-Madison, Department of Chemistry, Madison, WI

MP 383 GlycoNetwork: A software for relating glycan expression with glycoenzyme activity; Xavier A Holmes; Michael Russell S Alvarez; Armin Olumi; Erin K. Morissette; Carlito B. Lebrilla; University of California Davis, Davis, CA

MP 384 Sensitivity analysis of isotope ratio measurements by MC-ICP-MS; Piotr Radzinski; Jakub Karasinski; Andril Tupys; Michal Piotr Startek; Anna Barbara Gambin; University of Warsaw, Warsaw, Poland; University Medical Center of the Johannes-Gutenberg University Mainz, Mainz, Germany

MP 385 FTMStruct: a multi-source network traversal strategy to annotate lignin structure; Rongjun Gao; Jibao Liu; Qinglong Fu; Eunsang Kwon; Manabu Fujii; Tokyo
MONDAY POSTERS

MP 413 Chemical Transformations can Occur during DMS Separations: Lessons Learned from Beer’s Bittering Components; Christian Ierianto; Alexander Haack; Scott Hopkins; University of Waterloo, Waterloo, ON

MP 414 Rapid Separation and Quantitation of Δ8/Δ9-THC and other isobaric cannabinoids by Differential Mobility Spectrometry; Christian Ierianto; Patrick Thomas; Scott Hopkins; University of Waterloo, Waterloo, ON

MP 415 Exploring Isomer Separations and Structurally Specific Isotopic Shifts Using Next-Generation FAIMS Stages with Novel Buffers and Metal Cationization; Hayden A Thuman; Pratima Pathak; Gordon Anderson; Alexandre A Shvartsburg; Wichita State University, Wichita, KS; 2GAA Custom Electronics, LLC, Kennewick, Washington

MP 416 Orbitrap mass spectrometry and high-field asymmetric waveform ion mobility (FAIMS) enable in-depth, quantitative analysis of proteoforms <30 kDa; Jake Kline; Michael W Bellford; Cornelia L Boeser; Jingjing Huang; David Bergen; Kenneth R Durbin; Joseph B Greer; Graeme C McAlisterr; Christopher Mullen; Vlad Zarubsovskiy2; Luca Fornelli; University of Oklahoma, Norman, OK; 2Thermo Scientific, San Jose, CA; 3Proteinacious, Evanston, IL

MP 417 Exploring protein N-glycosylation alterations between wild-type and mutant forms of Irisin, Sayantani Chatterjee; Joshua A. Klein; Mu A1; Chuiyang Zhang; Bruce M. Spiegelman1, 4, Joseph Zaia1, 2; Department of Biochemistry, Center for Biomedical Mass Spectrometry, Boston University Chobanian & Avedisian School of Medicine, Boston, MA; 2Bioinformatics Program, Boston University, Boston, MA; 3Dana-Farber Cancer Institute, Boston, MA; 4Harvard Medical School, Boston, MA

MP 418 The development of new methods for formation, separation, detection, and identification of proteomers using differential mobility spectrometry and mass spectrometry; Andrew Finlay1; Allyson G. Yee1; Wojciech Gabryelski1; W. Scott Hopkins1; University of Guelph, Guelph, ON; University of Waterloo, Waterloo, ON

MP 419 Exploring FAIMS gas flow settings for optimal detection of post-translational modification using LC-MS/MS; Rosalie Chu1, 2; Chia-Feng Tsai1; Karl K Weltz1; Marina A Gritsenko1; Ronald J Moore1; Tao Liu1; Pacific Northwest National Laboratory, Richland, WA

MP 420 Improving Solvent Vapor Modification Through Ultrasonic Nebulization: Protic, Aromatic, and Nonclustering Solvent Systems for Isomeric Opioid Analysis with FAIMS-MS; Nathan a Grimes1; David Garibault1; Therese Evans Nguyen1; University of South Florida, Tampa, FL

MP 421 An Automated Workflow for the Quantification of 8-Different Antidepressants using LC-MS/MS; Ramisa Farih1; Oluwanifemi D Okoh1; Emma Rothkopf1; Adam Spooner1; Anubhav Tripathi1; Brown University, Providence, RI

MP 422 Challenges with the Bioanalysis of Phosphate Prodrugs and their Active Pharmaceutical Ingredients; Kasie Fang1; Timothy Sikorski1; Zhuo Chen1; Clara Andonian1; Hermes Licea-Perez1; GSK, Collegeville, PA

MP 423 Fully automated and integrated 96-channel proteomics sample preparation platform applied for high-throughput drug target identification; Ruijuan Tian; Southern University of Science and Technology, Shenzhen, China

MP 424 Chemical derivatization combined with supercritical fluid chromatography to improve the resolution of stereoisomers; Hermes Licea-Perez; Bioanalysis / GSK, Collegeville, PA

MP 425 In-line Derivatization of Fatty Acids for LC-ESI-MS/MS Identification; Anthony J Fanizza; Northern Illinois University (NIU), DeKalb, IL

MP 426 NRicher®: A Singular Low Abundance Proteome Enrichment Product Combines 6 Different Surface Features And Seamless Integration With On-Bead Digestion; Matt Kuruc1; Haiyan Zheng2; Amenah Soherwardy3; Swapan Roy1; Biotech Support Group LLC, Monmouth Junction, NJ; 2Rutgers University, New Brunswick, NJ

MP 427 Modular, scalable and automateable on-bead pipeline for bottom-up proteome and phosphoproteome profiling with built-in peptide and phosphopeptide fractionation; Previn Naicker1; Claire Koenig2; Ana Martinez Del Val2; Sipho Mamputha1; Sindiwse Buthelezi1; Ireshyn S Govender1, 3; Isak Gerber1, 3; Justin Jordaan1; Stoyan Stoychev1; Jesper Velgaard Olsen1; CSIR, Pretoria, South Africa; 2Novo Nordisk Foundation Center for Protein Research, Copenhagen, Denmark; 3ReSyn Biosciences, Pretoria, South Africa

MP 428 Miniaturization Strategies for Streamlined Drugs of Abuse Extraction prior to UHPLC-MS/MS Analysis; Charlotte Hayes1; Alan Edgington1; Thomas Smith1; Lee Williams1; Adam Senior1; Helen Lodder1; Russell Parry1; Lucy Lund1; Zainab Khin1; Brett Davies1; Claire Desbrow2; Dan Menasco1; Biogeom Limited, Cardiff, United Kingdom

MP 429 On-Column Digest Followed By SPE Desalting For Rapid And Simplified Sample Processing Without Sample Transfer; Heather Eastwood1; John D Laycock1; Manuel Bauer2; Fabian Wendt1; Qi Huang1; Shang Tsai1; Tecan, Baldwin Park, CA; 2Tecan, Männedorf, Switzerland

MP 430 Optimisation of sample preparation for the analysis of β-Methylamino-L-alanine in complex matrices; Siobhan J Peters1; Kenneth J Rogers1; Simon M Mitrovic1; David P Bishop1; UTS, Ultimo, Australia

MP 431 Determination of vedaprofen in livestock and fishery products using liquid chromatography-tandem mass spectrometry; Bohyun Shini1; Chehee Jeong1; Sang Beom Han1; Department of Pharmaceutical Analysis, College of Pharmacy, Chung-Ang University, Seoul, South Korea

MP 432 Comparison between trypsin digestion and weak acid hydrolysis for characterization of various proteins using nanoLC-MS/MS; Hyojin Hwang1; Dokyung Kwon1; Jeongwon Kim1; Chungnam National University, Daejeon, South Korea

MP 433 Sample preparation-related technical variability of proteomic workflows incorporating multiplexed isotopic labeling and LC-MS/MS analysis; Carly A. I. Twigg1; Stefani N. Thomas1; Department of Laboratory Medicine and Pathology, University of Minnesota, Minneapolis, MN

MP 434 Bottom-Up Proteomic Workflows for Low Cell Input Samples in a Core Facility Setting; Jennifer Roof1; Hossein Fazelinia1, 2; Asif Amin Dar2; Hua C Ding2; Lynn A Spruce1; CHOP-Penn Proteomics Core, Philadelphia, Pennsylvania; 2Department of Biomedical and Health Informatics, Children's Hospital of Philadelphia, Philadelphia, Pennsylvania; Children's hospital of Philadelphia, Philadelphia, Pennsylvania

MP 435 A novel two-cycle immunoffinity enrichment strategy to enhance assay sensitivity of biotherapeutics in tissues; Yipei Zhang1; Mark G. Qian1; Linlin Dong1; Takeda Development Center Americas, Cambridge, MA

MP 436 Identification of Low-Abundance Proteins in Biological Samples Using a Bottom-Up Approach on the ProTrap XK; Victoria A Miller1; Sara Lahsaei Little1; Jessica L Nickerson1; Angela Giraldo2; Jean-François Noé3; Jean-Philippe Couture2; Hugo Gagnon2; Alliumqs Corporation, Halifax, NS; 3PhenoSwitch Biosciences Inc., Sherbrooke, QC

MP 437 AutoPrep: fully automated, lossless proteomics sample preparation from lysate to protein concentration to contaminant-free, analysis-ready peptides - elute and shoot; John D Laycock1; Heather Eastwood1; Shang Tsai1; Manuel Bauer2; Fabian Wendt3; John Wilson3; Tecan, Baldwin Park, CA; 2Tecan, Männedorf, Switzerland; 3ProFi, LLC, Farmingdale, NY
MONDAY POSTERS

MP 438 Determination of atorvastatin calcium in human urine using LC-MS/MS; Jie-ni Wang1; He-Hsuan Hsiao2; 1Department of Chemistry, National Chung Hsing University, Taichung, Taiwan

MP 439 Normalizing MS Data: Extracted Lipids from Latent Fingerprints; Alessia E Chua1; Leah Pfeifer2; Heather Desaire3; 1University of Kansas, Lawrence, KS

MP 440 High-throughput method combining mass spectrometry and machine learning for analysis of fingerprint lipids for biomarker discovery; Madeline Isom1; Leah Pfeifer1; Eden Go1; Heather Desaire3; 1University of Kansas, Lawrence, KS

MP 441 Lipidomic and Proteomic Plasma Evaluations Reveal Biomarkers for the Diagnosis of Domic Acid Toxicosis in California Sea Lions; Amie M. Solosky1; Iliana M. Claudio2; Kaylie I. Kirkwood2; Rebecca L Beres1; Michael G. Janech2; Frances M.D. Guillard3; Benjamin A. Neely3; Erin S. Baker3; 1University of North Carolina Chapel Hill, Chapel Hill, NC; 2Department of Chemistry, North Carolina State University, Raleigh, NC; 3Department of Biology, College of Charleston, Charleston, SC; 4Wildlife Health Center, School of Veterinary Medicine, University of California, Davis, Davis, California; 5Chemical Sciences Division, National Institute of Standards and Technology, Charleston, SC; 6Department of Chemistry, University of North Carolina at Chapel Hill, Chapel Hill, NC

MP 442 Detailed kinetic measurements provide insights into competing fatty acyl chain loss from glycerophospholipid anions: why sn-2 loss is faster; Samantha A Mehner1; Kimberly C Fabijanczuk2; De'shovon M Shenault1; Scott A Mcluckey2; 1Purdue University, West Lafayette, IN

MP 443 Development of an offline 2D-LC lipidomics method; Fernando M Quintero1; Adriana Zarzini Buzzato2; Liang Li1,2; 1University of Alberta, Edmonton, AB; 2The Metabolomics Innovation Centre (TMIC), Edmonton, Alberta

MP 444 Development of automated MS/MS methods on an Orbitrap Fusion™ and a spectral database for in-depth lipidomic analysis of human plasma; Vincent Marie1; Benoît Colson1; François Fenaille1; 1Université Paris-Saclay, CE2, UMR 8225, Département Médicaments et Technologies pour la Santé (DMTS), MetaboHUB, Gif sur Yvette, France

MP 445 An Efficient Monophasic Extraction Method for High-Throughput Bacterial Lipidomics; Kingsley Bimpoh1; Kelly M Hines1; 1University of Georgia, Athens, GA

MP 446 Establishing an LC-HRMS workflow for targeted and untargeted lipidomic analyses; Rachel Harris1; Heidi Vitrac2; Michelle English1; James Atwood1; 1MOBILion Systems, Inc., Chadds Ford, PA

MP 447 Analysis of Lipids by Contained Electrospray Mass spectrometry with Online Fractionation using a Syringe-Based Solid Phase Extraction; Octavian Spears1; Benjamin J Burris2; Abraham Kwame Badu-Tawiah1; 1The Ohio State University, columbus, OH; 2agriculture and food, columbus, Ohio; 3The Ohio State University, Columbus, OH

MP 448 Electrospray ionization forms alkylated ammonium species that interfere with lipidomics analyses; Joshua A Roberts1; Aleksandra Bushueva1; Meaghan Harley1; Karl V Wasslen1; Jeffrey C Smith1; 1Carleton University, Ontario, Canada

MP 449 Functional role of ecysteostidens in awake and sleeping honey bee foragers; Deepika Bais1,2; Ohhaya Patole2; Susanne Neupert1; Axel Brockmann1; 1University of Kassel, Kassel, Germany; 2National Centre for Biological Sciences, Bengaluru, India

MP 450 Investigation of In situ Lipids from EAE Mouse Brain Tissue using Mass Spectrometry Imaging; Rawan Serana Kassim1; Krista Berlin2; Stephan B. Bach2; Thomas G. Forshuber1; 1University of Texas at San Antonio, San Antonio, TX; 2University of Texas at San Antonio, San Antonio, TX

MP 451 Untargeted lipidomics of the Gemmae obscuriglobus bacterium under sterol synthesis inhibition conditions; Franco Basile1; Shelby Wakefield1; Mitchell Helling1; Seifeddine Ben Tekaya1; Naomi Ward2; 1University of Wyoming, Laramie, WY; 2Colorado State University, Fort Collins, CO

MP 452 Identification of Complex Triacylglycerols in Mouse Epididymal Adipose Tissue Using Ultra-performance Convergence Chromatography-Mass Spectrometry; Yu-Ju Shih1; Mei-Ling Cheng1; 1Chang Gung University, Taoyuan, Taiwan

MP 453 Fingerprinting the Unique Lipidome of Membrane Proteins Using Liquid Chromatography, Ion Mobility Spectrometry and Mass Spectrometry; Jack P. Ryan1; Yun Zhu2; Melanie T. Odenkirk3; Arthur Laganowsky1; Erin S. Baker3; 1University of North Carolina at Chapel Hill, Chapel Hill, NC; 2Texas A&M University, College Station, TX; 3University of Texas at San Antonio, San Antonio, TX

MP 454 Automation of lipid extraction with Hamilton Vantage system; Weng Wong1; James Joubert1; Jay Leone1; Peter Liu2; Wendy Sandoval2; Qingling Li1; 1Genentech, South San Francisco, CA

MP 455 Omega-6 Fatty Acid Oxidative Metabolism in Inflamed Dental Pulp, Grace M Sørensen1; Ken M Hargreaves2; Qun Liu2; 1Stephan BH Bach1; 2Faculty of Medicine, University of Texas Health San Antonio, San Antonio, TX; 2University of Texas San Antonio, San Antonio, TX

MP 456 Chemical and Physical Separation of Singly and Doubly Charged Lipids Within the Mass Spectrometer; Kimberly Fabijanczuk1; James W. Hager1; Scott A. Mcluckey2; 1Purdue University, West Lafayette, IN; 2SCIEX, Concord, ON

MP 457 Using Lipid Exchange-Mass Spectrometry (LX-MS) to Uncover the Preferred Lipid Environment Surrounding Membrane Proteins; Melanie Odenkirk1; Guozhi Zhang1; Michael T Marty1; 1University of Arizona, Tucson, AZ

MP 458 Dual Metal Electrolysis Using a Theta Capillary for Lipid Analysis; Annessa Sengupta1; Madison Edwins1; Xin Yan1; 1Department of Chemistry, Texas A&M University, College Station, TX

MP 459 4D Analysis of Lipid Nanoparticles (LNP) Component using Elute-timsTOF Pro 2 with VIP-HESI Source; Beixi Wang1; Xuejun Peng2; Surendar Tadi1; Erica Forsberg2; 1Bruker Scientific, San Jose, CA; 2Bruker Scientific, Billerica, MA

MP 460 Discovery lipidomics workflow to maximize lipid identifications; Vanessa Linke1,2,3; Agnieszka Chacińska1,2; Joshua J. Coon1; 1Laboratory of Mitochondrial Biogenesis, IMol Polish Academy of Sciences, Warsaw, Poland; 2ReMedy International Research Agenda Unit, IMol Polish Academy of Sciences, Warsaw, Poland; 3Department of Chemistry, University of Wisconsin-Madison, Madison, WI

MP 461 LIPID MAPS classifier: Machine learning approach for the prediction of the lipid class using the theoretical aggregated isotope distribution; Annelies Agten1; Heiko Neuweger1; Dirk Valkenborg1; 1Hasselt University - DSI, Hasselt, Belgium; 2Bruker Daltonik GmbH, Bremen, Germany

MP 462 Comparative lipidomic analysis of green algae Chlorella sorokiniana under nutritional stresses; Hector Najera-Gonzalez1; Claudio Cessar Barrera-Duarte1; Luis R. Herrera-Estrella1; Damar Lopez-Arredondo1; 1Texas Tech University, Lubbock, Texas

MP 463 High Confidence Targeted Data Mining of Untargeted High-Resolution Data for Lipids, Shereh Banu Mohsin1; Mark Rartain1; Daniel Cuthbertson1; 1Agilent Technologies, Wood Dale, IL; 2Agilent Technologies, Santa Clara, CA
MONDAY POSTERS

MP 464 Cellular Lipidomics with C=C Specificity Enabled by Aziridination; Venush Pondaevdya; Xin Yan; Texas A&M University, College Station, TX

MP 465 Aziridination-assisted mass spectrometry for nonpolar lipid analysis with isomer resolution; Enri Hitzel; Mandison E Edwards; Dallas Freitas; Xin Yan; Texas A&M University, College Station, TX

MP 466 Structural Characterization and Accurate Relative Quantitation of Unsaturated Lipid Isomers Enabled by Aziridination; Xin Yan; Tingyuan Yang; Shuli Tang; Texas A&M University, College Station, TX

MP 467 Pigment profiles in microalgae extracts by electron-transfer MALDI: the analyzer's influence; Luis Miguel Diaz; Martha L. Chacón-Patiño; Chad R. Weisbrod; Cristian Blanco-Tirado; Marianny Y. Combariza; Universidad Industrial de Santander, Bucaramanga, Colombia; National High Magnetic Field Laboratory, Tallahassee, FL; Marine and Coastal Research Institute, Santa Marta, Colombia

MP 472 Novel MALDI-TOF screening workflow for rapid detection of host response to SARS-CoV-2; Ryan Walsh; Greg Ourednik; Les Edinboro; SpectraPass, Las Vegas, NV

MP 473 MALDI-MS for the analysis of cultural heritage materials; Signe Vahuri; Anu Teearu; University of Tartu, Institute of Chemistry, Tartu, Estonia

MP 474 Improvements in Tissue Mimetic Models Using Gelatin Reinforcement and Sprayed Standards; Andrew Bowman; Junhai Yang; David S. Wagner; AbbVie, Inc., North Chicago, IL; AbbVie Inc., North Chicago, IL

MP 475 Investigating the effect of protein 3D structure on MALDI when fitted to a modified DESI source; Jeff Brown; Emrys Jones; Michael Morris; Rainer Cramer; Waters Corporation, Wilmslow, United Kingdom; University of Reading, Reading, United Kingdom

MP 476 Development of a SALDI-MS approach for the specific and sensitive detection of biomolecules: focus on Alzheimer’s disease biomarkers; Kristina Kamp, Marius Pou, Mustizze; Yannick Coffinier; Christine Jenabali; Claudia Bich; University Montpellier, CNRS, ENSCM, IBMM, UMR5247, Montpellier, France; Univers Lille, CNRS, UMR8520, IEMN, Lille, France

MP 477 Linking MALDI-FT-ICR phytoplankton pigment profiles with community taxonomy in a marine ecosystem; Luis M. Diaz-Sánchez; Martha L. Chacón-Patiño; Chad R. Weisbrod; Julian Franco; Janet Vivas; Cristian Blanco-Tirado; Marianny Y. Combariza; Universidad Industrial de Santander, Bucaramanga, Colombia; National High Magnetic Field Laboratory, Tallahassee, FL; Marine and Coastal Research Institute, Santa Marta, Colombia

MP 478 Optimization of MALDI-MSI for spatial visualization of key metabolites in different sorghum root architectures; Robert K. Stanley; Ryan Park; Sanofi, Boston, MA; Robert K. Stanley; Ryan Park; Sanofi, Boston, MA

MP 479 Optimization of MALDI-MSI for spatial visualization of key metabolites in different sorghum root architectures; Robert K. Stanley; Ryan Park; Sanofi, Boston, MA; Robert K. Stanley; Ryan Park; Sanofi, Boston, MA

MP 480 Accurate mass calibration method for a target protein in the linear-mode of MALDI-TOF MS analysis; Saeevung Lee; Joon Park; Seung-won Kim; Won Suk Yang; Je-Hyun Baek; R&D Center for Clinical Mass Spectrometry, Seegene Medical Foundation, Seoul, South Korea

MP 481 Optimization of MALDI-TOF MS Analysis for Large Molecules by a Graphene-Coated Silicon Wafer Plate; Yoon Kyung Chol; Dong Huey Cheong; Heejung Jiang; Won Suk Yang; Je-Hyun Baek; R&D Center for Clinical Mass Spectrometry, Seegene Medical Foundation, Seoul, South Korea

MP 482 Peptides Decorated C18-StageTip for the Detection of As3+ in Environmental Water with MALDI-MS; Hua-Yun He; He-Hsuan Hsiao; Department of Chemistry, National Chung Hsing University, Taichung, Taiwan

MP 483 Development of a SALDI-MS approach for the specific and sensitive detection of biomolecules: focus on Alzheimer’s disease biomarkers; Kristina Kamp, Marius Pou, Mustizze; Yannick Coffinier; Christine Jenabali; Claudia Bich; University Montpellier, CNRS, ENSCM, IBMM, UMR5247, Montpellier, France; Univers Lille, CNRS, UMR8520, IEMN, Lille, France

MP 484 Enhanced Performance of MALDI-TOF MS Analysis for Large Molecules by a Graphene-Coated Silicon Wafer Plate; Yoon Kyung Chol; Dong Huey Cheong; Heejung Jiang; Won Suk Yang; Je-Hyun Baek; R&D Center for Clinical Mass Spectrometry, Seegene Medical Foundation, Seoul, South Korea

MP 485 Accurate mass calibration method for a target protein in the linear-mode of MALDI-TOF MS analysis; Saeevung Lee; Joon Park; Seung-won Kim; Won Suk Yang; Je-Hyun Baek; R&D Center for Clinical Mass Spectrometry, Seegene Medical Foundation, Seoul, South Korea

MP 486 Vapour deposition coated and recrystallised 9-aminocaridine method optimisation for MALDI MSI; Hugo Delattry; Ariadna Gonzalez; Chelsea Nikula; Lakshmi Nimishakavi; Daniel O’Connor; Melanie Bailey; Josephine Bunch; Ron Steven; National Physical Laboratory, Teddington, United Kingdom; Sanofi, Boston, MA; University of Surrey, Guildford, United Kingdom; Imperial College, London, London, United Kingdom

MP 487 Mobile ESI Sprayer Head for Matrix Application and On-Tissue Derivatization in MALDI-MSI; Andrew E Paulson; Evan A Larson; Young Jin Lee; Iowa State University, Ames, IA

MP 488 Optimization of small molecule MSI by delipidation, derivatization, and instrument tuning; Lisa Ficaro; Yik Siu; Mark Alu; Cynthia Loomis; Drew R. Jones; NYU Langone Health, New York, NY

MP 489 Spatial Distribution of Pentacystic Triterpenes in Cerecpia spp roots using MALDI Imaging Mass Spectrometry; Juan E. León-Jaimes; Luis M. Diaz-Sánchez; Guillermo Montoya; Cristian Blanco-Tirado; Marianny Y. Combariza; Universidad Industrial de Santander, Bucaramanga, Colombia; Universidad Icesi, Cali, Colombia

MP 490 Optimization of MALDI-MSI for spatial visualization of key metabolites in different sorghum root architectures; Robert K. Stanley; Ryan Park; Sanofi, Boston, MA; Robert K. Stanley; Ryan Park; Sanofi, Boston, MA

MP 491 Optimization of MALDI-MSI for spatial visualization of key metabolites in different sorghum root architectures; Robert K. Stanley; Ryan Park; Sanofi, Boston, MA; Robert K. Stanley; Ryan Park; Sanofi, Boston, MA

MP 492 Spatial Distribution of Pentacyclic Triterpenes in Cerecpia spp roots using MALDI Imaging Mass Spectrometry; Juan E. León-Jaimes; Luis M. Diaz-Sánchez; Guillermo Montoya; Cristian Blanco-Tirado; Marianny Y. Combariza; Universidad Industrial de Santander, Bucaramanga, Colombia; Universidad Icesi, Cali, Colombia

MP 493 Optimization of small molecule MSI by delipidation, derivatization, and instrument tuning; Lisa Ficaro; Yik Siu; Mark Alu; Cynthia Loomis; Drew R. Jones; NYU Langone Health, New York, NY

MP 494 Spatial Distribution of Pentacyclic Triterpenes in Cerecpia spp roots using MALDI Imaging Mass Spectrometry; Juan E. León-Jaimes; Luis M. Diaz-Sánchez; Guillermo Montoya; Cristian Blanco-Tirado; Marianny Y. Combariza; Universidad Industrial de Santander, Bucaramanga, Colombia; Universidad Icesi, Cali, Colombia

MP 495 Optimization of small molecule MSI by delipidation, derivatization, and instrument tuning; Lisa Ficaro; Yik Siu; Mark Alu; Cynthia Loomis; Drew R. Jones; NYU Langone Health, New York, NY
Northwest National Laboratory, Richland, WA; University of Arizona, Tuscon, Arizona; Lawrence Berkeley Laboratory, University of California, Berkeley, CA

MP 491 Automated well-to-well MALDI spotting and analysis using lower cost robotics and custom 3D-printed hardware: Sadie P. Schultz1; Garrett C. McFadden1; Matthew M. Champion1; University of Notre Dame, Notre Dame, IN

MP 492 MALDI-TOF Mass Spectrometry: A tool for characterization of CBD Oils; Les Edinboro1; Greg Ourendnik1; Ryan Walsh1; SpectraPass, Las Vegas, NV

MP 493 Supraphysiological intravenous vitamin C administration promotes fatty acid β-oxidation and energy metabolism in humans; Philenroza Thavrin1; Jaewoo Choi1; Ping Chen2; Qi Chen2; Jeanne Dirisko3; Jan F. Stevens1; Oregon State University, Corvallis, OR; University of Kansas Medical Center, Kansas City, KS

MP 494 Doo Dots: An investigational platform for performing Dried Fecal Spot (DFS)-based bioanalysis; Thomas D Horvath1; Melissa A. England1; Donald Chance2; Texas Children’s Hospital - Microbiome Center, Houston, TX; Medical University of South Carolina, Charleston, SC; Capitainer, Stockholm, Sweden

MP 495 A decision tree for diagnosing and phenotyping polycystic ovarian syndrome based on serum metabolic fingerprints; Ruimin Wang1; Lin Huang2; Kun Qian1; SJTU, Shanghai, China; Shanghai Chest Hospital, Shanghai, China

Clinical MS in practice: bias removal and research results in the multicentre SAPhIRE statin metabolism clinical trial; Eugene Goh1; Lie Hang Wu2; Leroy SPakkin2; E Shyong Tai3; Jack Wei Chieh Tan3; Chester L. Drum1; NUS, SINGAPORE, Singapore; National University of Singapore, Singapore, Singapore

Metabolic Phenotypes Reflect Patient Sex and Injury Status: A Cross-Sectional Analysis: Hope D Wellhaven1; Avery H Wellfey1; Prayag Pershad1; James Satalich1; Alexander C Vap2; Brian Bothe1; Ron K June1; Montana State University, Bozeman, MT; Virginia Commonwealth University, Richmond, VA

Quantitative analysis of omega fatty acids in human serum using Gas Chromatograph Mass Spectrometer: Dr. Aseem Wadde1; Prashant Hase1; Bhaumik Trivedi1; Sanket Chipunkar2; Durvesh Sawant2; Rahul Dwivedi2; Hemant Kesarkar2; Dheeraj Handique1; Dr. Pratap Rasam1; Dr. Jitendra Kelkar1; Shimadzu Analytical India Pvt. Ltd., Mumbai, India

Highly standardized metabolomic analysis of clinical samples using triple quadruple mass spectrometry: Chandrashhekar Honrado1; Masoumeh Dorrani1; Jifang Zhao1; Chen Dong1; Alessia Trimigno1; Keri Sheehan1; Elizabeth O’Day1; Jurre Kamphorst1; Olaris Inc, Framingham, MA

Five-hour bloodstream pathogen identification and antibiotic susceptibility testing using microbial metabolism directly from positive blood bottles with minimal sample preparation: Thomas Rydzak1; Ryan A Groves1; Railed Aburashed1; Maryam Mapar1; Ian A Lewis1; University of Calgary, Calgary, AB

Plasma Metabolomic Profiling for Diagnosis and Differentiation of Different Types of Cholestasis Diseases; Juliana Magalhães De Oliveira1; Martin Forbes2; Thais de Assis Lopes3; Alex Aparecido Rossini Silva4; Julianna Goldbaum Crescente4; Michelle Harriz Braga4; Andriá de Melo Porcari4; Stefan Kempa5; Eduardo Luiz Rachid Cançado1; Regina Vincenzi Oliveira1; Federal University of São Carlos, São Paulo, Brazil; Max Delbrück Center for Molecular Medicine in the Helmholtz Association, Berlin Institute for Medical Systems Biology, Berlin, Germany; University School of Medicine, Tokyo, Japan; Department of Pediatrics and Adolescent Medicine, Comprehensive Center for Pediatrics, Medical University of Vienna, Austria

Multi-class assessment of chemical exposure in dried blood spots: a pilot study; Vinicius Verri Hernandez1, 2; Maximilian Zeyda1; Lukas Wisiolli2; Benedikt Warth1;Faculty of Chemistry, Department of Food Chemistry and Toxicology, University of Vienna, Währinger Straße 38, 1090, Austria; Expose Austria, Research Infrastructure and National EIREN Hub, Vienna, Austria; Department of Pediatrics and Adolescent Medicine, Comprehensive Center for Pediatrics, Medical University of Vienna, Austria

Direct Probe Ionisation Mass Spectrometry applied to biomarker discovery in pancreatic cancer; Neil Lotus1; Alan Barnes1; Emily G Armitage1; Elon Correa1; Lynne Howells2; Sén Takeda2; Wen Chung1; Shimadzu Corporation, Manchester, United Kingdom; Liverpool John Moores University, Liverpool, United Kingdom; Institute for Precision Health, The University of Leicester, Leicester, United Kingdom; Department of Anatomy, Telkio University, School of Medicine, Helsinki, Finland; Leicester HPB Unit, Glenfield Hospital, Leicester, United Kingdom

MCB-MS/MS Analysis of amino acid derived neurotransmitters and their metabolites in cerebrospinal fluid, and serum; Rory M Doyle1; WuXi App-Tec Research Services Division, Cranbury, NJ

Development of a 96-well plate sample preparation method for multi-omics analysis using metabolomics and proteomics; Kazuki Ikeda1; Masatomo Takahashi1, 2; Hata Kosuke2; Kohta Nakatani2; Shunsuke Abaraya2; Takeshi Bamba2; Yoshihiro Izumi2; Kyushu University, Fukuoka, Japan; Medical Institute of Bioregulation, Fukuoka, Japan

Evaluation of dried blood spot extraction strategies for untargeted metabolomics workflow; Jiaon Lei1; Cara L. Sake1; John S. Chistyek1; Jonathan E. Katz1, 2; Lawrence J. Ellison Institute for Transformative Medicine, Los Angeles, CA; University of Southern California, Los Angeles, CA

Evaluation of the Biocrates MiXp Quant 500 kit on the Sciex 7500 QQQ LC-MS/MS for metabolomics analysis in liver; Dan Su; WuXi App-Tec Research Services Division, San Diego, CA

Development of Extraction Methods for Mitochondrial Membrane-Bound Products in Strain Engineering; Ju Eun Jeon1; Amy Lee1; Peter Jackson1; Nu Wang1; Andrea Liu1; Deborah Post1; Michael Leavell1; Mona Elbadawi1; Amyris, Emeryville, CA

Evaluation of Red Blood Cell Depletion in Whole Blood Fractionation Workflows: Sujatha Chilakala1; Cara L. Sake1; Ah Young Yoon1; Jonathan E. Katz1, 2; Lawrence J. Ellison Institute for Transformative Medicine, Los Angeles, CA; USC, Los Angeles, CA

Integration of MALDI-guided Laser Capture Microdissection to Enhance Spatial Metabolomics; Jong Hee Song1; Jessica K Lukowski1; Minsoo Son1; Antonia Zamacona Calderon1; Byoung-Kyu Cho1; Young Ah Goo1; Mass Spectrometry Technology Access Center, McDonnell Genome Institute, Washington School of Medicine, St. Louis, MO

Optimizing protocols to profile metabolites and lipids from individual organs of adult zebrafish; Darshak Gadara1; Michaela Schwager-Haber1; Madelyn M. Jackstadt1; Madison Barr1; Leah P. Shriver1; Gary J. Patti1; Washington University in St. Louis, St. Louis, MO

Adopting Orphan Metabolites of Microbiota: MS-based Biochemical and Metagenomic Characterization; Sungwahan F Oh; Brigham and Women’s Hospital, Boston, MA

A high-throughput microflow DIA workflow for bacterial proteomics; Miriam Abele1; Ettene Doll1; Florian P. Bay2; Chen Meng2; Klaus Neubauer1; Siegfried Schircher2; Bernhard Kuster1, 2; Christina Ludwig1; BayBioMS, TUM, Freising, Germany; Research Department Molecular Life Sciences, TUM, Freising, Germany; Chair of Proteomics

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and Bioanalytics, TUM, Freising, Germany; °Core Facility Microbiome, ZIEL – Institute for Food & Health, TUM, Freising, Germany

MP 514 Investigating Squid-Vibrio symbiosis using MALDI-tims-qTOF-IMS; Allison Mctamney1; Denise A Ludvik1; Shaimaa M Aboukhatwa4, Laura M Sanchez2; Mark J Mandel2; Terry W Moore1; 1Department of Chemistry and Biochemistry, University of California, Santa Cruz, Santa Cruz, California; 2Department of Medical Microbiology and Immunology, University of Wisconsin-Madison, Madison, WI; 3Department of Pharmaceutical Sciences, University of Illinois at Chicago, Chicago, IL; 4Department of Pharmaceutical Chemistry, Tanta University, Tanta, Egypt

MP 515 Metaproteomics with advanced phylogenetic search space filtering in MaxQuant; Jingyu Xia1; Shamil Urazbakhtin1; Jürgen Cox1; 1Computational Systems Biochemistry Research Group, Max-Planck Institute of Biochemistry, Martinsried, Germany

MP 516 The metabolic landscape of infant gut microbiome revealed by MS Proteomics in a gut simulator; Shigiy Zhang1; Li Chen2; Ming Hu1; Jianglei Zhu1, 2; 1The Ohio State University, Columbus, OH; 2The Ohio State University-Comprehensive Cancer Center, Columbus, OH

MP 517 Metaproteomics characterization of Svalbard permafrost active layer reveals posts-thaw metabolic activities and adoptions of subsurface microbes to a warming environment; Samantha Peters1; Richard Giannone1; Katie Sipes2; Fumumaya Abuah1; Renxing Liang3; Andrey Abramov1; Julia Boike1; Tatiana Vishnevskaya1, 2; Karen Lloyd2; Robert L Hettrich1; 1Oak Ridge National Laboratory, Oak Ridge, TN; 2University of Tennessee, Knoxville, TN; 3Princeton University, Princeton, NJ; 4Institute of Physiological and Biological Problems in Soil Science, Pushchino, Russia; 5Alfred Wegener Institute Helmholtz-Center for Polar and Marine Research, Potsdam, Germany; 6Humboldt-Universität zu Berlin, Berlin, Germany

MP 518 The role of microbial siderophores in the central nervous system and pulmonary infections; Dominika Luptáková1; Rutuja Hiraj Patil1; Miloš Petfik1; Jan Hrabčák1; Hynek Manač1; Andrea Patyžová1; Tereza Jufliková1; Radim Dobiáš1; David Alec Steveteck1; Vladimir Havlček1; 1Institute of Microbiology of the Czech Academy of Sciences, Prague 4, Czech Republic; 2Institute of Molecular and Translational Medicine, Olomouc, Czech Republic; 3Faculty Thomayer Hospital, Prague 4, Czech Republic; 4Public Health Institute, Ostrava, Czech Republic; 5California Institute for Medical Research, San Jose, CA; 6Stanford University School of Medicine, Stanford, Czech Republic

MP 519 Automated bacterial sample preparation from Agar to MALDI target for routine bacterial identification; Michael Douglas Nain1; Philip Kirk2; Matthew Oppenshaw2; Oliver Severn2; Leah Ashley1; 1Shimadzu, Manchester, UK; 2Manchester, United Kingdom; 3Singer Instruments, Roadwater, United Kingdom

MP 520 Comparison of Protein Extraction Methods and Data Analysis Strategies for Metaproteomic Soil Analysis; Abigale S Mikołitis1; Ethan McBride2; Marie Krogner1; Trevor Glaros1; Philip Mach1; 1Los Alamos National Laboratory, Los Alamos, NM

MP 521 Mass spectrometry-guided precision medicine: a new frontier for clinical microbiology; Ian Lewis1; Daniel B. Gregson1, 2; Fiona Clement1; Ashlee Ear1; Yonatze Grad1; Hallgrimur Benediktsson1, 2; Bruce Walker3; M. Ethan McDonald4; 1University of Calgary, Calgary, AB; 2Alberta Precision Laboratories, Calgary, AB, Canada, Calgary, AB; 3Broad Institute of MIT and Harvard, Cambridge, MA; 4Harvard T.H. Chan School of Public Health, Boston, MA

MP 522 Assessing the effects of exogenous fatty acids and FASII inhibitors on lipid profiles and daptomycin susceptibilities of Staphylococcus aureus; Keerthi Appala1; 1University of Georgia, Athens, GA

MP 523 Pseudomonas aeruginosa - Rhizopus microsporus interaction: a metabolomics hunt for an antifungal treatment for Mucormycosis; Emily C. Giedraitis1; Vanessa V. Phelan1; 1Department of Pharmaceutical Sciences, Skaggs School of Pharmacy and Pharmaceutical Sciences, University of Colorado, Anschutz Medical Campus, Aurora, CO

MP 524 A Targeted and Rapidly Expandable LC-MS/MS Platform for Deciphering the Relationship between SCFAs, Fiber, and the Gut Microbiome; Cheng-Yu Charlie Weng1; Christopher Suarez1; Karen Kalanetra1; Chad Masarweh1; 1David, Davis, CO; 2UC Davis, Davis, CA

MP 525 Simplified molecular imaging analysis of excreted microbial metabolites using a benchtop MALDI-TOF system; Sidrah Rahman1; Michael Douglas Nain1; Rian Griffiths2; Tom K. Abban1; 1School of Pharmacy, University of Nottingham, Nottingham, United Kingdom; 2Shimadzu, Manchester, UK, Manchester, United Kingdom; 3School of Pharmacy, University of Nottingham, Nottingham, United Kingdom; 4Shimadzu, Manchester, UK, Manchester, United Kingdom

MP 526 Spent media analysis and metabolic modelling of recombinant E. coli; Pramod P Wangikar1; Hardik Dodia1; Vivek Mishra2; Bhushan Burkur2; Charandatta Muddangi3; Anant Kedia3; Pravej Nakranti3; Sneh Rana3; 1Indian Institute of Technology Bombay, Mumbai, India; 2Indian Institute of Technology Bombay, Mumbai, India; 3Indian Institute of Technology Bombay, Mumbai, India

MP 527 Spent amino acid analysis opens paths to improve recombinant protein production in complex media; Hardik Dodia1; Vivek Mishra2; Deepi S1; Pramod P Wangikar1; 1Indian Institute of Technology Bombay, Mumbai, India; 2Indian Institute of Technology Bombay, Mumbai, India; 3Clarity Bio Systems India Pvt Ltd, Pune, India

MP 528 Method comparison of innovative bioinformatic tools for a rapid visualization of sample-specific signals of bacterial co-culture by mass spectrometry imaging; Pierre Burquette1; Raphaël La Rocca1; Christopher Kune1; Alexandre Bastin1; Déborah Tellatin1; Sébastien Rigali1; Loïc Quinton2; 1University of Liége, Liége, Belgium; 2University of Liége, Liége, Belgium

MP 529 Probability-based taxonomic profiling of microbiome samples using PegPM and Unipept; Tanja Holstein1, 2, 3; Pieter Verschaffelt4; Lennart Martens5; 1, 2, 4, 5Thilo Muth5; 6Bundesanstalt für Materialforschung und Prüfung, Berlin, Germany; 7VIB-Ugent Center for Medical Biotechnology, Gent, Belgium; 8Department of Applied Mathematics, Computer Science, and Statistics, Ghent University, Ghent, Belgium; 9Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, Germany

MP 530 Multiple targeted methods to elucidate dynamic changes to microbially-derived metabolites following xenobohumol supplementation in healthy adults; Paléc E. Jameson1; Eli Smart1; Gabriella Brown1; Jaewoo Choi1; 1Oregon State University, Corvallis, OR; 2National University of Natural Medicine, Portland, Oregon; 3PNNL, Richland, WA

MP 531 Using RTMS to Unravel the Microbiome Molecular Mechanisms of Carbon and Nutrient Cycling during Rewetting after Drought; Mary S Lipton1; Karl K Weltz1; Montana L Smith1; James J Moran2; 1Pacific Northwest National Laboratory, Richland, WA; 2Michigan State University, East Lansing, MI

MP 532 Changes in the gut metaproteome of women with different body mass index status; Gustavo Diaz1; Kitty Brown1; Anmahmor Hakim1; Corey Broekelman1; Jessica Prenni2; Mikayla A. Borton2; 1Analytical Resources Core: Bioanalysis and Omics, Colorado State University, Fort Collins, CO; 2ThermoFisher Scientific, San
Monday Posters

MP 533 Proteome-wide size exclusion ICPSM analysis of native metalloproteins complexes in bacteria and archaea:
James D Larson; Monika Tomkina-Lukaszewska; Hunter Faussett; Gwendolyn Cooper; Scott Spurzem; Savannah Cox; Rachel Spieß; Brooklyn Brekke; Jordan Pauley; Eric Boyd; Brian Bothner; ’Montana State University, Bozeman, MT

MP 534 Targeted Metabolomics to unveil gut metabolite signatures identifies quinic acid as disease promoting factor in endometriosis: Chandni Talwar; Pooja Popli; Satwikreddy Putturri; Chandrashekhar R. Ambati; Abu Hena Mostafa Kamal; Ramakrishna Kommagani; ’Department of Pathology and Immunology, Baylor College of Medicine, One Baylor Plaza, Houston, Texas; ’Department of Molecular and Cellular Biology, Baylor College of Medicine, One Baylor Plaza, Houston, TX; ’Department of Genetics, Texas, Denton, Texas

MP 535 The postnatal porcine urinary metabolome is associated with recurrent UTI and urobiome ecology: Michael L. Neuget; Neha V. Hulyalkar; Philippe E. Zimmern; Vladimir Shulava; Nicole J. De Nisco; ’Department of Biological Sciences, The University of Texas at Dallas, Richardson, Texas; ’Department of Urology, The University of Texas Southwestern Medical Center, Dallas, Texas; ’Department of Biological Sciences, The University of North Texas, Denton, Texas

MP 536 Accounting for chimeric spectra boosts the number of identifications in metaproteomics without impacting sensitivity: Tim Van Den Bossche; Lennart Martens; Viktoria Dorfer; ’VIB - UGent Center for Medical Biotechnology, Gent, Belgium; ’Department of Biomolecular Medicine, Ghent University, Gent, Belgium; ’Bioinformatics Research Group, University of Applied Sciences Upper Austria, Hagenberg, Austria

MP 537 Data-Independent Acquisition Mass Spectrometry as a Tool for Metaproteomics: Cross-Laboratory Methodological Comparisons Using a Model Microbiome: Andrew T. Raczewska; Jose Alfredo Blakely-Ruiu; Matthew R. McIlvain; Jose Alfredo Blakely-Ruiu; Matthew R. McIlvain; Tim Van Den Bossche; Brian C Sarle; Timothy J Griffin; Makoto Saito; Manuel Kleiner; Pratik D Jagtap; ’University of Minnesota, Minneapolis, MN; ’North Carolina State University, Raleigh, NC; ’Woods Hole Oceanographic Institution, Falmouth, MA; ’Ghent University, Gent, Belgium; ’Ohio State University, Columbus, OH

MP 538 LC-MS Analysis of the Effects of Oral Contraceptives on the Human Gut Microbiome: Daniella A Beerfas; Myedith R Damba; Ellen Kuang; Christopher R Harrison; ’San Diego State University, San Diego, CA

MP 539 Discovery and identification of a non-lethal mechanism for intercolony inhibition (“sibling rivalry”) in Marinobacter: Ellen Kuang; Heather Thorogood; Mary W Carey; Eric M Forberg; Carl J Carrano; San Diego State University, San Diego, CA; ’Bruker Scientific, LLC, Billerica, MA

MP 540 Nextgen Metaproteomics: Metaproteomics analysis using predicted deep learning library searching: Pratik Dilip Jagtap; Subina P Mehta; Wassim Gabriël; Andrew T. Raczewska; James Johnson; Reid Wagner; Mathias Wilhelm; Brian C Sarle; Timothy J Griffin; ’University of Minnesota, Minneapolis, MN; ’Computational Mass Spectrometry, Technical University of Munich, Freising, Germany; ’The Ohio State University, Columbus, OH

MP 541 Temporal profiling of the extracellular proteome secreted by Escherichia coli during biofilm formation on various mannoside surfaces: Mengfian Wang; Guoting Qin; Jennifer Copeland; Hamin Cai; ’University of Houston, Houston, TX; ’VICI Valco Instrument, Houston, TX

MP 542 Temporal profiling of the extracellular proteome secreted by Escherichia coli 83972 during biofilm formation on catheters pretreated with human urine: Rufena Li; Guoting Qin; Mengfian Wang; Jennifer Copeland; Humin Cai; Chengzhi Cai; ’University of Houston, Houston, TX; ’VICI Valco Instruments, Houston, TX

MP 543 Microbiota-Dependent Metabolic Changes Nutritional Intervention during Pregnancy: Emma R Guiberson; Brian Defelice; Josh Elias; Justin L Sonnenburg; ’Department of Microbiology and Immunology, Stanford University, Palo Alto, CA; ’Chancellor Zuckerberg Biohub, San Francisco, CA; ’Center for Human Microbiome Studies, Stanford University, Palo Alto, CA

MP 544 Thread-Based Microfluidic Device for Real-Time Reaction Monitoring by Thread Spray Mass Spectrometry: Salmika G Wairegi; Abuhrame Kwame Badu-Tawiah; ’The Ohio State University, Columbus, OH

MP 545 Photoswitch-decorated nanoparticle for on-chip protein separation and 2D Chromatogram determination: Tanushree Dutta; Julea Vlassakas; ’Rice University, Houston, TX

MP 546 High-Throughput Ultra-Low Flow LCMS platform for low sample amount proteome profiling: Paul Jacobs; Santosh Renuse; Xuefei Sun; Yuan Lin; Jeff Op De Beeck; ’Thermo Fisher Scientific - Belgium, Ghent, Belgium; ’Thermo Scientific - San Jose, CA; ’Thermo Fisher Scientific, Sunnyvale, CA

MP 547 Use of microchip capillary electrophoresis – mass spectrometry for automated rapid measurement of enzyme reaction kinetics: Gili Ben-Nissan; David Morgenstern; Simon Krabbe; J. Will Thompson; Scott Mellors; Yishai Levin; Michal Sharon; ’Weizmann Institute of Science, Rehovot, Israel; ’908 Devices, Inc., Boston, MA

MP 548 Combining capillary electrophoresis and trapped ion mobility spectrometry mass spectrometry to analyze epitranscriptomic marks mediating virus-host interactions in infectious diseases: Daniele Rollo; Adi M Kulkarni; Kate Yu; Guillaume Tremintini; Daniele Fabris; ’University of Connecticut, Storrs, CT; ’908 Devices, Inc., Boston, MA; ’Bruker Daltonics, San Jose, CA

MP 549 A Novel Sensitive Top-down RPLC-CE-MS System for the Analysis of Sub-microgram Intact Cell Lysate: Samin Anjum; Yanting Guo; Zhihao Zhao; Kellye A Cupp-Sutton; Si Wu; ’University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK

MP 550 Exploring the possibilities for Microchip SPE-CE-MS: J. Scott Mellors; J. Will Thompson; Erin A. Redman; ’908 Devices, Inc., Caryboro, NC

MP 551 Microfluidics: Streaming ink identification using mass spectrometry: Morgan Demmler; Nelson R Vinueza; ’Wilson College of Textiles, NC State University, Raleigh, NC; ’Department of Chemistry, NC State University, Raleigh, NC

MP 552 Mass spectrometry of primordial peptides for origins and astrobiology research: Jay G Forsythe; ’College of Charleston, Charleston, SC

MP 553 MAPPs (MHC-I/II-Associated Peptide ProteomicS) revolutions: an evolutive in vitro tool to assess immunogenicity risks: Axel Ducrot; Maureen Bardet; Katharina Hartman; Rebecca Kikuné; Céline Marban; Dora Carol; ’Roche Innovation Center Basel, Basel, Switzerland

MP 554 Evaluation of Multifarious MHC Class II Antibodies for Use as Immunoaffinity Enrichment Reagents in MHC Associated Peptide Proteomics (MAPPs): Jason Lamar; M. Violet Lee; Sylvia C Wong; Peter Tran; Ola Saad; ’Genentech Inc., South San Francisco, CA

MP 555 Spatial Neuroptidome Analysis of Small Neuronal Ganglia in Blue Crab Callinectes sapidus Informed by Multimodal Mass Spectrometry: Thao Duong; Ashley Phetsanthad; Peng-Hsuan Huang; Vu Ngoc Hung Tran;
Lingjun Li1,2; 1Department of Chemistry, University of Wisconsin-Madison, Madison, WI; 2School of Pharmacy, University of Wisconsin-Madison, Madison, WI

MP 557 Circadian neuropeptidomics for the analysis of coupling factors controlling multiscale behavioral rhythms in Drosophila melanogaster; Susanne Neupert1; Deepika Bais1; Anna-Sophie Kugeler1; Anna C Schneider1; 1University of Kassel, Kassel, Germany

MP 558 Improving Mass Spectrometry-Based Detection and Identification of Neuropeptides in Crustacean Hemolymph Using an Anticoagulant Buffer; Angel E. Ibara1; Wenxin Wu1; Lingjun Li1,2; 1University of Wisconsin-Madison, Department of Chemistry, Madison, WI; 2University of Wisconsin-Madison School of Pharmacy - Madison, University, Madison, WI

MP 559 Work for rapid automated immunopeptidome profiling; Stoyan Stoychev1; Justin Jordaan2; Terry Lim3; Pouya Fandii; ReSyn Biosciences, Pretoria, South Africa; 2ReSyn Biosciences, Pretoria, South Africa; 3Monash Biomedicine Discovery Institute, Melbourne, Australia

MP 560 Time-of-Day Analysis of the CSF Peptidome by nanoLC-QqTOF; Shannon D Berneche1; Taylor Jorgensen1; Wei-Chun Kao1; Dharmesh Parmar2; Martha Gillette1,3; Jonathan V. Sweedler2,1; 1Neuroscience Program, University of Illinois at Urbana-Champaign, Urbana, IL; 2Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana and Champaign, IL; 3Department of Cell and Developmental Biology, University of Illinois at Urbana-Champaign, Urbana, IL

MP 561 Immunopeptidomic profiling from soluble HLA in human plasma by ultra-high sensitive mass spectrometry; Maria Wahle1; Maximilian Zwiebel1; Wen-Feng Zeng1; Patricia Skowronek1; Marvin Thielert1; Matthias Mann1,2; Max-Planck-Institute for Biochemistry, Martinsried, Germany; 2Novo Nordisk Foundation Center for Protein Research, Copenhagen, Denmark

MP 562 An optimized biochemical and analytical workflow to unravel the human plasma peptidome; Andreas Zellner1; Steffen Tiedt1; Chien-Yun Lee1; 1Young Investigator Group: Mass Spectrometry in Systems Neurosciences, School of Life Sciences, Technical University of Munich, Munich, Germany; 2Institute for Stroke and Dementia Research, University Hospital, LMU Munich, Germany, Germany

MP 563 High sensitivity HLA-I and HLA-II immunopeptidomics on the TlmsTof Pro-2 Mass Spectrometer with Thunder-DDA-PASEF and HLA-tailored DIA-PASEF; David Gomez-Zepeda1,2; Annica Frekschat1,2; Julian Beyrer1,2; Stefan Tenzer1,2; 1Hi-TRON, Deutsches Krebsforschungszentrum (DKFZ), Mannheim, Germany; 2Institute for Immunology, University Medical Center of the Johannes-Gutenberg University Mainz, Mainz, Germany

MP 564 A novel deep learning-based workflow for analysing immunopeptidome data generated by Data Independent Acquisition (DIA); Qing Zhang1; Kyle Hoffman1; Sahar Rabinoviz1; Chao Peng1; Lei Xin1; Baozhen Shan1; 1Bioinformatics Solutions Inc, Waterloo, ON; 2BaizhenBio Inc., shanghai, China

MP 565 Sensitive, high-throughput single-shot HLA-I and HLA-II immunopeptidomics with improved coverage using data dependent parallel accumulation-serial fragmentation mass spectrometry; Kshiti Meera Phulphagar1; Claudia Crotecka1; Alvaro Sebastian Vaca Jaconme2; Susan Klaeger2; Eva Verzani2; Gabrielle Hernandez2; Karl R Clauser2; Jennifer G Abelin2; Steven A Carr2; 1Broad Institute of MIT and Harvard, Cambridge, MA; 2Barker Daltonics, San Jose, CA; 3Genentech Inc, South San Francisco, CA

MP 566 Neuropeptide Profiling of the Ascaris suum Body Cavity Fluid; Wenxin Wu1; Ciaran McCoy1; Dannib McKenize2; Laura Atkinson2; Lingjun Li1; 1University of Wisconsin Madison, Madison, WI; 2Queen’s University Belfast, Belfast, United Kingdom

MP 567 Enhancing the detection of MHC l-bound peptides on the TimsTOF Pro; Daniel Flender1,2; Geert Baggerman1,2; Kurt Boonen1,2; Elise Pepermans1; 1University of Antwerp, Antwerpen, Belgium; 2VITO - Flemish Institute for Technological Research, Mol, Belgium

MP 568 Investigation of the immunopeptidome from multiple genetically different major histocompatibility (MHC) alleles by mild acid elution (MAE) for vaccine development; Teesha C Baker1; Lucy Song2; Charley Cai1; Selwyn Gu1; Leonard J. Foster1; 1University of British Columbia, Vancouver, BC

MP 569 Algorithm-assisted peptidomic diagnostics of clinical microbiota isolates; Jia Fag1,2; Sudipa Malayi1; Duan Bao1; Bo Ning1; Adrian Zelazny2; Tony Hu1; Tulane University School of Medicine, New Orleans, LA; 1NIH/Clinical Center, Bethesda, MD

MP 570 Understanding Phosphoryrosine Signaling at the Single Spheroid Level; Brian D Fries1; Alissa Nelson1; Amanda B Hummon1; 1The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH; 2Cell Signaling Technology, Danvers, MA

MP 571 Assessing insulin signaling responses by protein phosphorylation surveillance in plasma extracellular vesicles; Yi-Kai Li1; Xiaofeng Wu1; Yury O. Nunez Lopez2; Richard E. Pratley1,2; Anton B. Iluk4,5; 1Wendy Tao1,2; 2Purdue University, WEST LAFAYETTE, IN; 3AdventHealth, Orlando, FL; 4Tymora Analytical Operations, West Lafayette, IN

MP 572 A guide to high-throughput dose-resolved phosphoproteomics to understand drug mechanism(s) of action; Florian P Bayer1; Jana Zecha1; 1Technical University of Munich, Freising, Germany

MP 573 Three-dimensional construction of mouse brain protein atlas based on spatial multiomics data; Shuang Yang1; Jia Yu1; Huai Shen1; Xiaohui Liu1; 1Fudan University, Shanghai, China; 2HuaZhong University of Science and Technology, Wuhan, China

MP 574 Streamlined protein extraction and cleanup for unbiasedly exploring pan-bacterial phosphoproteomics; Pei-Shan Wu1; Ting-An Chen1; 1Ying Lin1; Min-Hwa Lin1; 1Department of Microbiology, College of Medicine, National Taiwan University, Taipei City, Taiwan

MP 575 A Bio-Zr based enrichment for the phosphoproteins from human and animal tissues; Qidan Li1; Xiaolian Ning1; Zhoumei Zheng1; Siqi Li1; Ziyin Han1; Jie Liu1; Dongjie Wu1; Zhanlong Mei1; Jin Zi1; Siqi Liu1; 1BGI-Shenzhen, Shenzhen, China; 2National Institutes of Biomedical Imaging and Health, National Institutes of Health, Bethesda, MD

MP 576 High-throughput phosphoproteomics of formalin-fixed, paraffin-embedded rat tissues using microflow Zeno SWATH; Erin M Humphries1,2; Dylan Xavier1; Keith Ashman1; Peter G Hains3; Phillip J Robinson1,2; 1Children’s Medical Research Institute, Westmead, Australia; 2University of Sydney, Sydney, Australia; 3SCIEX, Sydney, Australia

MP 577 Phospho-site identification of multiple phosphorylated tau peptides in human brain; Gunnar Brinkmalm1; Juan Lantero Rodriguez1; Elena Camporesi1; Laia Montoliu-Gaya1; Johan Gobom1; Ann Brinkmalm1; Tammamry Lashley2; Henrik Zetterberg1; Kaj Blennow1; 1University of Gothenburg, Molndal, Sweden; 2University College London, London, United Kingdom

MP 578 Improving tryptic digestion efficiency for proteomic samples by metal ion additives; Kosuke Ogata1; Shunsuke Tanaka1; Ayana Tomioka1; Eisuke Kano1,2; Yasushi Ishihama1,3; 1Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, Japan; 2Kyoto University, Kyoto, Japan; 3National Institutes of Biomedical Innovation, Heart and Nutrition, Ibaraki, Japan

MP 579 Identifying MAPK signaling thresholds in melanoma using phosphoproteomics; Kristyn R Hayashi1,2; Natalie G Ahn1,2; 1Department of Biochemistry, University of
**MONDAY POSTERS**

Colorado, Boulder, CO; 1-BioFrontiers Institute, University of Colorado, Boulder, CO

**MP 580** Phosphotransomics V3: Expanding a web-based resource for online analysis of phosphoproteomics data; Michael G Leeming; Ching-Seng Ang; Shuai Nie; Swati Varshney; Nicholas Williamson; Melbourne Mass Spectrometry and Proteomics Facility, Bio21 Institute of Molecular Science and Biotechnology, The University of Melbourne, Parkville, Melbourne, Australia

**MP 581** A Suspension Trapping-based Sample Preparation Workflow for Sensitive Plant Phosphoproteomics; Chin-Wen Chen; Chia-Feng Tsai; Shu-Yu Lin; Chuan-Chih Hsu; 1-Institute of Plant and Microbial Biology, Academia Sinica, Taipei city, Taiwan; 2-Pacific Northwest National Laboratory, Richland, WA; 3-Academia Sinica Common Mass Spectrometry Facilities for Proteomics and Protein Modification Analysis, Academia Sinica, Taipei, Taiwan

**MP 582** Digging deeper into phosphoproteomes through Al-driven deconvolution of chimeric spectra; Florian Seefried; Daniel P. Zolc; Tobias Schmidt; Siegfried Gersten; Markus Graber; Patrick Kasmers; Markus Schneider; Layla Eljigah; Vishal Sukumaran; Pedro Navarro; Kai Fritzemeier; Yovany Cordero Hernandez; Frank Berg; Carmen Pasckie; David Horn; Bernhard Delange; Christoph Henrich; Martin Heinrich Freijo; 1-MSDA GmbH, Garching b.München, Germany; 2-Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany

**MP 583** Quantitative phosphoproteomics to identify candidate target engagement biomarkers related to efferocytosis and TAM RTK pathways; Manuel Tzouros; Emmanuelle Lezan; David Avila; Balazs Banfalvi; Florian Wanke; Nicolas Mercado; Barbara Geering; 1-Roche Innovation Center Basel, Pharmaceutical Sciences, F. Hoffmann-La Roche, Ltd., Basel, Switzerland; 2-Roche Innovation Center Basel, Medical Faculty, Rheinische Friedrich-Wilhelms-University of Bonn, Bonn, Germany; 3-Medical University of Innsbruck, Innsbruck, Austria; 4-University of Vienna, Vienna, Austria

**MP 584** Using large-scale phosphoproteomics to elucidate the regulation of Protein Kinase CK2 activity by peptidyl proline cis/trans isomerase Pin1; Scott E. Pease; Daniel P. Zolc; Christopher M. Rose; David W Litchfield; 1-Western University, London, ON

**MP 585** Phosphoproteomic analysis of the cellular response to lysosomal impairment; Pithamn Muthukottiyappan; Alireza Dehghani; Asisam Muchamedim; Fatema Akter; Mariana Eca Guimaraes De Araujo; Cristina Comin; Robert Ahrends; Lukas Huber; Volkmar Gieselmann; Dominic Winter; 1-Institute for Biochemistry and Molecular Biology, Medical Faculty, Rheinische Friedrich-Wilhelms-University of Bonn, Bonn, Germany; 2-Medical University of Innsbruck, Innsbruck, Austria; 3-University of Vienna, Vienna, Austria

**MP 586** Quantitative analysis of phosphorylated proteins from multiple signaling pathways using the TMTpro and SureQuant targeted mass spectrometry assay panel reagents; Ara Marcu; Bhavin Patel; Jae Chol; Dustin Frost; Penny Jenson; Amirmansoor Hakimi; Kay Opperman; Ryan Bomgardner; Christopher M. Rose; 1-Genentech Inc., South San Francisco, CA; 2-Thermo Fisher Scientific, Rockford, IL; 3-Thermo Fisher Scientific, San Jose, CA

**MP 587** Characterizing the effects of kinase inhibitors on the phosphorylation of transcription factors using subcellular fractionation; Andrea I. Gutierrez; Isabella T. Whitworth; Carolyn Allen; William E Fodrie; Daniele Canzani; Lindsay K Pino; Alexander J Federation; 1-Talus Bioscience, Seattle, WA; 2-University of Wisconsin-Madison, Madison, WI

**MP 588** Multi-species Benchmarking Phospho-DIA Comparison of Commercial Sample Prep Kits; Billy W Newton; Audrick Yang; Ying Zhu; Guanghui Han; 1-BGI Americas, San Jose, CA

**MP 589** Advances in phosphopeptide eludication is possible: permeation via TrEnDi improves LCMS detection of phosphopeptides; Samiksha Vij; Karl Wasslen; Jeffrey M MARNtorpe; Jeffrey C Smith; 1-Carleton University, Department of Chemistry, Ottawa, ON

**MP 590** Characterizing Root Exudate Composition Across 19 Cover Crop Species; Valerie Seliz; Colorado State University, Fort Collins, CO

**MP 591** GC-MS Profiling of Compounds Present in the Endangered Plant Ziziphus celata; Emily Boyette; Luc Alfred; Sarah Arman; Toby Ellison; Jenna Gutierrez; Stephanie Hicks; Nylla Wider; Kate Calvin; 1-South Florida State College, Avon Park, FL

**MP 592** Quantitative proteomic analysis of rice plants with different phosphatase activity to elucidate dynamic changes when grown in low and high phosphorus conditions; Yoshiaki Ueda; 1-Farhad Massomi-Aladizgeh; 2-Masaduzzaman Prodhان; Mehdi Mirzaei; Ghassem Hosseini Salekdeh; 3-Matthias Wissuwa; 4-Paul A. Haynes; 1-Japan International Research Center for Agricultural Sciences (JIRCAS), Tsukuba, Japan; 2-Macquarie University, North Ryde, Sydney, Australia; 3-University of Western Australia, Perth, Australia

**MP 593** The Detection by High Resolution Mass Spectrometry of Mogrosides Produced Through Metabolic Engineering of Diverse Plant Species; Matthew B. Kilgore; Anna Mathiassid; Devashri Selote; Jack Wilkinson; 1-Evo Life Systems, Durham, NC

**MP 594** Extending a Tandem Mass Spectrometry Library with High-Resolution Quality Spectra of 11,000 Plant Metabolites; Xiaoyu Yang; Pedatsur Neta; H. Martin Garraffo; Yuxue Liang; 1-Yamil Siomón-Manso; 2, 3-Yuri Litv; 4-Tchekhovskoi; 5-Yuri A. Mirokhin; 6-Stephen E. Stein; 7-NIST, Gaithersburg, MD

**MP 595** Metabolomics Revealed the Roles of Oxylinps and Melatonin in Stomatal Immunity; Chongyuan Xiang; Craig Dutresne; Suxue Chen; 1-Department of Biology, Genetics Institute, University of Florida, Gainesville, FL; 2-Thermo Scientific Training Institute, West Palm Beach, Florida; 3-Department of Biology, University of Mississippi, Oxford, MS

**MP 596** Comprehensive Lipidome Survey of the Tomato Suffered from Distinct Infection Phases of Late Blight Disease; Chia-Wen Hu; Ya-Ting Tseng; Scott E. Pease; 1-Academia Sinica, Taipei, Taiwan; 2-Academia Sinica Metabolomics Core Facility, Taipei, Taiwan

**MP 597** Dimensionality reduction methods and GNPs for plant metabolomics ofCentella asiatica cultivars; Luke C. Marrey; 1, 2-Md Alam Nure; 1, 2-Liping Yang; 1, 2-Jaewoo Choi; 2, 3-Natasha Cerruti; 2, 3-Armando Magana; 2, 3-Corey De la Cruz; 2, 3-Gerrard Johnson; 2, 3-Christopher M. Rose; 2, 3-Viswanathan; 1, 2-Sumanana Rajagopal; 1, 2-James Smith; 1, 2-Amal Soumyanath; 1, 2, 3-Jan F. Stevens; 1, 2, 3-Amanda Maier; 1, 2, 3-1-Department of Chemistry, Oregon State University, Corvallis, OR; 2-BENFRA Botanical Dietary Supplements Research Center, Oregon Health and Science University, Portland, OR; 3-Linus Pauling Institute, Oregon State University, Corvallis, OR; 4-Oregon Wild Harvest, Redmond, OR; 5-Biological & Ecological Engineering, Oregon State University, Corvallis, OR; 6-Department of Neurology, Oregon Health & Science University, Portland, Oregon; 7-School of Food Science & Nutrition, University of Leeds, Leeds, United Kingdom; 8-Department of Pharmaceutical Sciences, Oregon State University, Corvallis, OR

**MP 598** From exploratory analysis to high-throughput quantitative analysis ofWithania somniferaextract using LC-HRMS/MS and LC-MRM MS; Luke Marrey; 1, 2-Jaewoo Choi; 2; 3-Armando Alcalzar Magana; 1, 2, 3-Liping Yang; 1, 2, 3-Md Alam Nure; 1, 2, 3-Mikah Brandes; 1, 2, 3-Cody Neff; 1, 2, 3-Amala Soumyanath; 1, 2, 3-Jan Frederik Stevens; 1, 2, 3-Amanda Maier; 1, 2, 3-1-Department of Chemistry, Oregon State University, Corvallis, OR; 2-BENFRA Botanical Dietary Supplements Research Center, Oregon Health and Science University, Portland, OR; 3-Linus Pauling Institute, Oregon State University, Corvallis, OR; 4-Department of Neurology, Oregon State University, Corvallis, OR
Oregon Health & Science University, Portland, OR;
1Department of Neurology, Oregon Health & Science University, Portland, OR; 2Department of Pharmaceutical Sciences, Oregon State University, Corvallis, OR

MP 600 Inside into the proteome of Chelidonium majus latex; Joanna Gracz-Bernaciak1; Olivia Mazur2; Natalia Kielich1; Michalina Krkowiak1; Sophia Bradyyska1; Martyna Weglewsk1a; Oskar Musidzkia; Agata Malinowskia; Robert Nawrot1; 1Adam Mickiewicz University in Poznan, Faculty of Biology, Department of Molecular Virology, Poznan, Poland; 2Polish Academy of Sciences, Institute of Biochemistry and Biophysics, Mass Spectrometry Laboratory, Warsaw, Poland

MP 601 Peptide network analysis and metabolite correlation reveals primary metabolism contribution to susceptibility or resistance of Eucalyptus grandis to rust; Thais Regiani Cataldi1; Ana Lúcia Mendes Pinheiro1; Felipe Garbelini Marques1; Alline Sekiya1; Fabricio Edgar De Moraes1; Carlos Alberto Labate1; 1ESALQ, Piracicaba, Brazil

MP 602 Diversity and Antifungal Activity of Specialized Metabolites in Ecotypes of the Bioenergy Crop Switchgrass ( Panicum virgatum L.); Xiongxin Li1, 2; Meng-Yi Chou1, 2; Gregory Bonitou1, 2; Arthur Daniel Jones1, 2; Robert L. Last1, 2, 3; DOE Great Lakes Bioenergy Research Center, Michigan State University, East Lansing, MI; 1Department of Biochemistry and Molecular Biology, Michigan State University, East Lansing, MI; 2Department of Plant, Soil and Microbial Sciences, Michigan State University, East Lansing, MI; 3Department of Plant Biology, Michigan State University, East Lansing, MI

MP 603 Achieving higher productivity in cell line optimization by a streamlined middle-down workflow; Hirsh NANDA1; Andrew Mahan1; Zoe Zhang1; Partha Chowdhuri2; 1Janssen Research & Development, Spring House, PA; 2CSOX, Redwood city, CA

MP 604 Standard-Free Absolute Quantitation of Antibody Deamidation Degradation and Host Cell Proteins by Coulometric Mass Spectrometry; Yongling Ai1; Harsha P. Gunawardena2; Xuwen Li3; Yong-Ick Kim3; Howard D. Dewald4; Hao Chen5; 1New Jersey Institute of Technology, Newark, NJ; 2Janssen Research & Development, Spring House, PA; 3Analytical Research & Development, Merck & Co., Inc., Kenilworth, NJ; 4Ohio University, Athens, OH

MP 605 Top Down Analysis of a Multivalent PEGylated Fab-based Biotherapeutic in Cynomolgus Plasma to Assess in vivo Biotransformation using IA-LC-TOF-MS; Sylvia C Wong1; M. Violet Lee1; Ola Saad2; 1Genethinc Inc., South San Francisco, CA

MP 606 Newomics Microflow-Nanospray ESI-MS (Mn3ESI-MS) Platform for Sensitive and Robust Analysis of Monoclonal Antibody Glycograms; Nancy Fernandes; Lonza, Portsmouth, NH

MP 607 Recombinant chymotrypsin for improved peptide mapping of biotherapeutic proteins; Alba Katiria González Rivera1; Sergei Savelyev2; Michael M. Rosenblatt3; 1Promega Corporation, Madison, WI

MP 608 Peptide Mapping of a Monoclonal Antibody Using an Integrated Protein Digestion LCMS Platform (Perfinity-QTOF LCMS-9030); Kate (xiaoming) Xia1; Evelyn H. Wang1; Stephen Kurzyinski1; Taro Ogura1; Yoshiyuki Okamura1; Mohamed Boutaghou1; 1Shimadzu Scientific Instruments, Columbia, MD

MP 609 A Novel Approach to Mass Spec Sample Preparation of AAV Capsid Protein for Peptide Mapping and Host Cell Impurity analysis; Sergei Savelyev1; Chris Hosfield1; Alba Katiria González Rivera1; Marjeta Urh1; Michael M. Rosenblatt3; 1Promega Corporation, Madison, WI

MP 610 Effect of in-source CID on non-Specific truncation in Characterization of Antibody-based Therapeutics using Reduced LC-MS Analysis; Roshanak Aslebagh1; Kai Zheng1; 1CytomX Therapeutics, South San Francisco, CA

MP 611 Intact Mass Analysis of Biotherapeutic Stability in Tissues; Yunan Wang1; Mei Han2; Justin Iwuagwu1; Fang Xie1; Lin Zeng3; Kip Conner1; 1Amgen, Inc., South San Francisco, CA

MP 612 Enhanced biopharmaceutical characterization using next generation multireflecting time-of-flight technology; Guillaume Bechade1; Dale A Cooper-Shepherd2; Emma Marsden-Edwards2; Martin E. Palmer2; 1Waters S.S.A.S, Saint-Quentin, France; 2Waters Corporation, Wilmslow, United Kingdom

MP 613 Characterization of carbamoylated lysine in a therapeutic recombinant protein top-down electron fragmentation; Jhoan Frankel1; Rachel Joseph Meewissen1; Mike Hare2; Yury Vasil’ev3; Joseph Beckman2; 1Xemptiva, Montevideo, Uruguay; 2-eMSion, Corvallis, OR

MP 614 Monitoring mAb proteoforms in mouse plasma using an automated immunocapture combined with top-down and middle-down mass spectrometry; Jonathan Dhenin1; 1Valérie Lafont; Mathieu Dupré2; Jean-Baptiste3; Alain Krick2; Christine Mauriac1; Julia Chamot-Rooke1, 2, 3, 4; 1Institut Pasteur, Paris, France; 2Sanofi, Chilly-Mazarin, France; 3Université Paris Cité, Paris, France; 4CNRS, Paris, France

MP 615 Characterization of Charge Variants by Ion Exchange Chromatography and Mass Spectrometry; Yun Zhang1; Li-Li Tsao1; Tiffany Hawkins1; Brian Woodrow1; 1RockwellSigma, Rockville, MD

MP 616 “Flash Characterization” of Antibodies via Microdroplet Reactions in an Unmodified Jet Stream Source; Michael D Krienerman1; Jim Lau2; Hui Zhao2; Harsha P. Gunawardena2; 1Agilent Technologies, Santa Clara, CA; 2Agilent Technologies, Wilmington, DE; 3Janssen Research & Development, Spring House, PA

MP 617 Chemical labeling and mass spectrometry for characterization of the higher order structure of a bispecific antigen-bridging biotherapeutic (BABB) and its complexes; Arnik Shah1, 2; Dipa Batabyal3; Dayong Qiu1; Weidong Cui1; John Harrahyl; 4Alexander R. Ivanov2; 1Amgen, Inc., Cambridge, MA; 2Northeastern University, Boston, MA; 3Amgen, Thousand Oaks, CA; 4Sanofi, Cambridge, MA

MP 618 Multi-attribute method (MAM) for biotherapeutics characterization: biosimilarity assessment, high-throughput and low-flow analytical methods applications; Silvia Millan Martin1; Craig Jakes2; Lisa Strasser3; Sara Carillo1; Jonathan Bones1, 2, 3; 1NIBRT, Dublin, Ireland; 2University College Dublin, Belfield, Ireland

MP 619 Peptide mapping workflow for direct microchip CE-MS analysis of biotherapeutics; Sara Carillo1; Jonathan Bones1, 2; 1NIBRT, Dublin, Ireland; 2University College Dublin, Belfield, Ireland

MP 620 Mass spectrometry-based approaches to investigate allosteric modulation and biased signaling of GPCR’s; Parth Kapoor1; Idir Liko1; Fernando Almeida1; Jonathan Hopper1; Joanna Toporowska2; Argyris Politis3; 1NIBRT, Dublin, Ireland; 2908 Devices, Inc., Boston, MA; 3908 Devices, Inc., Carboro, NC

MP 621 Development of Multi-Attribute method (MAM) for heavily glycosylated protein vaccines; Asif Shajahan1; Vera B. Ivleva1; Jason G. Gall2; Q. Paula Lei1; 1Vaccine
**MONDAY POSTERS**

**MP 622** Novel approach to achieve high spectral quality without compromising identification for biopharma applications; Stephens Hoyle; Sara Carillo; Craig Jakob; Silvia Millán-Martin; Sona Nidayev; Kevin L. Schafer; Jonathan Jones; Shannon Ellik; 1ThermoFisher Scientific, San Jose, CA; 2NIBRT, Dublin, Ireland; 3Thermo Fisher Scientific, Courtaboeuf, France

**MP 623** In Vivo Structural Analysis of Membrane Proteins via Hydroxyl Radical Footprinting; James Dowell; Daniel Benjamin; Faraz Choudhury; 1Immuno Scientific, Madison, WI

**MP 624** Investigations of a Bispecific Antibody Dimerization via Hydroxyl Radical Footprinting; Harsha Gunawardena; Andrew Mahan; Hirsh Nanda; Daniel Benjamin; 1JOHNSON AND JOHNSON, Spring House, PA; 2Immuno Scientific Inc., Madison, WI

**MP 625** A native multi-dimensional MAM workflow for at-line characterization of mAb titer, size, charge, and glycoform heterogeneities in cell culture supernatant; Sanghati Bhattacharya; Srishti Joshi; Anurag Singh Rathore; 1Indian Institute of Technology, Delhi, Delhi, India

**MP 626** Multi-attribute monitoring of aggregates and charge variants of monoclonal antibody through native 2D-SEC-MS-WCX-MS; Sunil Kumar; Tushar Sharad Savane; Vadiraj Bhat; Anurag Singh Rathore; 1Indian Institute of Technology Delhi, New Delhi, India; 2Indian Institute of Technology, Delhi, New Delhi, India; 3Agilent Technologies, Bangalore, India

**MP 627** A Disruptive Approach for Characterization of mAb Charge Variants by Imaged Capillary Isoelectric Focusing (iIEF)-UV/IMS; Greg Adams; Hunter Walker; Margo Wilson; Scott Mack; Maggie Ostrowski; FUJIFILM Diosynth Biotechnologies USA, Morrisville, NC; 2SCIEX, Fremont, CA

**MP 628** Top/Middle-Down Protein Sequencing: a novel automated data processing tool for the Top-Down/Middle-Down analysis of biological therapeutics; Mona Hamada; Stefano Gotta; Wen Jin; Amy Claydon; Amandine Boudreau; 1SCIEX, concord; 2Genedata, Basel; 3Switzerland; 4Aude Tartiere; 1SCIEX, concord; 2Genedata, Cambridge, United Kingdom; 3Switzerland; 4Aude Tartiere

**MP 629** A Single Data Workflow Leveraging Middle-Down Sequencing to Validate Intact Mass Analysis Characterization of Therapeutic Antibodies; Stephen Koh; Mauricio Bronzetti; Aude Tartiere; 1Amy Claydon; 2Arnd Brandenburg; 3Genedata, San Francisco, CA; 4Genedata, Cambridge, United Kingdom; 5Genedata, Basel, Switzerland

**MP 630** Rapid analysis of titre, aggregate and intact mass of antibody therapeutics using multi-dimensional liquid chromatography coupled with native mass spectroscopy; Tushar Sharad Savane; Sunil Kumar; Vadiraj Bhat; Anurag Singh Rathore; 1Indian Institute of Technology Delhi, New Delhi, India; 2Indian Institute of Technology Delhi, New Delhi, India; 3Agilent technologies, Bangalore, India

**MP 631** Investigating the conformational dynamics of the inteceptor calmodulin-nitric oxide synthase complex by cross-linking mass spectrometry; Ting Jiang; Guanghua Wan; Haikun Zhang; Eric Underbakke; Changjian Feng; 1UNM College of Pharmacy, Albuquerque, NM; 2Roy J. Carver Department of Biochemistry, Biophysics and Molecular Biology, Ames, Iowa

**MP 632** Mass Spectrometric Recognition Motif Discovery by Intact Transition Epitope Mapping – Force differences between Original and Unusual Residues (ITEM-FOUR) Analyses; Claudia Röwer; Christian Ortmann; André Neumann; Raghavendra R. Elkesar; Michael Becker; 1Proteome Center Rostock, Rostock, Germany; 2Waters Corporation - TA Instruments, Eschborn, Germany; 3TRANSCEND Centre, Regional Institute of Oncology (IRO), Guelph, Guelph, ON; 4The British University in Egypt, El Sherouk City, Egypt

**MP 633** Identification and structural modeling of the nuclear receptor liver receptor homolog-1 with a novel corepressor peptideidropyoli cis/trans isomerase B; Valentine V Courouble; 1Biel Bdr; 2Roberto Vera Alveare; 3Bruce D Pascal; 4Theodore Kamenec; 5Patrick R. Griffin; 1, 2The Herbert Wertheim UF Scripps Institute for Biomedical Innovation & Technology, Jupiter, FL; 2Skaggs Graduate School of Chemical and Biological Sciences, The Scripps Research Institute, Jupiter, FL; 3Omicson Informatics, Honolulu, HI

**MP 634** Examining the Structure-Function Relationship of Enzymes using Temperature-Controlled Nanoelectrospray Mass Spectrometry; Julien Harrison; 1Adam Pruska; 2Renato Zenobi; 1ETH Zurich, Zurich, Switzerland

**MP 635** Limited proteolysis-mass spectrometry (LiP-MS) enables global profiling of the effects of glycosylation on protein conformational changes; Haiyan Lu; Xudong Shi; Lauren Fields; Hua Zhang; 1Tianyi Wang; 1, 2Nathan V. Weilham; 1, 2Lingjun Li; 1School of Pharmacy, University of Wisconsin-Madison, Madison, WI; 2School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI; 3Department of Chemistry, University of Wisconsin-Madison, Madison, WI

**MP 636** Understanding the role of conformational dynamics in the substrate promiscuity of the Pup-proteasome system in mycobacterium; Alicia Plourde; 1Siavash Vahidi; 1University of Guelph, Guelph, ON

**MP 637** Tracking the Mechanistic Origins of Irreversible Protein Unfolding; Evelyn H MacKay-Bar; 1Lars Konermann; 1University of Western Ontario, London, ON

**MP 638** Determining Collision Cross Sections Using Orbitrap Charge Detection Mass Spectrometry; Kyle Patrick Bowen; 1Michael Senko; 1Thermo Fisher Scientific, San Jose, CA

**MP 639** Establishing a decision tree for native mass spectrometry analysis of membrane proteins in complex membrane mimetics; Weijing Liu; 1Christopher Mullen; 2Donggyun Kim; 1Vadim Cherevazov; 2Gregory J. Dodge; 1Barbara Impalari; 1, 2Barun S. Jayasinghe; 2Michael T. Marty; 2Rosa Viner; 1Thermo Fisher Scientific, San Jose, CA; 2University of Southern California, Los Angeles, CA; 3Massachusetts Institute of Technology, Cambridge, MA; 4University of Arizona, Tucson, AZ

**MP 640** Monitoring of conformational changes in transmembrane proteins using HDX and FFAP radical labeling; Lukas Foda; 1, 2Jasmin Rodriková; 1, 2Pet Pompach; 1, 2Zdeněk Kukačka; 1, 2Pet Novák; 1, 2Pet Man; 1, 2; 1Institute of Microbiology of the CAS, v. v. i., Prague, Czech Republic; 2Charles University, Faculty of science, Prague, Czech Republic; 3Institute of Biotechnology of the CAS, v. i., Prague, Czech Republic

**MP 641** Characterizing Macromolecular Dipeptide Moments via Differential Ion Mobility Spectrometry with Linked Field/Pressure Scans; Alexandre A Stvarzburg; 1Roch Andrzejewski; 2Andrew Entwistle; 1Monika Gomola; 2Patrick Knight; 1Wichita State University, Wichita, KS; 2Shimadzu Research Laboratory (Europe), Manchester, United Kingdom

**MP 642** Altered dimerization kinetics and dynamics of SARS-CoV-2 main protease determined by native and hydrogen-deuterium exchange mass spectrometry; Syuan-Ting Kuo; 1Yin Xin; 2David Russell; 2Texas A&M, College Station, TX

**MP 643** Dysregulation of mitochondrial CipP protease using orthosteric and allosteric inhibitors; Monica M Goncalves; 1Angelina S Kim; 2Aligars Velvise; 2Taylor Forrest; 3Vincente Trude; 2Matthew Kimberly; 1, 4Michael Schimmer; 1Andrei Yudin; 1Siavash Vahidi; 1University of Guelph, Guelph, ON; 2University of Toronto, Toronto, ON; 3University of Toronto, Toronto, ON; 4The British University in Egypt, El Sherouk City, Egypt
PM 644  Cryo-EM atomic structure determination from macromolecular samples produced by native electrospray ion beam deposition (ESIBD); Tim K Esser; Jan Bohning; Paul Fremdling; Carol V Robinson; Justin L. P. Benesch; Lindsay Baker; Tammy A.M. Bharat; Stephan Rauschenbach; University of Oxford, Oxford, United Kingdom; Structural Studies Division, MRC Laboratory of Molecular Biology, Cambridge, United Kingdom; Oxford University, Oxford, United Kingdom; University of Oxford, Dept. of Chemistry, Oxford, United Kingdom.

PM 645  Structural interactomics and structure prediction reveal protein binding sites within disordered regions: Julia Rutla; Cong Wang; Ying Zhu; Pin-Liang Jiang; Arne Elofsson; Boris Bogdanow; Fan Liu; Department of Structural Biology, Leibniz Forschungsinstitut für Molekulare Pharmacologie (FMP), Berlin, Germany; Department of United Kingdom; Biophysics, Stockholm University, Stockholm, Sweden; Science for Life Laboratory, Stockholm University, Solna, Sweden; Charité – Universitätsmedizin Berlin, Berlin, Germany.

PM 646  Structural investigation of large eye lens β-crystallin heterooligomers using native ion mobility-mass spectrometry and computations; Michał T. Dzieniak; Amber Rolland; Takuto Takeda; Kirsten J. Lamp; James S. Prei; George Fox University, Newberg, OR; Utrecht University, Utrecht, Netherlands; University of Oregon, Department of Chemistry and Biochemistry, Eugene, OR; Kyoto University, Kyoto, Japan; Oregon Health & Science University, Portland, Oregon.

PM 647  Reactivity of proteins with singlet molecular oxygen as a probe for structural mass spectrometry; Michael Volny; Giovanni Tomno; Marek Polák; Lukáš Fojtík; Daniel Kavan; Petr Man; Petr Novák; Charles University, Faculty of Science, Prague, Czech Republic; BioCEV – Institute of Microbiology, Prague, Czech Republic; University of Padua, Department of Pharmacy, Padua, Italy.

PM 648  Supercharging reagent improves nanoHPLC–ESI-MS/MS analysis of disulfide bonds and His-tagged peptides; Chia-Wei Lin; Fabia Canonica; Simone Wüthrich; Paolo Nanni; Ralph Schlaphbach; Functional Genomics Center Zurich, University of Zurich & ETH Zurich, Zurich, Switzerland; Department of Dermatology, University of Zurich, Zurich, Switzerland.

PM 649  Millisecond time-resolved hydrogen/deuterium-exchange mass spectrometry at single amino acid resolution resolves conformers of α-synuclein familial mutants; Lindsay Cole; Ulrik H Mistorz; Andrew J Williamson; Ken Cook; Jenny Ho; Yuqi Shi; Rosa Viner; Jonathan J Phillips; Applied Photophysics Ltd, Leatherhead, United Kingdom; Thermo Fisher Scientific, Copenhagen, Denmark; Thermo Fisher Scientific, Hemel Hempstead, United Kingdom; Thermofisher Scientific, San Jose, CA; Living Systems Institute, University of Exeter, Exeter, United Kingdom.

PM 650  Application of a Benchtop Method for Oxidative Footprinting to Detect Structural Changes in a Protein Complex from Staphylococcus Aureus; Maria C Panepeptide; Juliana Ilman; Victor Torres; Beatrix Uberheide; NYU Grossman School of Medicine, New York, NY.

PM 651  Investigating binding interactions between SARS-CoV-2 PLpro and inhibitors, interferons and viral targets using ultraviolet photodissociation and collision cross section analysis; Virginia K. James; Katel Lyn S. Zuercher; Jennifer S. Brodbelt; University of Texas at Austin, Austin, TX.

PM 652  Characterization of loading efficiency of protein nanocages with native MS and limited charge reduction; Kevin Cheung; Daniil G Ivanov; Igor A Kaltashov; University of Massachusetts at Amherst, Amherst, MA.

PM 653  Mapping the C-terminus of α-Synuclein conformers by native crosslinking and ion mobility mass spectrometry; Melanie Cheung See Kil; Ian K. Webb; Indiana University Purdue University Indianapolis, Indianapolis, IN.

PM 654  Insights into the Fission Yeast Rp6, Br1 and Br2 Complex using Crosslinking-MS; Enrique Arevalo; Chu Thet Ywe; Sara Magoun; Jonathan Garcia; Prakash K. Shukla; Mahesh B. Chandrasekharan; Spectrus, Beverly, MA; Department of Radiation Oncology and Huntsman Cancer Institute, University of Utah School of Medicine, Salt Lake City, Utah.

PM 655  Variable-Temperature Electrospray Ionization Coupled with Electron Capture Dissociation to Study Temperature Induced Solution Phase Structural Changes; Kristie L. Baker; Philip C. Lacey; Yuan Gao; Benjamin J. Jones; Vicki H Wysocki; The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH.

PM 656  Assay for solvent accessibility of methionine residues in complex sample using methionine oxidation footprinting and top-down proteomics; Anju Teresa Sunny; Yanting Guo; Kellye A Cupp-Sutton; Si Wu; University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK.

PM 657  Mass spectrometry-based structural investigations of S100b; Nolan K McLaughlin; Nicole D. Wagner; Michael L. Gross; Washington University in Saint Louis, Saint Louis, MO; Washington University School of Medicine, St. Louis, MO.

PM 658  Aggregation pathways of Transthyretins: a mass spectrometry study on health-related mutants; Lili Fan; David H. Russell; Texas A&M University, College Station, TX.

PM 659  Monitoring MsBA Activity under Turnover Conditions; Tianqi Zhang; Jixing Lyu; Arthur Laganowsky; Texas A&M University, College Station, TX.

PM 660  Enabling simultaneous photoluminescence spectroscopy and X-ray Footprinting to study protein conformation and interactions; Pablo Scrosati; Sayan Gupta; Line G Kristensen; Brandon Russell; Shawn M Costello; Susan Marquesse; Corie Y Ralston; Lawrence Berkeley National Laboratory, Berkeley, CA; University of California, Berkeley, CA.

PM 661  AlphaCross-XL: A rapid and robust tool for the identification of cross-linking of proteins using XL-MS; Deepatkar Biswas; Sanjyot Vinayak Shenoy; Kail Mandadi; Arthur Zalevsky; Ayushi Verma; Audrey Kishishita; Andrej Salj; Sanjeeva Srivastava; Arun P. Wilita; IIT Bombay, Mumbai, India; UCSF, San Francisco, CA.

PM 662  Electrochemical Oxidation-State Switching of Heme in Cytochrome c Reveals Associated Covalent Modifications; Pablo Scrosati; Lars Konermann; Western University, London, ON.

PM 663  Enzyme-based arginylome discovery in whole proteomes using isotopic labeling; Zonglao Lin; Joanna M Gongora; Yixuan (Axe) Xie; Samaneh G. Kondalaji; Xingyu Liu; Mingzhu Zhou; Faith M Robison; Dongwen Lv; Anna S. Kashina; Michael J. Greenberg; Benjamin A Garcia; Washington University in St. Louis, St. Louis, MO; University of Texas Health Science Center at San Antonio, San Antonio, Texas; University of Pennsylvania, Philadelphia, PA.

PM 664  Identification of 113 new histone marks by CHIMA, a tailored database search strategy; Jinjun Gao; Xintei Sheng; Jianfeng Du; Di Zhang; Chang Han; Yue Chen; Chu Wang; Yining Zhao; The University of Chicago, Chicago, IL; Peking University, Beijing, China; University of Minnesota, Minneapolis, MN.
MP 665 Integrating mass spectrometry and iEF: a state of the art technology for high-resolution characterization of protein charge heterogeneity; Teresa Kwok1; Mike Zhou1; She Lin Chan1; Anna Schaefer1; Xiaoyi Zhang2; Min Du2; 1Advanced Electrophoresis Solutions Ltd., Cambridge, ON, Canada; 2Thermo Fisher Scientific, Shanghai, China; 2Thermo Fisher Scientific, Boston, MA

MP 666 Engineering an enzymatic tool for chemoselective C-terminal modification; Clara Frazier1; Amy Weeks1; 1Biochemistry, University of Wisconsin Madison, Madison, WI

MP 667 An in situ chemically-induced modular strategy to profile E2 ubiquitination events in living cells; Suprama Datta1; Caitlin J. Hill1; Nicholas P. McCurtin1; Rebecca A. Scheck1; 1Tufts University, Medford, MA

MP 668 The regulation and functions of lysine lactylome in Escherichia coli; Hanyang Dong1; Jianji Zhang2; Kai Zhang1; Tianjin Medical University, Tianjin, China

MP 669 Utilizing SILAC Labeling for Imrhe Absolute and Relative Quantification of Glycation and Other PTMs; Sonal Priya1; Ron Orlando1; Marta Popov1; 1University of Georgia, Athens, GA; 2Glycoscientific, Athens, GA

MP 670 Identification and differentiation of positional isomers of O-linked glycopeptides of etanercept using an alternative electron-based MS/MS approach; Zoe Zhang1; Haichuan Liu2; Xuezhi Bi2; 1Sciex, Redwood City, CA; 2SCIEX, Redwood City, CA; 2Bioprocessing Technology Institute (BTI), Singapore, Singapore

MP 671 A single-injection workflow for enhanced peptide mapping using collision-induced dissociation (CID) and electron activated dissociation (EAD); Elliott Jones1; 1Sciex, Redwood City, CA

MP 672 Ion Mobility Separations of Largest Peptide Epimers and Intact Isoformic Protein Peptides with Variant PTM Localizations; Gayani Wijegunawardana1; Hayden A Thurman1; Francis Berthias2; David Williamson3; Haifan Wu1; Gabe Nagy1; Ole Jensen1; Alexandre A Shvarko1; 1Wichita State University, Wichita, KS; 2Southern Denmark University, Odense, Denmark; 3University of Utah, Salt Lake City, UT

MP 673 Redox proteomics of how Trx1 promotes autophagy through transnitrosylation of Atg7 during myocardial ischemia: Narayan Nagarajan1; Shinichi Oka1; Tong Liu1; Hong Li1; Junichi Sadoshima1; 1Rutgers New Jersey Medical School, Newark, NJ

MP 674 Revealing non-canonical phosphorylation of the SARS-CoV-2 nucleocapsid serine/arginine-rich domain using top-down electron capture dissociation and sequence tag generation; Rachel Franklin1,2; Phillip Zhu1; Adrian Guthals2; Joseph Meeuwesen2; Stephen Madden2; Michael C. Hare2; Richard Cooley1; Joseph Beckman2; 1Oregon State University, Corvallis, OR; 2-eMSion, Corvallis, OR; 2Oregon State University, Corvallis

MP 675 Exploring multiplexing strategies for ADP-Ribosylation; Martin Rykar1; Holda Awah Anagho1; Ivo A Hendriks1; Michael L Nielsen1; 1University of Copenhagen, Copenhagen, Denmark

MP 676 A mass spectrometric based characterization of protein aggregates isolated from a cohort of Progressive Supranuclear Palsy patients; Maaike Beuvink1; Mukesh Kumar1; Arthur Viode1; Christoph N Schlaiffer1; Kathrin Wengen1; Timothy Chang1; Michael Dutere2; Daniel Geschwind2; Dennis W Dickson2; Hanno Steen1; Judith Steen1; 1Boston Childrens Hospital, Boston, MA; 2UCLA Mednet, Los Angeles, CA; 3Mayo Clinic, Rochester, MN

MP 677 Site-specific Detection of Protein S-acylation by iodoTMT Labeling and Immobilized anti-TMT Antibody Resin Enrichment; Jian Cal1; Ming Song1; Ming-Dong Yang1; Michael Merchant1; Frederick Benz1; Jon Klein1,2; Craig McClain2,3,7,8, 1Division of Nephrology and Hypertension, Department of Medicine, University of Louisville School of Medicine, Louisville, Kentucky; 2Division of Gastroenterology, Hepatology and Nutrition, Department of Medicine, University of Louisville School of Medicine, Louisville, KY; 3Department of Pharmacology and Toxicology, University of Louisville School of Medicine, Louisville, KY; 5Robley Rex Veterans Affairs Medical Center, Louisville, Kentucky; 6Alcohol Research Center, University of Louisville, Louisville, KY; 7Hepatology and Toxicology Center, University of Louisville, Louisville, KY; 8Robley Rex Veterans Affairs Medical Center, Louisville, KY

MP 678 Global succinylome and proteome of human brain reveal succinylation of key lysine residues of hallmark proteins associated with Alzheimer’s disease; Elizabeth T Anderson1; Yun Yang2; Victor Tapia3; Hui Xu4; Ruchika Bhawal1; Qin Fu5; Gary E. Gibson6; Sheng Zhang1; 1Proteomics and Metabolomics Facility, Cornell University, Ithaca, NY; 2Burke Neurological Institute, Weill Cornell Medical College, New York, NY

MP 679 BioPlexPTM: Linking Cell-Specific Interactions to Differential Protein Expression and Post-Translational Modifications; David R Vanderwall1; Brandon Gassaway2; Laura Pantono Vaites1; David P Nusinow2; Donald S Kirkpatrick3; J. Wade Harper1; Steven P Gyg3; Edward L Huttlin4; 1Harvard Medical School, Boston, MA; 2Interline Therapeutics, Bosto, MA

MP 680 Systematic Profiling Histone Lysine Glycerylation with Chemical Proteomics Analysis; Yi-Cheng Sin1; Yue Chen1; 1University of Minnesota, Minneapolis, MN

MP 681 Emerging role of leumag in innate immune response – potential link to anti-inflammatory effects; Robert Vidmar1; Matej Vizovilek1; Tilen Sever1; Matej Kolaric1; Petra Matjan Stefil2; Georgy Mkhaylov3; Andrea Kozak3; Thomas Reinheckel4; Boris Turk4; Marko Fonovic5; Uozef Stefan Institute, Ljubljana, Slovenia; 4Jozef Stefan Institute, Jamova cesta 39, Slovenia; 5Institute of Molecular Medicine, University of Freiburg, Freiburg, Germany

MP 682 Defining Ubiquitin Role in DNA-Protein Crosslink Repair using Mass Spectrometry; Luke Erber1; Natalia Tretyakova1; 1University of Minnesota, Minneapolis, MN; 2University of Minnesota, Twin Cities, MN

MP 683 Development of Improved Detection Methods for Proteomic Analysis of Tyrosine Sulfation; Cavila Rose1; Matt Davison1; Charles Dann1; 1Indiana University Bloomington, Bloomington, IN

MP 684 LC-MS Identified Esterification of Glutamic Acid by Sorbitol in a Monoclonal Antibody Stability Assessment; Bin Yu1; Sharen Williams1; Glen Young1; 1coherus bioscience, Camarillo, CA

MP 685 Boosting the sensitivity of electron-based fragmentation with cyclic ion mobility; Dale A Cooper-Shepherd1; Emma Madsen-Edwards1; Darren Hewitt1; Jason Wildgoose1; Samantha Ippoliti1; James I. Langridge1; 1Waters Corporation, Wimslow, United Kingdom

MP 686 In-depth and integrated proteomics of thiol oxidation and phosphorylation for a holistic view of cell signaling; Austin Gluth1,2; Xiaolu Li1; Matthew J Gaffrey1; Marina A Gritsenko1; Kiall Francis G Suazo1; 1Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA; 2Department of Biological Systems Engineering, Washington State University, Richland, WA; 3Chemical Biology, Pacific Northwest National Lab, Richland, WA; 4Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, Washington; 5Chemical and Biological Signatures Division, Pacific Northwest National Lab, Richland, WA

MP 687 Inhibition of Demethylation and Oxidation Artifacts in LC-MS Multi-attribute Method (MAM): Pinoli Wei1; Gordon Nicol1; Ping Jiang1; Jie Ding1; 1PPD Inc, Madison, WI
MP 688 Chemical proteomics and data independent acquisition enable drug target identification in Mycobacterium tuberculosis; Dietrich Moster1; Josef Braun2; Stephan Sieber1; 1Technical University of Munich, Munich, Germany; 2Technical, Munich, Germany

MP 689 A Proteomic Investigation of Clarithromycin Resistance and Susceptibility in Mycobacterium abcessus and Mycobacterium massiliense; Sung Hwan Yoon1; Ebru Selen2; Eva Le Run2; Shamira Shalam2; Adrian Zelazny2; Aleksandra Nita-Lazar1; 1NIH/NAID, Bethesda, MD; 2NIH/Clinical Center, Bethesda, MD

MP 690 Assessment of mRNA vaccine stability by evaluating protein expression of SARS-CoV-2 spike protein with isoole dilution mass spectrometry; Paul Branhamp1; Yulanda M. Williamson2; Hans C. Cooper2; Fabio N. Najjar3; John R Barr3; Tracie L. Williams2; 1Oak Ridge Institute for Science and Education, Atlanta, GA; 2NIH/Clinical Center, Bethesda, MD; 3National Center for Environmental Health, Centers for Disease Control and Prevention, Atlanta, GA

MP 691 Novel collection resistance profiles of Acinetobacter nosocomialis clinical isolate, KANO2; Hayoung Lee1,2; Sung Ho Yoon1; Sang-Yeop Lee1; Changkyun Edmond Park1,2; Seung Il Kim1; 1Korea Basic Science Institute, Ochang, South Korea; 2Korea Research Institute of Bioscience and Biotechnology, Yuseong-gu, South Korea

MP 692 Serum Proteomics of COVID-19 Samples Analysed by Liquid Chromatography and Thermo Fisher Scientific Cyclic Ion Mobility Mass Spectrometer: Aishath Shaufa Shareef1; Eleanor Matthews1; Leroy B. Martin III1; Matthew E. Daly1,3,3; Christopher J. Hughes1; Lee Gettings1,3,4,3; Robert Plumb2; Simpson Angela1; Timothy Felton3; Fowler Stephen4; Clare Mills1,4; 1The University of Manchester NHS Foundation Trust, Manchester, United Kingdom; 2Waters, Milford, MA; 3Waters Corporation, Milwauk, United Kingdom; 4The University of Surrey, Guildford, United Kingdom

MP 693 Mass Spectrometry Reveals How Iron and Zinc Accumulation Pathways Promote Azole Resistance in a Clinical Isolate of Aspergillus fumigatus; Catalina Avendano1; Margarita Semis1; Daniel Roth2; Rose S. Atukunda3; Karine Bagramyan4; Lotus Logren1; Sanjeet Dadwal2; Jason E. Stajich5; Markus Kalum6; 1City of Hope, Duarte, CA; 2University of California, Riverside, Riverside, CA

MP 694 Malaria’s Plasmodium vivax invasion Receptors? Mass Spectrometric Comparison of the Membrane Proteomes of Erythrocytes, Reticulocytes, JK-1, and BEL-A Cells; Jessica S Molina1; Daniel Roth2; Manuel Alfonso Palatnik3,3,4; Markus Kalum5; 1City of Hope, Duarte, CA; 2Fundación Instituto de Inmunología de Colombia, Bogotá, Colombia; 3Faculty of Medicine, Universidad Nacional de Colombia, Bogotá, Colombia

MP 695 A novel immunoproteomic approach to MHC class I-restricted peptide discovery for influenza CD8+ T cell adaptive vaccine development; Richard Brase1; Sutopa Dwivedi1; Hager Mohamed2; Aykan Karabudak1; Patrick Romano1; Brian Pfister1; Xiaofang Huang1; 1Emergex USA, Doylestown, PA

MP 696 Novel gene identification in the influenza virus infection model using multi-omics approach, reveals potential CD8+ T-cell adaptive vaccine candidates; Sutopa Dwivedi1; Richard Brase1; Hager Mohamed2; Aykan Karabudak1; Patrick Romano1; Brian Pfister1; Xiaofang Huang1; 1Emergex USA, Doylestown, PA

MP 697 Borellia PeptideAtlas: A proteome resource for the Lyme disease community; Helisa Wippel1; Jaipal P Reddy1; Zhi Sun1; David H Baxter1; David D. Shetzeyberg1; Melissa Caimano2; Robert L. Moritz1; 1Institute for Systems Biology, Seattle, WA; 2University of Connecticut School of Medicine, Farmington, CT

MP 698 Fast and sensitive detection of Urinary Tract Infections through SRM monitoring of machine learning defined peptide signatures; Clarisse Goti1; Florence Roux-Dalvai1; Antoine Lacombre-Rastoll1; Charles Maxey2; Cristina Jacob2; Eve Bérubé2; Maurice Boissoinot2; Michel G. Bergeron2; Neloni Wijeratne3; Claudia Martins4; Arnaud Droit1; 1Proteomics Platform and Computational Biology Laboratory, CHU de Québec Université Laval Research Centre, Québec, QC; 2Thermo Fisher Scientific, San Jose, CA; 3Infectiology Research Centre, CHU de Québec Université Laval Research Center, Québec, QC

MP 699 Lipidomic and proteomic analysis of the ferropotosis-like killing of S. aureus by arachidonic acid; Rutan Zhang1; Ismael A. Barreras Beltran1; Quynh Do3; Brian J. Wenth1; Lbin Xu1; 1University of Washington, Seattle, WA

MP 700 In-containment Orbitrap mass spectrometry analysis of proteomic changes during SARS-CoV-2 infection in a Syrian golden hamster (Mesocricetus auratus) model; Kayla Adcock1; Daniel G. Mead1; Franklin E. Leach1; 1University of Georgia, Athens, GA

MP 701 DDA- and DIA-PASEF profiling of cross-kingdom infections reveals new mechanisms driving disease; Brianna Ball1; Ayman Abou-Hamze1; Xiaofang Huang1; 1Emergex USA, Doylestown, PA

MP 702 Top-Down Proteomics Platform Enabled by Photocleavable Surfactant Azo for the Comprehensive Characterization of Endogenous Phospholamban; Holden T. Rogers1,2; David S Roberts1; Eli J. Larson1,3; Jake A. Melby2; Kalina A. Kostin4; Austin V. Carr1; 1Emergex USA, Doylestown, PA; 2Waters Corporation, Milford, MA; 3Waters Corporation, San Jose, CA; 4Oak Ridge Institute for Science and Technology, Oak Ridge, TN

MP 703 Comprehensive Characterization of Protein Kinases by Native Top-Down Mass Spectrometry: Hein-Ju Chan1; Brad H. Li1,2; Boris Krchev1; David S. Roberts2; Ying Ge1,2,3; 1Department of Chemistry, University of Wisconsin-Madison, Madison, WI; 2Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI; 3Department of Surgery, University of Wisconsin-Madison, Madison, WI; 4Human Proteomics Program, University of Wisconsin-Madison, Madison, WI

MP 704 Systematic optimization of electron activated dissociation for top-down targeted protein sequencing; Jason Caison1; Ihor Batruch1; 1SCIX, Concord, ON

MP 705 Identifying and characterizing heme-acquisition mechanisms in C. diphtheriae using a combination of bottom-up and native top-down proteomics; Andrew K. Goring1; Robert T. Clubb1; Rachel R. Ogorzalek Loo1; Joseph A. Loo1; 1University of California, Los Angeles, Los Angeles, CA

MP 706 An integrated structural proteomics pipeline to study membrane proteins in Arabidopsis thaliana tissues; Stephanie Thibert1; Jesse Wilson1; Vimal Balasubramanian1; Deseree Reid1; John Melchior4,5,6; Kim Hixson2; Tanya Winkler1; Ronal Woljak2; Akelt Bilbao1; Jennifer E. Kyle1; Mowezi Zhou1; 1Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, Washington; 2National Security Directorate, Pacific Northwest National Laboratory, Richland, Washington; 3Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA; 4Department of Pathology and Laboratory Medicine, University of Cincinnati Medical School, Cincinnati, Ohio; 5Physical and Computational Sciences Division, Pacific Northwest National Laboratory, Richland, Washington

MP 707 Enhanced Top-Down Mass Spectrometry Performance with a Hybrid Quadrupole-Multireflecting Time-of-Flight System; Brad J. Williams1; Dale A. Cooper-Shepherd1; Barbara J. Sullivan; James J. Lang, Medical, Farming, PA; 1Waters Corporation, Milford, MA; 2Waters Corporation, Wilmsow, United Kingdom; 3Waters Corporation, Milford, MA; 4Waters Corporation, Wilmsow, United Kingdom; 5Waters Corporation, Milford, MA; 6Waters Corporation, Wilmsow, United Kingdom
MP 708  Capillary Zone Electrophoresis-Mass Spectrometry Reveals Histone Modification Patterns during Zebrafish Embryonic Development: Fei Fang1; Qianyi Wang1; Liangliang Sun2; “Michigan State University, East Lansing, MI

MP 709  Evaluation of Protein Identification by Top-Down Data-Dependent and Data-Independent Acquisition Mass Spectrometry: Abdul Rehan Basharat1; Tian Xu2; Yong Zhang3; Liangliang Sun2; Xiaowen Liu2; “Indiana University - Purdue University Indianapolis, Indianapolis, IN; Michigan State University, East Lansing, MI; Indiana University School of Medicine, Indianapolis, IN; Tulane University School of Medicine, New Orleans, LA

MP 710  Structural diversity of kinase complexes revealed by top-down mass spectrometry with micro-scale size exclusion chromatography: Boris Khriel1, 2, 3; Jake A Melby1; Holden T Rogers1; Eli J Larson1; Kevin M. Buck1; Emily A Reasoner1; Hsin-Ju Chan1; Charlotte Jette1, 2, 3, 5; Ying Ge1, 4, 7; “Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI; 2University of Siegen, Siegen, Germany; 3CSSB, Center for Structural Systems Biology, Hamburg, Germany; 4Department of Chemistry, University of Wisconsin-Madison, Madison, WI; 5German Electron Synchrotron DESY, Hamburg, Germany; 6Leibniz Institute of Virology (LIV), Hamburg, Germany; 7Human Proteomics Program, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI

MP 711  Improved Dissociation Efficiency of Protein Ions within a Trapped Ion Mobility Device via Supercharging and Dynamic Control of Ion Count: Katherine A Graham1; Charles F Lawlor1; Nicholas B Borotta1; “University of Nevada Reno, Reno, NV

MP 712  Towards top-down proteomics of large proteoforms using capillary zone electrophoresis-tandem mass spectrometry: Olivia Gordon1; Liangliang Sun2; “Michigan State University, East Lansing, MI

MP 713  Increased Dimensional Analysis of Native Proteins via Synthetic Nanopore: Mario Rodriguez Garcia1; John R. Yates III1; “Scripps Research, La Jolla, CA

MP 714  Towards deep top-down protein analysis by tandem-trapped ion mobility spectrometry/mass spectrometry coupled with parallel accumulation serial fragmentation (tandem-TIMS/PASEF): Christian Bleiholder1; Fanny C Liu1; Jusung Lee1; Melvin A Park2; Mark E Ridgway3; Alina Thiesen3; Christopher A Wotton4; Stephen Fried5; “Florida State University, Tallahassee, FL; 2Bruker Daltonics, Billerica, MA; 3Bruker Daltonics GmbH & Co. KG, Bremen, Germany; 4Bruker Daltonics GmbH & Co.KG, Bremen, Germany; 5John Hopkins University, Baltimore, MD

MP 715  MASH Native: A Unified Solution for Native Top-Down Proteomics Data Processing: Sean J. Mellwain1; Eli J. Larson1; Melissa R. Pergande1; Michelle E. Moss1; Kalina J. Rossler1; R. Kent Werner1; Boris Khriel1, 2; Harini Josyer1; Jake A. Melby1; David S Roberts1; Kyndallane A. Pike1; Zhouxin Shi1; Hsin-Ju Chan1; Bridget Knight1; Holden T. Rogers1; Kyle A. Brown1; Irene M. Ong1; Ky Gron-Jaeng1; Michael T. Marty1; Ying Ge1; “University of Wisconsin-Madison, Madison, WI; 2University of Siegen, Siegen, Germany; 3University of Tübingen, Tübingen, Germany; 4University of Arizona, Tucson, AZ

MP 716  Improved Dissociation Efficiency of Protein Ions within a Trapped Ion Mobility Device via Supercharging and Dynamic Control of Ion Count: Katherine A Graham1; Charles F Lawlor1; Nicholas B Borotta1; “University of Nevada Reno, Reno, NV

MP 717  Application of Mass Spectrometry-Based Methods to Define the Cell-Surface Proteome of Murine Intestinal Organoids: Dylan Z Dieters-Castador1; Paolo Manzanillo1; Daryl Bulloch1; Han-Yin Yang1; David Chow1; Aman Makaju2; Bradford Gibson1; “School of Pharmacy, University of Wisconsin-Madison, Madison, WI

MP 718  Proteome profiling of rat brain cortical changes during the early postnatal brain development using a surfactant-free protocol and label-free quantitation: Witold M Winiak1; William Padgett1; Emily M Pitzer1; David W Herr1; “US EPA Research Triangle Park, NC

MP 719  AbsoluteQuantitation of Peptides and Proteins AfterDerivatization by Coulometric Mass Spectrometry: Praneeth Ivan Joel Fru1; Md Tamirul-A-Hassan1; Yongling Ai1; Hao Chen1; “New Jersey Institute of Technology, Newark, NJ

MP 720  Proteome profiling of rat brain cortical changes during the early postnatal brain development using a surfactant-free protocol and label-free quantitation: Witold M Winiak1; William Padgett1; Emily M Pitzer1; David W Herr1; “US EPA Research Triangle Park, NC

MP 721  APEX Labeling and LC-MS/MS Analysis for Exploring the Proximity Proteome of YY1: Zhongwen Cao1; Yenyu Yang1; Yuncheng Wang1; “900 University Ave, Riverside, CA 92521, Moreno Valley, CA

MP 722  After Derivatization by Coulometric Mass Spectrometry: Praneeth Ivan Joel Fru1; Md Tamirul-A-Hassan1; Yongling Ai1; Hao Chen1; “New Jersey Institute of Technology, Newark, NJ

MP 723  Application of Mass Spectrometry-Based Methods to Define the Cell-Surface Proteome of Murine Intestinal Organoids: Dylan Z Dieters-Castador1; Paolo Manzanillo1; Daryl Bulloch1; Han-Yin Yang1; David Chow1; Aman Makaju2; Bradford Gibson1; “School of Pharmacy, University of Wisconsin-Madison, Madison, WI

MP 724  APEX Labeling and LC-MS/MS Analysis for Exploring the Proximity Proteome of YY1: Zhongwen Cao1; Yenyu Yang1; Yuncheng Wang1; “900 University Ave, Riverside, CA 92521, Moreno Valley, CA

MP 725  Solution-stabilized TMT & TMTpro reagents in 96-well plates for high-throughput sample processing: Dustin Frost1; Ryan Bomgardner1; “Thermo Fisher Scientific, Rockford, IL

MP 726  Proteome profiling of rat brain cortical changes during the early postnatal brain development using a surfactant-free protocol and label-free quantitation: Witold M Winiak1; William Padgett1; Emily M Pitzer1; David W Herr1; “US EPA Research Triangle Park, NC

MP 727  14-plex DeAla Isobaric Tags for High-Throughput Quantitative Proteomics: Pei-Kai Liu1; Ting-Jia Gu2; Danqing Wang3; Yanyan Liu1; “Bruker Daltonics, Billerica, MA; 2University of Wisconsin-Madison, Madison, WI; 3School of Pharmacy, University of Wisconsin-Madison, Madison, WI

MP 728  Deciphering phytocannabinoid pharmacological effects using C. elegans, proteomics and bioinformatics: Fatma Boujour1; Jennifer Ben Salem1; Bruno Nkambou1; Francis Beaudry1; “Universite de Montreal, St-Hyacinthe, QC

MP 729  Determination of vanilloid targets in Caenorhabditis elegans using Thermal proteome profiling: Bruno Nkambou1; Jennifer Ben Salem1; Francis Beaudry1; “Universite de Montreal, St-Hyacinthe, QC

MP 730  Systematic investigation of the N-terminal effect on protein stability: Zewu Yang1; Senhan Xu1; Kejun Yin1; Xing Xu1; Ronghu Wu1; “School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA
MP 731  A Benchmarking Workflow for High-Throughput DIA Label-Free Quantification using a Novel High-Resolution Accurate Mass Platform; Anna V. Pashkova¹; Julia Kraegenbring¹; Pedro Navarro¹; Tabiwan Ng An. Arrey¹; Eduard Denisov¹; Hamish Stewart¹; Jeff Op De Beeck²; Nicolaie Eugen Damoc³; ¹Thermo Fisher Scientific, Bremen, Germany; ²Thermo Fisher Scientific, Ghent, Belgium

MP 732  A Comparative Spatial Quantitative Proteomics Analysis of LBD Human Brain; Ju Wang¹; Huan Sun¹; Zhiping Wu¹; Junmin Peng¹; ¹St.Jude Children Research Hospital, Memphis

MP 733  Proteomic and Phosphoproteomic Investigation of Neural Stem Cell to Oligodendrocyte Precursor Cell Differentiation Reveals Phosphorylation-Dependent Processing of Dclk1; Robert Hardt¹; Alireza Deghghi¹; Carmen Schoor¹; Markus Gödderz²; Nur Cengiz³; Shiva Ahmadi¹; Ramesh Sharma¹; Karin Schork²-³; Martin Eisenacher²-³; Volkmar Gieselmann¹; Dominic Winter¹; ¹Institute for Biochemistry and Molecular Biology, Medical Faculty, Rheinische Friedrich-Wilhelms-University of Bonn, Bonn, Germany; ²Medizinisches Proteom-Center, Medical Faculty, Ruhr-University Bochum, Bochum, Germany; ³Medical Proteome Analysis, Center for Protein Diagnostics, Ruhr-University Bochum, Bochum, Germany

MP 734  Quantitative spatial proteomics combined with lipidomic analysis of human hippocampus using laser capture microdissected cells from MALDI-imaged tissue sections; Lauren R. DeVine¹; Caitlin M. Tressler¹; Rahul A. Bharadwaj¹; Kristine Glunde¹; Daniel Weinberger¹; Robert N. Cole¹; ¹Johns Hopkins School of Medicine, Baltimore, MD; ²Lieber Institute for Brain Development, Baltimore, MD

MP 735  Ultra-high-resolution MS1-quantification combined with deconvolution of chimeric MS/MS spectra enables in-depth quantitative proteomics and application in high-quality spatial proteomics; Shuo Qian¹; Shichen Shen¹; Shihan Huo²; Salee Rasam¹; Min Ma¹; Jun Qu¹-²; ¹Roswell Park Comprehensive Cancer Center, Buffalo, NY; ²University at Buffalo, Buffalo, NY

MP 736  Spatiotemporally Resolved Notch Interactions on its Path from Membrane to Nucleus; Marian Kalocsay¹; Alexandre P Martin¹; Gary Bradshaw¹; Robyn J Elser¹; Stephen C Blacklow²; ¹UT MD Anderson Cancer Center, Houston, TX; ²Harvard Medical School, Boston, MA

MP 737  A Chemoproteomic Approach for the Quantitative Identification of Arsenic-Binding Nuclear Proteins; Shiyuan Guo¹; Pengcheng Wang²; Yinsheng Wang²; ¹University of California Riverside, Riverside, CA; ²University of California, Riverside, Riverside, CA

MP 738  Quantitative Assessment of Epitranscriptomic Reader, Writer and Eraser Proteins Modulated by H4K16ac and H3K36me3; Jiekai Yin¹; Tianyu Qi¹; Lin Li¹; Yinsheng Wang¹; ¹University of California, Riverside, Riverside, CA

MP 739  FragPipe-Analyzer: an interactive and user-friendly web application for the analysis of quantitative proteomics data; Yi Hsiang¹; Haijian Zhang¹; Ginny Xiaohe Li¹; Fengchao Yu²; Felipe Da Veiga Leprevost²; Ralf B Schittenhelm²; Alexey I. Nesvizhskii¹-²-³; ¹Department of Computational Medicine and Bioinformatics, Ann Arbor, MI; ²Monash Proteomics & Metabolomics Facility, Department of Biochemistry and Molecular Biology, Biomedicine Discovery Institute, Monash University, Clayton, Australia; ³Department of Pathology, University of Michigan, Ann Arbor, MI

MP 740  Targeted proteomics analysis of metabolic pathway proteins to develop and optimize Chinese Hamster Ovary (CHO) cell culture medium and feed; Km Shams Ud Doha¹; Chengjian Tu¹; Asik Didar¹; Jie Qiu¹; ¹Thermo Fisher Scientific, Grand Island, NY

MP 741  Benchmarking the performances of label-free protein quantitation: Data dependent acquisition (DDA) vs. data independent acquisition (DIA); Ling Li¹; Belinda Willard¹; ¹Cleveland Clinic, Cleveland, OH
TP 001 Single Fiber Quantitation of Solid-Phase Microextraction Samples with Five-shot Direct Analysis: G. Ascher Newsome; Erin R. Birdsell; Hannah A. Lawther; Smithsonian Museum Conservation Institute, Sulland, MD; "Smithsonian National Museum of the American Indian, Sulland, MD

TP 002 Time-course monitoring of Hexafluorophosphate decay using Soft Ionization by Chemical Reaction In Transfer (SICRIT) ion source; Motoshi Sakakura; Teruhisa Shiota; AMR Inc., Meguro-Ku, Japan

TP 003 The Role of Ion Suppression in Secondary Electrospray Ionization-Mass Spectrometry; Cedric Wetheril; Stamatiou Giannoukos; Renato Zenobi; ETH Zurich, Zurich, Switzerland

TP 004 Understanding of phenomena of Si deposition on the electrode in counter flow atmospheric pressure chemical ionization source; Shun Kumano; Satoshi Wakiita; Tatsuo Norig; Research & Development Group, Hitachi Ltd., Kokubunji-Shi, Japan; "Digital Systems & Services, Hitachi Ltd., Omika, Japan

TP 005 A new frontier of direct analysis: real-time in electron ionization detection (REI) first coupling of ambient sampling with electron ionization; Adriana Ario; Giovanna Nevola; Giorgio Famignini; Pierangela Palma; Achille Cappiello; UNIVERSITY OF URBINO CARLO BO. URBINO, Italy; "Vancouver Island University, Nanaimo, BC

TP 006 Infrared Matrix-Assisted Laser Desorption Electrospray Ionization with a Heated Electrospray Emitter; Kevan T. Knizner; David C. Muddiman; "FTMS Laboratory for Human Health Research, Department of Chemistry, Raleigh, NC

TP 007 Biocompatible solid-phase microextraction pin-probe electrospray ionization-mass spectrometry system facilitates high sensitivity and ease of automation; Wei Zhou; Janusz Pawliszyn; "University of Waterloo, Waterloo, ON

TP 008 Comprehensive characterization of an engineered Cas9 protein and its post-translational modifications (PTMs) by LC-MS/MS; Zhichang Yang; Sahana Mollari; Chao-Xuan Zhang; Alicja Powers; Yan Lu; SCIEX, CA, USA; "Scri, CA; "St. Jude Children's research hospital, Memphis, TN; "St. Jude Children's Research Hospital, Memphis, TN

TP 009 Contained Secondary Electrospray Ionization Mass Spectrometry: Toward High-Throughput Screening of Amines as CO2 Capture Reagents; Dmytro S. Kulyk; Taghi Sahraei; Ayesha Sethi; Abraham Kwame Badu-Tawiah; "The Ohio State University, Columbus, OH; "Siberian State Medical University, Tomsk, Russia; "Skolkovo Institute of Science and Technology, Skolkovo, Russian Federation

TP 010 Single Spot (<1mm) Dewaxing and Analysis of Paraffin-Embedded Tissue sections using Liquid Microjunction Sampling Probe (LMJ-SSP) mass spectrometry (MS); Haiy Metwally; Malek Hassan; Jessie Deng; Richard D. Oleschuk; "Queen's University, Kingston, ON

TP 011 Rapid in-line solvent switching for liquid micro-junction surface sampling probe (LMJ-SSP) based mass spectrometry detection; Jian Yu; Malek Hassan; Richard D. Oleschuk; "Queen's University, Kingston, ON

TP 012 Real-time subsurface analysis and depth profiling using a sharpened liquid micro-junction surface sampling probe (LMJ-SSP); Julia McPhail; Jian Yu; Richard D. Oleschuk; "Queen's University, Kingston, ON

TP 013 ESI from surface of spherical probe made of inert fibrous material as a tool for investigation of rude biological samples; Igor Popov; Mariya Shamraeva; Ekaterina Shamara; Stanislav Pekov; "MIPT, Dolgoprudny, Russian Federation; "Siberian State Medical University, Tomsk, Russia; "Skolkovo Institute of Science and Technology, Skolkovo, Russian Federation

TP 014 Optimization of Enclosure for introduction of Polar Organic Modifiers to Protein Analysis in DESI-MS;
Improved cation exchange chromatography of monoclonal antibody on a monodisperse particle column enables deep characterization and biosimilarity assessment; Sara Carillo1; Florian Fuess1; Silvia Millan Martin1; Shanhua Lin1; Jonathan Bones1;2; NIBRT, Dublin, Ireland;2Thermo Fisher Scientific, Sunnyvale, CA;3School of Chemical and Bioprocess Engineering, University College Dublin, Dublin, Ireland

TP 027
A High-Resolution UHPLC-MS based method for quantifying monoclonal antibody from human serum; Connor E Gould1; Jake Ocque2; Robin Difrancesco2; Qin Ma3; Raymond Cha3; Gene Morse3; Troy D. Wood1;1Department of Chemistry, University at Buffalo, Buffalo, NY;2Department of Pharmacy Practice School of Pharmacy and pharmaceutical sciences, University at Buffalo, Buffalo, NY

TP 028
Multiplexed Bioanalysis ofVariousAntibody–Drug Conjugates (ADCs) in Cynomolgus Monkey Plasma/Using Immunoaffinity LC-MS/MS; Eric W. Ma1; Minghao Sun1; William R. Mylott Jr.1; David Roos2; PPD, Richmond, VA;1Boehringer Ingelheim, Ridgefield, CT

Unambiguous Identification and Localization of Isoaspartic Acid in Therapeutic Proteins by Optimized Enzymatic Digestion and Electron Transfer Dissociation; Lidong He1; Jason L. Richardson1; Zhongqi Zhang2; Les Miranda3; Suminda Hapuarachchi3; Jun Zhang4; Jiu-Li Song5; Argen, Thousand Oaks, CA

Polyclonal antibody epitope mapping at single amino acid resolution for pregnancy malaria vaccine design; Santosh A Misal1; Robert Morrison2; Jonathan Renn1; Yai Donitchamou1; Martin Burkhart3; Alessane Dicko2; Patrick Duffy2; Michal Fried1; Molecular and Pathogenesis Biomarkers Section, Laboratory of Malaria Immunology and Vaccinology (LMIV), National Institute of Allergy and Infectious Diseases (NIAID), National Institutes of Health (NIH), Bethesda, MD;2Pathogenesis and Immunity Section, Laboratory of Malaria Immunology and Vaccinology (LMIV), National Institute of Allergy and Infectious Diseases (NIAID), National Institutes of Health (NIH), Bethesda, MD;3Malaria Research & Training Center, Faculty of Medicine, Pharmacy and Dentistry, University of Sciences Techniques and Technologies of Bamako, Bamako, Mali

TP 030
Orthogonal techniques for LCMS characterization of a lysine conjugated ADC; Lucy Fernandes1; St. John Skitoni1; Marshall Bern1; Kriatza Radd1; Andreas Nageli2; Sabrina Forri1; Protiva Mettler, LLC, Cupertino, CA;1Genovis AB, Lund, Sweden

TP 031
Zero False Positives in Multi-Attribute Method New Peak Detection with a Statistics Guided Approach; Qiningwen Cao1; John Guan1; Delia Li1; Jennifer Zhang1; Riley Togashi1; Elizabeth Johnson1; Jia Guo2; Peilu Liu1; Lance Cadang1; Monica Sadek1; Feng Yang1; Genetech, Inc., South San Francisco, CA;1Amy Genentech, Inc., South San Francisco, CA;2Amgen Inc., Thousand Oaks, CA;3Amgen Inc., Bumaby, BC

TP 032
Targeted Determination of the Abundant Therapeutic Monoclonal Antibody Interactome in Human Plasma, Serum, and Synthetic Mimics; G. Reid Bshog1; John J. Correia1;1University of Mississippi Medical Center, Jackson, MS

TP 033
Detection of antibody Fab glycosylation impact on antigen binding and blocking of endogenous protein Interactions by SEC and intact LC-MS; Daniel Woodall1;2; Arnold McAuley1; Christy A Thomson1; Thomas M Dillon2; Arnold McAuley1; Pavel Bondarenko1;2; Amgen Inc, Thousand Oaks, CA;1Amgen Inc., Bumaby, BC

TP 034
Increasing Coverage of Host Cell Proteins by FAIMS Depletion Using Low, High, and Combined Edge Retention Times; Craig P Dunfee; Thermo Fisher Scientific, West Palm Beach, FL

TP 035
TP 036 Facilitating LC-MS Analysis of Fusion Protein Therapeutics by Enzymatic Hydrolysis of Flexible Linkers; Andreas Naegeli1; Magdalena Widgren-Sandberg1; Maria Nordgren1; Camilla Sivertsson1; John Lindsay1; Rikke Ryttel1; Genovis AB, Lund, Sweden; 2Genovis Inc, Cambridge, MA

TP 037 Comprehensive characterization of monoclonal antibodies (mAbs) and Antibody Drug Conjugates (ADCs) on a novel high-resolution accurate mass platform; Kristina Szrzenzi1; Angela Crescuiolo2; Kai Scheffler1; Nicolaie Eugen Damoc2; 1ThermoFisher Scientific, Basel, Switzerland; 2Thermo Fisher Scientific, Bremen, Germany

TP 038 Super-immunity by pan-sarbecovirus nanobodies; Yuefei Xiang1; Wei Huang2; Hejun Liu3; Zhe Sang4; Sham Nambulli5; Jérémie Thibaud4; 5University of Antwerp, Antwerpen, Belgium; 1Rapid Novor Inc., Kitchener, ON; 2Rapid Novor Inc, Kitchener

TP 042 MALDI-TOF Mass Spectrometry with Machine Learning for High-Throughput Screening of Raw Milk for Evidence of Mastitis; Jon Thompson1; Savana Everhart1; Sumon Sarkar1; Beth Clayton2; 2Texas Tech University, Amarillo, TX; 2Texas Dairy Herd Improvement Association, Canyon, Texas

TP 043 Diving deeper with depthcharge: A transformer deep learning framework for modeling mass spectrometry data; William E Fondie1; Wout Bittiumereux2; Meihi Yilmaz3; William S Nolen4; 1Talus Biosciences, Seattle, WA; 2University of Antwerp, Antwerpen, Belgium; 3University of Washington, Seattle, WA

TP 044 Mapping Competitive Activity Based Protein Profiling Data to AlphaFold2 Models; Adam L Borne1; Yusuf Adeshina1; Natalia Zaliznyak2; Luca Naël1; Zachary Carpenter1; 1VantAI, New York, NY

TP 045 GlycoNovo: Deep learning based framework for N-linked glycan DeNovo sequencing; Qianqiu Zhang1; Zeqin Mao1; Weiping Sun2; Xiuyu Zhang2; Ngoc Hieu Tran1; Xin Lei2; Baozhun Shan2; Ming Li2; 1University of Waterloo, Waterloo, ON; 2Bioinformatics Solutions Inc, Waterloo, ON

TP 046 Machine learning of cancer type and tissue of origin from proteomes of 1,277 human tissue samples and 975 cell lines; Zhaoxiana Cai1; Zainab Noor1; Adel T Aref1; Emma L Boys2; Dylan Xavier2; Natasha Lucas3; Steven G Williams3; Jennifer M Koh4; Erin Sykes4; Rebecca C Poulos4; Peter G Hains4; Phillip J Robinson5; Rosemary Balleine5; Roger R Reddel5; Qing Zhong6; ProCan8; Children’s Medical Research Institute, Faculty of Medicine and Health, The University of Sydney, Westmead, Australia; 2Westmead Institute for Medical Research, Westmead, Australia

TP 047 Using protein structures predicted by Alphafold2 to understand the fragmentation of proteins from pathogenic bacteria analyzed by MALDI-TOF-TOF-MS/MS; Jiyun Park1; Clifton K Fagerquist1; Produce Safety & Microbiology, Western Regional Research Center, Agricultural Research Service, USDA, Albany, CA; 2Oak Ridge Institute of Science Education, Oak Ridge, TN

TP 048 Al-based Comprehensive Prediction of Tandem Mass Spectra of Tryptic Peptides to Generate Proteome-Scale Mass Spectral Libraries; Joel S Lapin1; Xinjian Yan1; Qian Dong1; 1NIST, Gaithersburg, MD; 2Georgetown University, Washington DC, DC

TP 049 Transfer Learning Methods Improve Deep Fragmentation Model; Alexandros Pachos1; Anna Susmeli1; Oliver M Bernhardt1; An-phi Nguyen; Tejas Gandhi1; Lukas Reiter1; Biognoys AG, Zurich, Switzerland

TP 050 AllMSPeak: a Convolutional Neural Network-Based Model for Ground-Truth Liquid Chromatography/Mass Spectrometry Features Selection; Hiu-Lok Nga1; Zongwei Cai1; 1Hong Kong Baptist University, Hong Kong, China

TP 051 Exploring the Temporal Metabolome of "Hyperfood" Kimchi with Data-Driven Trajectory Cluster Analysis; Ali Lotfi1; Alla Veselkova1; Alexey Melnik2; Kirill Veselkov2; Alexander Aksenov3; 3University of Connecticut, Storrs, CT

TP 053 Applying Automated Machine Learning for Classification and Regression in Large-Scale Clinical Proteomics Datasets; Amir Aalavii1; Harendra Guturu1; Guhan Venkataraman1; Jane Lange1; Matthew Chang2; Travis Moore2; Khater Mohamedelshok2; Anna Halamia3; Frank Schmidt3; Karsten Suhre3; Mark Flory4; Serafin Batzoglou1; 1Seer, Inc., Redwood City, CA; 2Oregon Health & Science University, Portland, Oregon; 3Weill Cornell Medicine - Qatar, Education City, Qatar

TP 054 Estimating the uncertainty of AI predictions of the Kovats retention index; Lewis Geer1; Douglas Siotta2; 1NIST, Gaithersburg, MD; 2NIST, Gaithersburg, MD

TP 056 Improving Identification Confidence in Suspect Screening of Consumer Products using Machine Learning; William D Watson1; Kristin A Favela1; Jake A Janssen1; Michael J Hartnett1; Heath A Spidle1; Bertis R&D Division, Bertis Inc., South Korea;

TP 057 Realistic in silico generation and augmentation of mass spectrometry based proteomics data using generative adversarial networks; Varitha Tewari; Sunghyun Huh2; Sangtae Kim; Olga Vitek1; 1Northeastern University, Boston, MA; 2Bertis R&D Division, Bertis Inc., Seongnam-si, South Korea

TP 058 A novel deep learning approach to reconstruct sub-micron spatial and FT-ICR spectral mass spectrometry imaging using co-registered multimodal data; Md
Novel supervised learning algorithms for real-time optimization of mass spectrometry-based proteomics data acquisition to improve proteome and interactome coverage; Iryna Abramchuk; Yun-En Chung; Alona Petrová; Changhai Zhan; Jonathan R Krieger; Tharan Srikumar; Mathieu Lavallée-Adam; University of Ottawa, Ottawa, ON; Bruker Scientific LLC, San Jose, CA; Bruker Ltd., Milton, ON

Automating GC/MS peak integration using Machine Learning Modelling for maximizing throughput, quality and enhancing consistency; Thomas Bliszpam; Tamas King; Winnie Ouyang; Steve Pruimzanger; Agilent Technologies, Cedar Creek, TX; Agilent Technologies, Inc, Houston, Hong Kong

Comparative Analysis of Protein Folding Stability-Based Profiling Methods for the Characterization of Breast Cancer; Morgan Bailey; Hyejin Park; Michael C. Fitzgerald; Duke University, Durham, NC

Analysis of serum metabolomics characteristics of 63 acute leukemia patients by liquid chromatography-mass spectrometry; Wang Lei; Beijing Lu Daopei Institute of Hematology, Beijing, China

Identification of Lyso-Platelet Activating Factors as Central Nervous System Biomarkers for Tay-Sachs Disease; Pamela Kell; Sonali Mishra; Tobo Taghiari; Heather L Gray; Daniel S Ory; Xuntian Jiang; Washington University School of Medicine, St. Louis, MO; University of Massachusetts Medical School, Worcester, MA; Casma Therapeutics, Cambridge, MA; Washington University School of Medicine, St. Louis, MO

Development of a dia-PASEF based workflow for single-shot 3K global proteomics of cerebrospinal fluid amenable to high-throughput and large cohort analysis; Kuznari Sandeep; Takeo Kamakura; Yuetang Ye; Satya Saxena; Viewanath Devanarayan; Pallavi Sachdev; Kanta Horie; Eisai Co., Ltd., Tsukuba-shi, Japan; Eisai Inc., Nutley, NJ

High-performance serum metabolic fingerprints encode breast cancer; Yida Huang; Kun Qian; Shanghai Jiao Tong University, Shanghai, China; Shanghai Jiao Tong University, Chicago, IL

Multi-omic landscapes of Nasopharyngeal Carcinoma reveal patterns associated with induction chemotherapy response; Dongxue Wang; Yingqin Li; Xiantong Shao; Chunxian Ou; Jun Ma; Fuchu He; Beijing Proteome Research Center, National Center for Protein Sciences, Beijing, China; Sun Yat-Sen University Cancer Center, guangzhou, China

Energy Depletion and Metabolic Alterations in Cellular Model of Fabry Disease; Ryan W. Pearce; Jillian Kedger; Igor Radzik; Yana I Sanders; Cleveland State University, Cleveland, OH

Discovery proteomics identifies specific alterations in lysosomal and autophagy protein pathways in a neuronal model of preamyloidogenic brain disorders; Hilary Andaluz Aquilari; Mali Cosden; Lei Ma; Jacob Marcus; Robert Drolet; Nathan Hatcher; Merck & Co., Inc., West Point, PA

Development of Click-Chemistry-based Affinity Purification for Sequencing (Click-seq) and Analysis of Global Interactions of Estrogen with Chromatin Molecules; Quynh-Trang Do; Husam Katefan; Shu-Hui Chen; National Cheng Kung University, Tainan, Taiwan

Determining pathogenicity of gangliosides in urine of patients suffering from diabetic kidney disease by high resolution tandem mass spectrometry; Raluca Ioga; Anca Suteanu-Simulescu; Mirea Sarbu; Ligia Petrică; Alina D. Zamfir; Department of Condensed Matter, National Institute for Research and Development in Electrochemistry and Condensed Matter, Timisoara, Romania; Department of Medical Chemistry, University of Nephrology, “Victor Babes” University of Medicine and Pharmacy, Timisoara, Romania; Department of Technical and Natural Sciences, “Aurel Vlaicu” University of Arad, Arad, Romania

Non target TOF-analysis of oxidation products of aromatic amino acids with chlorine dioxide as potential marker of cell death; Ferdinand Maer Wachtler; Hendrik Kersten; Thorsten Benter; University of Wuppertal, Wuppertal, Germany

Untargeted, deep plasma proteomics and metabolomics analysis in ΔCLN3 porcine model enabling biomarker discovery and mechanistic insights into Batten disease; Brittany Lee; Christine Neville; Ting Huang; Mitchell Reichert; Anna Haimova; Alina D. Zamfir; Daniel Hornburg; Jon Brudvig; Seer Inc., Redwood City, CA; Amicus Therapeutics, Philadelphia, Pennsylvania; Pediatrics and Rare Disease Group, Sanford Research, Sioux Falls, South Dakota; Sanford Burnham Prebys, San Diego, California

Proteoform Detection in Deep Plasma Proteomics through Peptide Expression Correlation; Yixing Huang; Jiong Wang; Alexey Stukalov; Ting Huang; Amanda Heit; Douglas Siler; Daniel Hornburg; Jon Brudvig; Seer Inc., Redwood City, CA; Amicus Therapeutics, Philadelphia, Pennsylvania; Pediatrics and Rare Disease Group, Sanford Research, Sioux Falls, South Dakota; Sanford Burnham Prebys, San Diego, California

Untargeted metabolomics reveals predictive biomarkers for Type 2 diabetes mellitus in the Indian population; Sheena A Rana; Pramod P Mangalkar; Vivek Mishra; Bhushan Borkar; Pralay Nigalkar; Rakesh Kumar Sahay; Lakshman Kumar; Indian Institute of Technology Bombay, Mumbai, India; Clarity Bio Systems
TP 079  Very large-scale cerebrospinal fluid proteomics for biomarker discovery in multiple sclerosis; Jakob Bader1; Christine Makarov2; Sabrina Richter2; Friederike Heid1; Patricia Skowronski3; Maximilian Strauss4; Constantin Ammar5; Marvin Thieler5; Wen-Feng Zeng4; Isabella Bludau4; Benjamin Schubert4; Fabian Theis5; Christiane Gasperi6; Bernhard Hemmer7; Matthias Mann1; 1Department of Proteomics, Max Planck Institute of Biochemistry, Martinsried, Germany; 2Clinical Neuroimmunology Unit, University Hospital rechts der Isar, Technical University Munich, Munich, Germany; 3Institute of Computational Biology, Helmholtz center Munich, Neuherberg, Germany; 4Department of Proteomics, Max Planck Institute of Biochemistry, Martinsried, Munich, Germany; 5NFN Center for Protein Research, University of Copenhagen, Copenhagen, Denmark

TP 080  diAPOSEF-based comparative proteomics analysis of blood-derived exosomes from drug naïve Parkinson’s disease (PD) patients in two independent patient cohorts; Laura F Dagley1, 2; Ai Huey Tan3; Samantha J Emery-Corbin4; Jamuna M Yousef1, 2; Ahmed Mohamed1, 2; Andrew Evans5; Seong-Seng Tan6; Shen-Yang Lim4; Han-Joon Kim7; Andrew I Webb1, 2; 1Advanced Technology and Biology Division, The Walter and Eliza Hall Institute of Medical Research, Parkville, Australia; 2Department of Medical Biology, University of Melbourne, Parkville, Australia; 3Faculty of Medicine, University of Malaya, Kuala Lumpur, Malaysia; 4Bioinformatics Division, The Walter and Eliza Hall Institute of Medical Research, Parkville, Australia; 5Movement Disorders Service, Department of Neurology, Royal Melbourne Hospital, Parkville, Australia; 6Department of Medicine, Royal Melbourne Hospital, Parkville, Australia; 7Department of Neurology and Movement Disorder Center, Seoul National University Hospital, Jongno-gu, South Korea

TP 081  Interferon-γ modulates tissue metabolic response during Chagas disease; Azadeh Nasuhidehnavi; Mahboob Lesani; Jarrod A Roach; Monica Ness; Micah D’Armand De Chateauvix; Laura-Isobel McCaill; 1University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK; 2University of Oklahoma, Department of Microbiology and Plant Biology, Norman, OK

TP 082  A machine learning approach of metabolomic, clinical and comorbidity data to predict COVID-19 severity and hospitalization duration; Georgia Charkoftaki1; Reza Aalizadeh2; Alvaro Santos-Neto3; Wan Ying Tang4; Emily A. Davidson3; Varvara Nikolopoulou2; Yewei Wang4; Brian Thompson2; Tristan Furnary2; Ying Chen4; Andreas Copp1; Wade Schult1; Akiko Iwasaki1, 2; Richard W. Pierce1; Charles S. Dela Cruz1; Gary V. Desir1; Naftali Kaminski1; Shelli Farhadian1; Kirill Veselkov1, 2; Rupak Datta1; Melissa Campbell1; Nikolaos S. Thomaidis1; Albert I. Ko1; David C. Thompson1; Vasiliu Basiliu1; 1Yale University, New Haven, CT; 2National and Kapodistrian University of Athens, Greece; 3University of São Paulo, São Carlos, Brazil; 4Yale School of Public Health, New Haven, CT; 5Harvard Medical School, Boston, MA; 6Howard Hughes Medical Institute, Chevy Chase, MD; 7Imperial College, London, London, United Kingdom; 8Duke University, Durham, NC

TP 083  Peptidomic characterization of protease activity and biomarker discovery of COPD pathogenesis associated with HIV in clinical BALF samples; Monica E. Kruk1, 2; Danielle Weise1; Sarah Samorodnitsky3; Carmen Martin-Alonso1; Erick Lock3; Subina Mehta3; Pratik D Japtap3; Chris Wendt4, 5; Timothy J Griffin4; 1Department of Medicine, University of Minnesota, Minneapolis, MN; 2Biochemistry, Mol. Biology and Biophysics, University of Minnesota, Minneapolis, MN; 3Division of Statistics, School of Public Health, University of Minnesota, Minneapolis, MN; 4Harvard-MIT Division of Health Sciences and Technology, MIT, Cambridge, Massachusetts; 5Minneapolis Veterans Affairs Healthcare System, Minneapolis, MN

TP 084  Integrated workflows for mass-spectrometry based profiling of cancer cell derived extracellular vesicles in biofluids and tissues; Jody Vyuktuka1; Taketo Kato2; Hirokuya Maximayama2; Allison Stewart2; Ehsan Iraijzad2; Yining Cai1; Fuchung Hsiao1; Jennifer B Dennisson1; Edwin J Ostrin1; Hai T Tran1; Carl M Gay1; Lauren A Byers1; Johannes Fahrmann1; Samir M Hanash1; 1The University of Texas MD Anderson Cancer Center, Houston, TX; 2Nagoya University, Nagoya, Japan

Proteomics identification of a potential biomarker of the malnutrition associated Konzo disease in human blood plasma samples; Victor Fourcassié1; Matthew S. Bramble2; Florence Roux-Dalval1; Neerja Vashist1; Dieudonné Mumba Ngoiy4; Desiré Tshala-Katumbay3; Eric Vilain2; Arnaud Droit1, 2; 1Proteomics platform, CHU de Québec - Université Laval Research Center, Quebec City, Québec, Canada; 2Center for Genetic Medicine Research, Children’s Research Institute at Children’s National Hospital, Washington, DC USA, Washington, DC; 3Center for Genetic Medicine Research, Children’s Research Institute, Children’s National Hospital, Washington, DC; 4National Institute of Biomedical Research, Kinshasa, The Democratic Republic Of Congo; 5Department of Genomics and Precision Medicine, The George Washington University School of Medicine and Health Sciences, Washington, DC; 6Computational Biology Laboratory, CHU de Québec - Université Laval Research Center, Quebec, Quebec

Application of Proton Induced X-ray Emission (PIXE) spectroscopy for quantifying biomarker levels; Gary A Glass1, 2; Todd A. Byers1; Darshpreet Kaur Saini3; 1Charles T. Bowen1; Bibhudutta Rout4; 1University of North Texas, Denton, TX; 5University of North Texas, Denton, Texas

TP 085  Dual-column ZENO-TOF System to Achieve Robust and High-Quality Plasma Proteomics; Yi (Jimmy) Zeng1; Hao Qian1; Mark Marispini1; Jessica Chan1; Megan Mora1; Robert Zawada1; Philip Ma1; Bruce Wilcox1; 1PrognomIQ Inc, San Mateo, CA

Peptidomics analysis reveals changes in small urinary peptides in patients with intestinal cystitis/bladder pain syndrome; Mohammad N. Khan1; John Chen1, 2; Chengjie Ji2; Bridget A. Tripp3; Aline de Lima Leite4, 5; Heidi E. Roth1, 3; Jiri Viljanen1; Sabrina Richter5; 1University of North Texas, Denton, TX; 2University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK; 3University of Kansas, Department of Neurology and Movement Disorder Center, Seoul National University Hospital, Jongno-gu, South Korea; 4Center for Biotechnology, University of Nebraska-Lincoln, LINCOLN, NE; 5Department of Biotechnology, University of Nebraska-Lincoln, LINCOLN, NE; 6The Nebraska Center for Integrated Biomolecular Communication (NCIB), University of Nebraska-Lincoln, LINCOLN, NE; 7Department of Biochemistry, University of Nebraska-Lincoln, LINCOLN, NE; 8Redox Biology Center, University of Nebraska-Lincoln, LINCOLN, NE

TP 086  2D LC-MS/MS with Direct Digestion to Enhance Quantitation of Monkey Serum hIDUA in the Presence of ADA and Endogenous Enzyme; Wenchu Yang2; Drew Tietz3; Jiang Wu2; Eugene Goh2; Poh Leong Lim2; A. Mark Richards1, 2; Brian Libby2; 1National University of Singapore, Singapore, Singapore; 2National University of Singapore, Singapore, Singapore; 3Children’s National Hospital, Washington, DC, USA; 4National university hospital, Singapore, Singapore

TP 087  Development of Liquid Chromatography – Mass Spectrometry-Based Targetted Metabolomic Assays To Screen For Heart Failure and other Chronic diseases; Leroy S Pakkiri1, 2; Lik Hang Wu1, 2; Eugene Goh3, 4; Poh Leong Lim2; A. Mark Richards1, 2; Chester L. Drum1, 3, 4; 1National University of Singapore, Singapore, Singapore; 2National University of Singapore, Singapore, Singapore; 3cardiovascular research institute, Singapore, Singapore; 4Chirstchurch heart institute, Univ. of Otago, Christchurch central city, New Zealand; 5national university hospital, Singapore, Singapore

TP 088  Peptidomics analysis reveals changes in small urinary peptides in patients with intestinal cystitis/bladder pain syndrome; Mohammad N. Khan1; John Chen1, 2; Chengjie Ji2; Bridget A. Tripp3; Aline de Lima Leite4, 5; Heidi E. Roth1, 3; Jiri Viljanen1; Sabrina Richter5; 1University of North Texas, Denton, TX; 2University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK; 3University of Kansas, Department of Neurology and Movement Disorder Center, Seoul National University Hospital, Jongno-gu, South Korea; 4Center for Biotechnology, University of Nebraska-Lincoln, LINCOLN, NE; 5Department of Biotechnology, University of Nebraska-Lincoln, LINCOLN, NE; 6The Nebraska Center for Integrated Biomolecular Communication (NCIB), University of Nebraska-Lincoln, LINCOLN, NE; 7Department of Biochemistry, University of Nebraska-Lincoln, LINCOLN, NE; 8Redox Biology Center, University of Nebraska-Lincoln, LINCOLN, NE

TP 089  Peptidomic characterization of protease activity and biomarker discovery of COPD pathogenesis associated with HIV in clinical BALF samples; Monica E. Kruk1, 2; Danielle Weise1; Sarah Samorodnitsky3; Carmen Martin-Alonso1; Erick Lock3; Subina Mehta3; Pratik D Japtap3; Chris Wendt4, 5; Timothy J Griffin4; 1Department of Medicine, University of Minnesota, Minneapolis, MN; 2Biochemistry, Mol. Biology and Biophysics, University of Minnesota, Minneapolis, MN; 3Division of Statistics, School of Public Health, University of Minnesota, Minneapolis, MN; 4Harvard-MIT Division of Health Sciences and Technology, MIT, Cambridge, Massachusetts; 5Minneapolis Veterans Affairs Healthcare System, Minneapolis, MN

TP 090  A Universal Surrogate Matrix Assay for Urea Analysis in Biological Matrix to Support Clinical Pharmacokinetic Studies of Respiratory Diseases; Yang
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Tang; Micheal Van Parys; Xiaorong Liang; Brian Dean; Liuxi Chen; Genentech Inc., South San Francisco, CA; Labcorp, Madison, WI

TP 092 A multiplexed mass spectrometric assay of 42 biomarkers for high-throughput screening obesity-related clinical samples: Tanul L; Parsnak Dakup; Athena A. Schepmoes; Thomas L. Fillmore; Adam C. Swensen; Tong Zhang; James P. Delany; Bret H. Goodpasture; Jie Pu; Tfujin Shi; Jun Qu; Wei-Jun Qian; PNNL, Richland, WA; AdventHealth, Orlando, FL; University at Buffalo, Buffalo, NY

TP 093 A Multi-Omics Strategy to Develop and Optimize Cell Culture Media in Fed-Batch Cultivation of CHO-S, DG44, and CHO-K1 GS cells; Chenjiong Tu; Vyncent Nguyen; Km Shams Ud Doha; Alex Abreu; Sarah Baron; Didar Asik; Scott J. Jacobia; Andrew M. Campbell; thermo Fisher Scientific, Grand Island, NY; thermo Fisher Scientific, Buffalo, NY

TP 094 Assessment of a 60-biomarker health surveillance panel (HSP) on whole blood from remote sampling devices by LC/HRMS-MS and DIA-MS analysis; Stephen A. Whelan; Nathan Hendricks; Zachary L. Dwight; Qin Fu; Annie Moradian; Jennifer E. Van Eyk; Susan M. Mockus; Precision Biomarker Laboratories, Cedars-Sinai Medical Center, Beverly Hills, CA; Smit Heart Institute, Advanced Clinical Biosystems Research Institute, Cedars-Sinai Medical Center, Los Angeles, California

TP 095 Quantitative metabolomics and lipidomics of more than 1,400 biomarkers using cloud-based workflow management software with machine learning peak integration algorithm; Gregor Omer; Markus Langsdorf; Tuan Hai Pham; Cornelia Röhring; Therese Koal; biocrates life sciences ag, Innsbruck, Austria

TP 096 A novel quantification method for RPE phagocytosis using a VLP-PUTA-based strategy; Fangyuan Gao; UC Irvine, Irvine 92617, CA

TP 097 Determination of Benzenophones in human Placenta from Northern Taiwan using a Solid-liquid Extraction-based UHPLC-MS/MS; Ming-Hung Hsieh; Mei-Lien Chen; Pei-Wei Wang; Wen-Po Cheng; Yu-Fang Huang; Department of Safety, Health and Environmental Engineering, National United University, Miaoli, Taiwan; Institute of Environmental and Occupational Health Sciences, National Yang-Ming Chiao Tung University, Taipei, Taiwan; Department of Pediatrics, Heping Fuyou Branch, Taipei City Hospital, Taipei, Taiwan

TP 098 Development of a workflow to assess gastric cancer antigenic biomarkers in circulation using ion-mobility mass spectrometry and enzyme-linked immunosorbent assays; Rongzheng Dou; Hiroyuki Katayama; Ehsan Irajizad; Yining Cai; Nan Jiang; Yatao Shi; Tyler Chen; Jianhui Li; Yi Tao; Ming Chiao; Ming Chiao; Life Sciences, Rüsselsheim am Main, Germany; Department of Child Neurology, Giessen, Germany

TP 099 LC-FAIMS/dcV-MS Method Enabled Ultra-Sensitive Antigen-Free Quantification of Low-abundance Biomarkers in Clinical Cohorts, with High Accuracy and Sensitivity; Qingqing Shen; Jie Pu; Chao Xue; Wei-Jun Qian; Cornelia L Boeser; Claudia Martins; Scott M Peterman; Jun Qu; University at Buffalo, Buffalo, NY; Pacific Northwest National Lab, richland, WA; ThermoFisher Scientific, San Jose, CA; New York State Center of Excellence in Bioinformatics & Life Sciences, Buffalo, NY

TP 100 Molecular determination of survival motor neuron protein provides a breakthrough for gene therapy and newborn diagnostics of spinal muscular atrophy; Michael Przybylski; Pascal Wiegand; Tamsila Khan; Stefan Maeser; Wolfgang Kleinekotter; Andreas Hahn; Centre for Analytical Biochemistry and Biomedical Mass Spectrometry, Rüsselsheim am Main, Germany; Department of Child Neurology, Giessen, Germany

TP 101 Quantitative Proteomics for Selectivity and Mechanism of Action Analysis of a Heterobifunctional STAT3 degrader In Vitro and In Vivo; Yatao Shi; Eric Kuhn; Karen Yuan; Yogesh Chutake; Kaishal Dixit; Michele Mayo; Joyoti Dey; Bin Yang; Haojing Rong; Phillip Liu; Dirk M Wathler; Chris De Savi; Kirti Sharma; Kymera Therapeutics, Watertown, MA

TP 102 Serum N-Glycan Profiling of Patients with Narcolepsy type 1 Using LC-MS/MS; Akeem Adeyemi Sanni; Md Abdul Hakim; Mona Goli; Samer El Hayek; Farid Talih; Bartolo Lanuzza; Firas Kobeissy; Giuseppe Pazzi; Stefania Mondello; Raffaele Ferri; Yehia Mechref; Texas Tech University, Lubbock, TX; Department of Psychiatry and Behavioral Sciences, University of Miami Miller School of Medicine, Miami, FL; Department of Psychiatry, Faculty of Medicine, American University of Beirut, Beirut, Lebanon; Sleep Research Centre, Department of Neurology IC, Oasi Research Institute-IRCCS, Troina, Italy; Faculty of Biochemistry and Molecular Genetics, American University of Beirut, Beirut, Lebanon; Morehouse School of Medicine (MSM), Center for Neurotrauma, Multiomics & Biomarkers, Department of Neurobiology, Atlanta, Georgia; IRCCS, Istituto delle Scienze Neurologiche di Bologna, Bologna, Italy; Department of Biomedical, Metabolic and Neural Sciences, University of Modena and Reggio Emilia, Modena, Italy; Department of Biomedical and Neural Sciences and Neurofunctional Imaging, University of Messina, Messina, Italy

TP 103 Clinical proteomic analysis across the Alzheimer’s disease continuum; Sophia Weiner; Mathias Sauer; Nicholas Ashton; Pedro Rosa-Neto; Henrik Zetterberg; Kai Blennow; University of Gothenburg, Gothenburg, Sweden; McGill University, Montreal, Quebec; Sahlgrenska University Hospital, Gothenburg, Sweden

TP 104 Development of a Highly-specific LC-MS-based Quantitative Fecal Occult Blood Test for Canine; Zhiyu Li; Hefeng Zhang; Siyu Liu; Zhiren Yu; Lili Xing; Yi Tao; Liang Sheng; WuXi AppTec, Shanghai, China

TP 105 Evaluating co-expression of tagged proteins in isolated EVs with attomole sensitivity; Michael A Shaw; Dmitriy Verkhoutrov; Soumya Kandi; Nicholas Ashton; Kenneth Jetter; Nicholas Ashton; Michael J. Eller; Alexander Revzin; Emile A. Schweikert; Department of Chemistry and Biochemistry, California State University Northridge, Northridge, California; Department of Chemistry, Texas A&M University, College Station, Texas; Department of Physiology and Biomedical Engineering, Mayo Clinic, Rochester, Minnesota

TP 106 High-throughput biomarker discovery (BA) of serum biomarker 7aC4 using tandem LC/MS: devising an end-to-end single-vial approach in a sample-limited setting; Soumya Kandi; Qin C Ji; John P. Savary; Sarah-link Polakow; Gary J Jenkins; Kenneth Ruterbories; Mary Saltarello; Mario Richter; Abbvie, North Chicago, IL

TP 107 Integration of enhanced and quantitative plasma proteomics with immunoassays for discovery of blood biomarkers for early detection of papillary thyroid carcinoma; Hong Wang; Nan Jiang; Linzhen Song; Huanjun Ling; Juan Ling; Junli Gao; Junshun Gao; Shengpeng Ying; Qi Chen; Hangzhou Cosmos Wisdom Mass Spectrometry Center of Zhejiang University Medical School, Hangzhou, China; Hangzhou Cosmos Wisdom Mass Spectrometry Center of Zhejiang University Medical School, Hangzhou, China; Taizhou Central Hospital, Taizhou, China

TP 108 Investigation of systemic inflammation induced FcRn dysregulation with sensitive LC-FAIMS/dCV-MSR; Chao Xue; Qingqing Shen; Jie Pu; Yang Liu; Ming Zhang; Jun Qu; University at Buffalo, Buffalo, NY; New York State Center of Excellence in Bioinformatics & Life Sciences, Buffalo, NY
TP 109 LC-MS based Discovery of Plasma Phosphopeptide Markers for Alzheimer’s Disease Staging and Clinical trials; Kyungdo Kim1; Min-Kyung Jun1; Se Hwan Jang1; Byeong C. Kim2; Zee-yong Park3; 1School of Life Science, Gwangju Institute of Science and Technology, Cheonmungwagiro123, Buk-gu, Gwangju, South Korea; 2Department of Neurology, Chonnam National University Hospital, Gwangju, South Korea

TP 110 NanoLC-timsTOF platform-assisted analysis of glycosylated albumin in diabetes-affected plasma and tear film; Yangi Tan; University of Illinois, Urbana, IL

TP 111 A Comparison of Tribrass Metalloproteome Architectures for Deep Blood Plasma Proteinomes; Johannes Kreuzer1,2; Jingjing Huang3; Eric F Zaniewski1,2; Sorosh Hajizadeh1,2,4; Benedikt C. Clemens1,2; David Bergen2; Jesse D. Canterbury2; Michael W. Senko5; Graeme C McAllister6; Wilhelm Haas7,8,9; 1MGH Cancer Center, Charlestown, MA; 2Harvard Medical School, Boston, MA; 3Thermo Fisher Scientific, San Jose, California; 4Babraham Institute, Cambridge, Cambridge, MA; 5ThermoFisher Scientific, San Jose, California

TP 112 The proteome of urinary extracellular vesicles informs tumor progression in localized prostate cancer; Amanda Khoo1,2,3; Meinusha Govindarajan1,2,4; Zhuyi Qiu5; Vladimir Ignatchenko6; Danny Vesprini6,7,8; O. John Semmes9; Julius O Nyalwidde7; Stanley Liu1,2,4; Paul C Boutros2,4; Thomas Kislinger3; 1Department of Medical Biophysics, University of Toronto, Toronto, ON; 2Princess Margaret Cancer Centre, University Health Network, Toronto, ON; 3Jonsson Comprehensive Cancer Center, University of California, Los Angeles, Los Angeles, CA; 4Odette Cancer Centre, Sunnybrook Health Sciences Centre, Toronto, ON; 5Leroy T. Canoles, Jr. Cancer Research Center, Eastern Virginia Medical School, Norfolk, VA

TP 113 Inoperative Margin Detection of Head and Neck Cancer with Rapid Evaporative Ionisation Mass Spectrometry; James Anthony Higgison1,2; Jasmin Werner1,2; Stefania Maneta-Stavrakaki1,2; Lauren Ford1; Dani Simon1; Yuchen Xiang1,2; Jagtar Dhand2,3; Zoltan Takats1; 1Imperial College, London, London, United Kingdom; 2Brighton and Sussex Medical School, Brighton, United Kingdom

TP 114 Media Compromised Analysis during Human Primary T Cell Culture using a Triple Quadrupole Mass Spectrometer; Evelyn H. Wang1; Stephen Kurzyniec1; Erin Strom1; Tammy Jones-Lepp2; Amanda Leisgang1; Andrew Ortiz2; Jefferson Kinney2; Yoshiyuki Okumura2; 1Shimadzu Scientific Instrument, Columbia, MD; 2University of Nevada Las Vegas, Las Vegas, NV

TP 115 Studying Off-Target Effects of Small Molecule Covalent Cysteine Modifiers Using Thermal Protein Profiling; Andrew J Pericacciante1; Kate Brown2; Tapan K Maiti1; Massimiliano Bissas1; Genoveffa Franchini1; Daniel H Appella1; Ettore Appella1; Lisa M Jenkins1; 1Laboratory of Cell Biology, Center for Cancer Research, National Cancer Institute, Bethesda, MD; 2Vaccine Branch, Center for Cancer Research, National Cancer Institute, Bethesda, MD; 3Laboratory of Bioorganic Chemistry, National Institute of Diabetes and Digestive and Kidney Diseases, Bethesda, MD

TP 116 Millions of cellular drug assays created by dose-resolved (phospho)proteomics reveal drug mechanism of action and decrypt post-translational modifications; Jan Zech1; Florian P. Bayer1; Nicola Bernet1; Stephan Eckert1; Svenja Wiechmann1; Matthew The1; Julian Mueller1; Karl Kramer1; Guillaume Medard1; Mathias Wilhelm1; Annika Schneider1; Maria Reincke1; Julia Woortman1; Severin Lechner1; Patroklos Samaras1; Ludwig Lautenbacher1; Firas Hamood2; Polina Prokofeva3; Stephanie Heintzmeir1; Benjamin Ruprecht1; Bernhard Kuster1; 1Technical University of Munich, Freising, Germany

TP 117 HDAC inhibitors induce proteome remodeling of diverse lung cancer cells; Chwee Lin4; Devin Schweppe1; 1University of Washington, Seattle, WA

TP 118 DIA proteomics method applied to probing p53-independent functions of Mdm2 and Mdmx in a human melanoma cell line; Anu Jain5; Rafaela Muniz De Queniriz6; Jayanta K. Chakrabarty1; Liodas1; Carol Prives2; Lewis M. Brown1; 1Department of Biological Sciences, Quantitative Proteomics and Metabolomics Center, Columbia University, New York, NY; 2Department of Biological Sciences, Columbia University, New York, NY

TP 119 Parallel analysis of the proteome, histone PTMs and RNA modifications from frozen tissue sections by MS; Joanna K Lempiainen1; Yuxuan (axe) Xie1; Angela C Hirbe1; Benjamin A Garcia1; 1Washington University in St Louis, Department of Biochemistry and Molecular Biophysics, St Louis, MO; 2Washington University in St Louis, School of Medicine, Division of Oncology, St. Louis, MO

TP 120 Phosphoproteome and cDNA-Seq by typing of gastric cancer reveals dynamic transformation with chemotherapy; Jun Adachi1; Hirokazu Shoji2; Masahiko Aoki3,1,2; HideKazu Hirano1; Yuichi Abe1; Kazufumi Honda4,5; Takeshi Tomonaga1; Kenji Mizuguchi1; Takaki Yoshikawa1; Narikazu Boku1,2; 1National Institutes of Biomedical Innovation, Health and Nutrition, Ibaraki, Japan; 2National Cancer Center Hospital, Tokyo, Japan; 3Kyoto University, Kyoto, Japan; 4Nippon Medical School, Tokyo, Japan; 5University of Tokyo, Tokyo, Japan

TP 121 High-Throughput proteome profiling of in-vitro generated tumor associated macrophages reveals key signatures of immune response proteins for therapeutic applications; Shreya Ahuja1; Becki Dudley1,2; Abby J. Chiang1,2; Matthew S. Glover2; Lisa H Cazares2; Luca Melchior2,3; Robert Wilkinson4; Dmitry Gabrilovich5; Des Jones6; Sonja Hess7; 1Astrazeneca, Gaithersburg, MD; 2AstraZeneca, Cambridge, United Kingdom; 3AstraZeneca, Cambridge, United Kingdom; 4AstraZeneca, Gaithersburg, MD

TP 122 Molecular Landscapes of Breast Cancer Subtypes: Data Independent Acquisition and Identification of Potential Therapeutic Targets for Stroma Reprogramming; Jordin J. Pan1; Joanne Bons1; Rosemary Ba2; Chira Chen3; Deborah Collyar2; Christie L Hunter1; Philippe Gascard1; Thea D Tisty1; Birgit Schilling1; 1Buck Institute for Research on Aging, Novato, CA; 2University of California San Francisco, San Francisco, CA; 3SCIX, Redwood city, CA

TP 123 Metabolic landscape identified altered Arachidonic acid pathway in bladder cancer; Mohammad Khurshid1; Hassan1; Dhanasinghe Waduge Badrjaye Piyarathna2; Vasanta Puttur1; Roni J. Bolla3; Martha K Terris4; Leomar Y Ballester4; 1Imperial College, London, London, United Kingdom; 2Department of Nutrition Science, Purdue University, West Lafayette, IN; 3Purdue Proteomics Facility, Bindley Bioscience Center, Purdue University, West Lafayette, Indiana

TP 124 The Proteomic Changes inHCT 116 Colon Cancer Spheroids During Growth; Catherine B Edgington1; Nicole C. Belter1; Amanda B. Hummon1; 1The Ohio State University, Columbus, OH; 2The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH

TP 125 Differing Cytoplasmic Lipid Droplet Proteomes from Vehicle-Treated and Fatty Acid Synthase-Inhibited Metastatic Breast Cancer Cells Generate Novel, Testable Hypotheses; Chaylen J Andolino1,2; Kimberly K Buhman1; Dorothy Teegarden1; 1Department of Nutrition Science, Purdue University, West Lafayette, IN; 2Purdue Proteomics Facility, Bindley Bioscience Center, Purdue University, West Lafayette, Indiana

TP 126 Identification of Celecoxib as a new e3 ligase ligand for PROTAC design; Yufen Xia1; Y Li2; Zongtao Lin1; Jing Pei1; Guangrong Zheng1; Dongwen Lv3,4; 1Department of
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Proteogenomic Characterization of Chemotherapy Response in Muscle Invasive Bladder Cancer: Matthew V. Holt; Yongchao Dou; Meggie N. Young; Antrix Jain; Alexander B. Saltzman; Jonathan T. Lei; Kyle D. Drinnon; Sung Han Kim; Meenakshee Anurag; Bing Zhang; Anna Malovannaya; Seth P Lerner; Baylor College of Medicine, Houston, Texas

TP 135 
Identifications of metabolic changes upon microbiome depletion in pancreatic tumor bearing mice models: Pongrak Awiwi; Zhang; Xiang Li; Peter Sajjakulrukkit;

TP 136 
Multi-Omics approach to identify the molecular signature of primary non function prior to transplantation in deceased donor kidneys: Sadr ul Shahheed; Fenna E.M. Van De Lemmens; Corinna M Snashall; Maria Letizia Lo Faro; Chris W. Sutton; Jan H.N. Lindeman; Rutger J. Ploeg; Nuffield Department of Surgical Sciences, University of Oxford, Oxford, United Kingdom; Department of Surgery, Transplant Center Leiden University Medical Center, Netherlands; Institute of Cancer Therapeutics, University of Bradford, Bradford, United Kingdom

TP 137 
Data Acquisition and Intraoperative Analysis on a mobile, battery-operated orbitrap mass spectrometer: Michael Keating; Charles A. Wolfe; Andréia de Melo Porcari; Alexander Makarov; Livia S. Eberlin; University of Texas at Austin, Austin, TX; Division of Surgical Oncology, Baylor College of Medicine, Houston, Texas; Thermo Fisher Scientific, Beverly, MA; West Point, PA

TP 138 
Moving towards digitally-enabled clinical trials with metabolomics analysis of dried blood samples (DBS) using an at-home microsampling collection device: Thomas P. Wyché; Corinne Thomas; Melanie Anderson; Brad R. Evans; Kevin P. Bateman; Theodore R. Sana; Merck & Co., Inc., Cambridge, MA; Merck & Co., Inc., West Point, PA

TP 139 
Investigating Lipid Sources Contributing to Resistance to Lysosomal Autophagy Inhibition in Melanoma: Sandra L. Harper; Vaibhav Jain; Ravi K. Amaravadi; David W. Speicher; Aaron R. Goldman; The Wistar Institute, Philadelphia, PA; University of Pennsylvania, Philadelphia, PA

TP 140 
A Simplified Proteomics LC-MS/MS Assay for Determination of ApoE Genotypes in Plasma Samples: Deema Q. Qasrawi; Rania M Khan; Evgeniy V. Petrotenko; Manuel Montero-Odasso; Christoph H. Borchers; Mikhail Khafizov; Vladimir Ignatchenko; Marcus O. Bernardini; Thomas Kislinger; Princess Margaret Cancer Centre, University Health Network, Toronto, ON; Division of Gynecologic Oncology, Princess Margaret Cancer Centre, University Health Network, Toronto, ON; Department of Obstetrics and Gynaecology, University of Toronto, Toronto, ON; Department of Medical Biophysics, University of Toronto, Toronto, ON

TP 133 
Spatial N-Glycan Profiling of an Ovarian Cancer Mouse Model Using MALDI Mass Spectrometry Imaging: Xin Ma; Soojin Park; Thu-Huyen Pham; Andro Botos; Sylvia R. Yum; Eun Young Park; Olga Kim; Grace Grimslay; Jaeyeon Kim; Richard R. Drake; Facundo M. Fernandez; School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA; Department of Biochemistry and Molecular Biology, Indiana University School of Medicine, Indianapolis, IN; Department of Cell and Molecular Pharmacology and Experimental Therapeutics, Medical University of South Carolina, Charleston, SC

TP 132 
Verification of Serum Biomarkers for High-Grade Serous Ovarian Carcinoma Recurrence by Targeted Proteomics: Deborah W. Borchers; Borchers; S. A. Khair; Vladimir Ignatchenko; Marcus O. Bernardini; Thomas Kislinger; Princess Margaret Cancer Centre, University Health Network, Toronto, ON; Division of Gynecologic Oncology, Princess Margaret Cancer Centre, University Health Network, Toronto, ON; Department of Obstetrics and Gynaecology, University of Toronto, Toronto, ON; Department of Medical Biophysics, University of Toronto, Toronto, ON

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Sumo Inhibition Unveils the Dark Immunopeptidome in Acute Myeloid Leukemia: Léa Christophe; Mirela Pascaaru; Chantal Durette; Eric Bonneil; Joel Lanoix; Marie-Pierre Hardy; Krystel Vincent; Claude Prerault; Pierre Thibault; Institute of Research in Immunology and Cancer, Université de Montréal, Montréal, QC; Department of Medicine, Université de Montréal, Montréal, Québec, Canada

TP 120 
Determination of ApoE Genotypes in Plasma Samples: Deema Q. Qasrawi; Rania M Khan; Evgeniy V. Petrotenko; Manuel Montero-Odasso; Christoph H. Borchers; Mikhail Khafizov; Vladimir Ignatchenko; Marcus O. Bernardini; Thomas Kislinger; Princess Margaret Cancer Centre, University Health Network, Toronto, ON; Division of Gynecologic Oncology, Princess Margaret Cancer Centre, University Health Network, Toronto, ON; Department of Obstetrics and Gynaecology, University of Toronto, Toronto, ON; Department of Medical Biophysics, University of Toronto, Toronto, ON

TP 121 
Cell Viability, Purity, and Drug-Protein Interactions of Novel Gold (I) Compounds Within Various Cancer Types: Kyle L. Wilhelmen; Charli Worth; Neda Feizi; Shyam Pokhrel; Ahmad Ahmad; Mitchell Bruce; Alice Bruce; Joseph Taube; Touradj Solouki; Baylor University, Waco, TX; University of Maine, Orono, ME

TP 123 
SUMO inhibition unveils the dark immunopeptidome in acute myeloid leukemia: Léa Christophe; Mirela Pascaaru; Chantal Durette; Eric Bonneil; Joel Lanoix; Marie-Pierre Hardy; Krystel Vincent; Claude Prerault; Pierre Thibault; Institute of Research in Immunology and Cancer, Université de Montréal, Montréal, QC; Department of Medicine, Université de Montréal, Montréal, Québec, Canada

TP 124 
Proteogenomic Characterization of Chemotherapy Response in Muscle Invasive Bladder Cancer: Matthew V. Holt; Yongchao Dou; Meggie N. Young; Antrix Jain; Alexander B. Saltzman; Jonathan T. Lei; Kyle D. Drinnon; Sung Han Kim; Meenakshee Anurag; Bing Zhang; Anna Malovannaya; Seth P Lerner; Baylor College of Medicine, Houston, Texas

TP 125 
Identifications of metabolic changes upon microbiome depletion in pancreatic tumor bearing mice models: Pongrak Awiwi; Zhang; Xiang Li; Peter Sajjakulrukkit;
TP 144 A new MALDI-based diagnostic method for the detection of C. difficile in humans: Josef Dvorak1, 2; Petr Pompač1, 2; Jaroslav Hrabák1; Lukáš Fojtík1, 2; Petr Novák1, 2; 1Department of Biochemistry, Charles University, Prague, Czech Republic; 2Institute of Microbiology of the CAS, v. v. i., Prague, Czech Republic; 3Institute of Biotechnology of the CAS, v. v. i., Prague, Czech Republic; 4Biomedical Center, Faculty of Medicine, Charles University, Pilsen, Czech Republic

TP 145 LC-MS/MS innovations geared to address the changing landscape of newborn screening: Konstantinos Petritis1; Samantha L Isenberg1; C. Austin Pickens1; Carla Cuthbert1; 1Centers for Disease Control and Prevention, Atlanta, GA; 2Shimadzu Scientific Instruments, Carlsbad, CA; 3Department of Biochemistry, Purdue University, West Lafayette, Indiana; 4Department of Emergency Medicine, National Taiwan University Hospital, Taipei, Taiwan; 5Department of Forensic Medicine, College of Medicine, National Taiwan University, Taipei, Taiwan; 6Forensic and Clinical Toxicology Center, National Taiwan University Hospital, Taipei, Taiwan; 7Department of Pharmacy, College of Medicine, National Taiwan University, Taipei, Taiwan; 8Department of Biomedical Data Sciences and Statistics, Stanford, CA, Stanford, CA; 9Department of Emergency Medicine, National Taiwan University Hospital, Taipei, Taiwan; 10Department of Urology, Indiana University School of Medicine, Indianapolis, IN

TP 146 Simultaneous Quantification of 13 Clinically Significant Simple and Macrocytic Trichoethenes in Human Urine Using Liquid Chromatography with Tandem Mass Spectrometry: Claudia G Beck1; Matthew R McIntyre1; Dennis G Hooper1; 1Realtime Laboratories, Carrollton, TX

TP 147 Rapid identification of Methicillin-resistant Staphylococcus aureus (MRSA) and methicillin-susceptible Staphylococcus aureus (MSSA) using the MasSpec Pen Technology: Manoj Kumar1; Coreen L. Johnson2; Michael Keating1; James J. Dunn1; Min Woo Sun1; Robert Tibshirani1; Rachel D. Downey1; Lindsey M. Kirkpatrick1; Livia S. Eberlin2; 1Bruker Scientific, Billerica, MA; 2Robert International, Odense, Denmark; 3Department of Biochemistry, Purdue University, West Lafayette, Indiana; 4Department of Chemistry, Purdue University, West Lafayette, Indiana; 5Tymora Analytical Operations, West Lafayette, Indiana; 6Department of Urology, Indiana University School of Medicine, Indianapolis, IN

TP 148 Therapeutic Drug Monitoring Using Miniature Mass spectrometer for ICU: Jixun Bu1; Nan Zhang1; Wenpeng Zhang2; Zheng Ouyang3; 1PURSPEC Technology (Beijing) Ltd., Beijing, China; 2Department of Precision Instrument, Tsinghua University, Beijing, China; 3Institute of Precision Instrument, Tsinghua University, Beijing, China

TP 149 Development and validation of LC-MS/MS method for the measurement of plasma aldosterone revealed interference in patient samples: Yi Ting Tan1; Troy Puar1; Daryl Hee1; 1CHANGI GENERAL HOSPITAL, Singapore, Singapore

TP 150 A complete, automated end-to-end workflow for high-throughput therapeutic drug monitoring using Evosep DRM: Angela Mc Ardle1; Magnus Husufeldt2; Bharath Kumar Raghuraman1; Dorte Bekker-Jensen1; Ole Vorn1; 1Copenhagen, Denmark; 2Evosep, Odense, Denmark

TP 151 Intelligent Reflex: A novel approach for higher throughput; improved clinical specificity and enhanced QA/QC. Application in newborn screening: Lindsay M MasNarra1; Doug Jaffe2; Samantha L Isenberg3; Carla Cuthbert4; Konstantinos Petritis5; 1ODC, Atlanta, GA; 2Bruker Scientific, Billerica, MA; 3Shimadzu Scientific Instruments, Carlsbad, CA; 4Department of Biochemistry, Purdue University, West Lafayette, Indiana; 5Department of Urology, Indiana University School of Medicine, Indianapolis, IN

TP 152 Multiple LC-MS/MS method development and validation for the simultaneous analysis of seven antibiotics from pediatric whole blood volumetric absorptive microsamples: John Takyi-Williams; Ruling Li; Amanda Bwint; Bo Wen; Duxin Sun; Marc Schectez; Kevin J. Downes; Athena F. Ziuppa; Minjounath P. Padi; 1University of Michigan, Ann Arbor, MI; 2University of Michigan Ann Arbor, Ann Arbor, MI; 3Children’s hospital of Philadelphia, Philadelphia, Pennsylvania; 4Midwestern University, Downers Grove, Illinois

TP 153 Chemical biopsy acupuncture needles for direct-mass spectrometry via microfluidic open interface applied to in-vivo tissue monitoring in surgery: Runshan W Jiang1; Janusz B Pawliszyn1; 1University of Waterloo, Waterloo, ON

TP 154 High-throughput end-to-end automated Evosep-MRM workflow for the quantification of glycerated albumin in diabetes: Bharath Kumar Raghuraman; Angela Mc Ardle; Ole Vorn; Nicolai Bache; Martin Overgaard; Christian Ravensborg; Evosep Biosystems, Odense, Denmark

TP 155 A fast and novel workflow with DART-LC-MS/MS platform for urine toxicolgy screening and confirmation with orthogonal methods: Francois Espouvert1; Terry Bates2; Bruker Corporation, Billerica, MA; 3Bruker Scientific, Billerica, MA

TP 156 FragFinder: Automatic selection of unique and selective EI fragment ions for GC-MS-based metabolic screening: Guan-yuan Chen1; Ju-Yu Chen2; Mei-Ling Lai3; Kun-Chen Lee3; Te-I Weng1, 2, 5; 1Department and Graduate Institute of Forensic Medicine, College of Medicine, National Taiwan University, Taipei, Taiwan; 2Forensic and Clinical Toxicology Center, National Taiwan University Hospital, Taipei, Taiwan; 3Department of Pharmacy, College of Medicine, National Taiwan University, Taipei, Taiwan; 4Department of Biomedical Data Sciences and Statistics, Stanford, CA, Stanford, CA; 5Department of Emergency Medicine, National Taiwan University Hospital, Taipei, Taiwan

TP 157 Personalized extracellular vesicle phosphoproteomics identifies relevant functional signaling for renal cell carcinoma monitor: Marco Hadisurya1, 2; Zhuojun Luo1; Xiaofeng Wu1; 1Department of Biochemistry, Purdue University, West Lafayette, Indiana; 2Department of Chemistry, Purdue University, West Lafayette, Indiana

TP 158 Quantitation of endogenous steroids in serum using dried blood spot serum separator card and triple quadrupole mass spectrometry: Vikki Johnson1; Nicholas Chestara2; Yoshiyuki Okamura; Shimadzu Scientific Instruments, Carlsbad, CA; 2DPX Technologies, La Jolla, CA; 3Shimadzu Scientific Instrument, Columbia, Maryland

TP 159 Rapid diagnosis of brain tumors by onco-metabolic detection using miniature mass spectrometry system: Junhan Wu1; Xinqi Fang1; Haoyue Zhang1; Bin Jiao1; Nan Wang1; Jixun Bu2; Xiao Chen1; Wei Hua1; Ying Mao1; Wenpeng Zhang1; Zheng Ouyang1; Tsinghua University, Beijing, China; 2Huashan Hospital, Fudan University, Shanghai, China; 3PURSPEC Technology (Beijing) Ltd., Beijing, China

TP 160 Human Biofluid Benchmark Study comparing different workflows for deep and unbiased Clinical Proteomics;
Kinetic study of trisulfide to disulfide conversion in IgG1 mAbs under physiological conditions using Mass Spectrometry
Zhao W Gao; Xuefei Zhong; Yuan Mao; Ning Li; Albert Torri; Analytical Chemistry Group, Regeneron Pharmaceuticals Inc., Tarrytown, New York; 

FOLLOWING molecular changes during wound skin healing with topical statin treatment: Lilian Valadares-Tose; Ahmed Hawash; Ivan Jozic; Francisco Fernandez-Lima; Florida International University, Miami, FL; University of Miami, Miami, FL

CardioCarePack – personalized medicine system to improve the quality of patients suffering from cardiac arrhythmias: Maciej Stopa; Rafał Szewczyk; Anna Lenartowicz; Julia Mironenk a; Katarzyna Krupcyńska - Krupczyńska - Stopa; Adrian Sobon; Leszek Kalinowski; Adrianna Radulsk a; Tomasz Borkowski; Ewelina Marciniak; Bioanalytical Sp. z o.o., Gdańsk, Poland; LabExperts sp. z o.o., Gdańsk, Poland; Gdańsk Medical University, Gdańsk, Poland

Development and validation of a comprehensive liquid chromatography-tandem mass spectrometry-based test for plasma amino acid analysis in pediatric patients: Lily Olayinka; An_if K Chokkalla; Deepthi Rajapakse; Emily Garnett; Sridive Devaraj; Department of Pathology and Immunology, Baylor College of Medicine, One Baylor Plaza, Houston, Texas; Department of Pathology, Texas Children’s Hospital, Houston, Texas

Higher Order Structure Characterization of a Monoclonal Antibody by Fast Photochemical Oxidation of Protein (FPOP)-Mass Spectrometry: Yanchun Lin; Austin B. Moyle; Victor A. Beaumont; Lucy L. Liu; Sharon Polleck; Don L. Rempel; Hailun Liu; Heilang Shi; Jason C. Rouse; Hai-Young Kim; Ying Zhang; Michael L. Gross; Washington University in St. Louis, MO; Abbvie Inc., North Chicago, IL; Pfizer, Inc., Sandwich, United Kingdom; Pfizer, Inc., Andover, MA; Pfizer, Inc., New York City, NY; Sarepta Therapeutics, Inc., Cambridge, MA

Monoc and IntraLink Filter (Mi-Filter) To Reduce False Identifications in Cross-Linking Mass Spectrometry Data: Yingxi Li; Ling Hao; Min Miao; Randy Gariglio; David Wolfer; University of Arizona, Tucson, Arizona; Massachusetts Institute of Technology, Cambridge, MA; Pfizer, Inc., San Diego, CA

Chemopectrographic approaches to decipher novel mechanisms of non-vesicular cholesteryl transport: Miranda Villanueva; Nikolaus Burton; Andrew Flippin; Sho Takechi; Rohith Nagara; Liujuan Cui; Peter Tontonoz; Keriann Backus; UCLA, LOS ANGELES, CA; UCLA, Los Angeles, CA

Investigating daptomycin–membrane interactions using mass spectrometry: Tapasayanu Dash; Deseree Reid; Michael T. Marty; The University of Arizona, Tucson, Arizona

New regions of interaction revealed for Aquaporin-9 binding partners via XL-MS: Carla O’Neal; Zhen Wang; Kevin Schey; Vanderbilt University, Nashville, TN

A photo-tagging approach for studying the interactions between model peptides and membrane lipids: Jing Zhao; Lipeng Giao; Yu Xia; Tsinghua University, Beijing, China

In vitro to In vivo Characterization of Amyloid Beta 1-42 using Mass Spectrometry-based Footprinting: Cynthia (xinjyi) Kuang; Yanchun Lin; Zhao Sun; Andrew Yoo; Michael L. Gross; Washington University in St. Louis, MO; Washington University School of Medicine, St. Louis, MO; Washington University in St. Louis, MO

Ving: A New Tool in the Trans-Proteomic Pipeline for XL-MS Using Cleaveable Cross-Linking Reagents: Michael R. Hoopman; David D. Shteynberg; Luis Mendoza; Kamal Mandal; Arun P. Wila; Eric W. Deutsch; Robert L. Moritz; Institute for Systems Biology, Seattle, WA; University of California San Francisco, San Francisco, CA

A Covalent Labeling-Mass Spectrometry Method for Identifying Protein Amyloid Inhibitors: Kanin Khammong; Richard W. Vachet; University of Massachusetts Amherst, Amherst, MA

Optimized XL-MS workflows for membrane protein analysis: Yi He; Gregory J Dodge; Barbara Imperiali; Rosa Viner; Therma Fisher Scientific, San Jose, CA; Massachusetts Institute of Technology, Cambridge, MA

Carbone Crosslinking in Gas-Phase Peptide Ion Scaffolds: Hongyi Zhu; Václav Zima; Emily Ding; František Tureček; University of Washington, Seattle, WA

Dimethylithioure a as a Quencher in Hydroxyl Radical Protein Footprinting Experiments: Anter A Shami; Sandeep K. Misra; Lisa Jones; Joshua S. Sharp; University of Mississippi, University, MS; University of California San Diego, CA

A simple method for 'click-enabled' covalent labeling of hydrophobic protein microenvironments using radical mediated azidylation of amino acid sidechains: Benjamin B. Minkoff; Heather L. Burch; Jamison D. Wolfer; Michael R. Sussman; University of Wisconsin, Madison, WI

Conventional cell fixation improves performance of in situ crosslinking mass spectrometry while preserving ultrastructure: Andrzej Gołębski; Anil K Chokkalla; David C Schriemer; Pfizer, Inc., San Diego, CA

Real-time library search improves the sensitivity and throughput of cross-link identification: Max Ruwolt; Boris Bogdanoiu; Fan Liu; Leibniz-Forschungsinstitut für Molekulare Pharmakologie, Berlin, Germany

CFI Confidently Identifying protein-protein interactions by harmonizing cross-link scores with machine learning: Pin-Liang Jiang; Max Ruwolt; Boris Bogdanoiu; Fan Liu; Leibniz-Forschungsinstitut für Molekulare Pharmakologie (FMP), Berlin, Germany; Thermo Fisher Scientific, San Jose, CA

High-throughput XL-MS analysis on a new high-resolution accurate mass platform: Yi He; Tabiwang Arrey; Martin Zeller; Nicole Eugen Damoc; Rosa Viner; Thermo Fisher Scientific, San Jose, CA; Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany

Protein Footprinting Using Water Photolysis: Oluwatosin A. Ogundairo; Kermit K. Murray; Louisiana State University, Baton Rouge, LA

Development of Fast Photochemical Footprinting of Glycans for Topographical Analysis of Glycans: Sandeep K. Misra; Hao Liu; Sidney Stuckett; Joshua S. Sharp; University of Mississippi, University, MS

Cross-link assisted spatial proteomics to map sub-organelle proteomes and membrane protein topology: Ying Zhu; Kerem Can Akayka; Diogo Borges Lima; Max Ruwolt; Cong Wang; Martin Lehrman; Fan Liu; Department of Structural Biology, Leibniz-Forschungsinstitut für Molekulare Pharmakologie (FMP), Berlin, Germany
TP 188 Fluidic platform for enrichment of protein complexes for crosslinking-MS on a magnetic particle-based trap; Shaunak Raval1; David C Schriemer1; Vladimir Sarpe2; Alex D Crowder2; Pauline Douglas3; Susan P Lees-Miller4; Danny Laurent1; 1University of Calgary, Calgary, AB

TP 190 Are these crosslinking results significant? Bring on the bootstraps! Lindsey D Ulmer1; Christopher N Woods2; Natalie L Stone2; Rachel E Klevit3; Matthew F Bush4; 1Department of Chemistry, University of Washington, Seattle, WA; 2Department of Biochemistry, University of Washington, Seattle, WA

TP 191 Thrombin-DiolWaf APTT Assay Binding Investigated by DEPC Covalent Labeling-MS; Zachary J Kirsch1; Jonathan Ashby2; Richard W. Vachet1; 1University of Massachusetts Amherst, Amherst, MA; 2Mount Holyoke College, Holyoke, MA

TP 192 Unique Protein Identifications Improve Protein-Protein Interaction Identification Rate in CRIMP 2.0; D Alex Crowder1; Vladimir Sarpe1; David C Schriemer1; 1University of Calgary, Calgary, AB

TP 193 Few seconds range time-points for semi-automated Fenton Chemistry HRF reaction. Robust and inexpensive HOS monitoring method in vaccine antigen design; Alessandro Vadi1; Alessio Corrado1; 1GSK vaccines, Siena, Italy

TP 194 Accelerating Drug Discovery using an Automated High-Throughput Desorption Electrospray Ionization Mass Spectrometry Platform; Nicolas M. Morato1; Kai-Hung Huang2; Samadhi C. Kulathunga1; Veronica Fong3; Beinan Liu4; 1Department of Chemistry, University of Washington, Seattle, WA; 2Department of Biochemistry, University of Washington, Seattle, WA

TP 196 Quantitative Workflow for xC/UV/MS Data using a Single Vendor-Neutral Interface; Anne Marie Smith1; Yury Zhukov1; Sofya Chudova2; Vitaly Lashkin3; 1ACD/Labs, Toronto, ON

TP 197 Development and validation of an LC-MS/MS method for quantitation of IACS-10759, a novel OxPhos inhibitor, in human plasma; Quanyun Xu1; Yongying Jiang2; Emilia Di Francesc03; Philip Jones2; 1Institute for Applied Cancer Science, UT MD Anderson Cancer Center, Houston, TX

TP 198 Developing Novel Bioanalytical Method for Direct Quantification of Pegylated Lipid CDN Nanodiscs in Mouse Serum Using LC-MS/MS and In-Source CID; Ji Zhang1; Eric L Dano2; Jiaxiang Wang3; 1Millennium Pharmaceuticals, Inc., cambridge, MA; 2Koch Institute for Integrative Cancer Research, Massachusetts Institute of Technology, Cambridge, MA

TP 199 Affinity Selection of Double-Click Triazole Libraries for Rapid Discovery of Allosteric Modulators for GLP-1 Receptor; Ye Xin1; Shuo Liu2; Karl Barry Sharpless3; Jiajia Dong2; Wenqiong Shui1; 1ShanghaiTech University, Shanghai, China; 2Shanghai Jiao Tong University, Shanghai, China; 3The Scripps Research Institute, La Jolla, CA

TP 200 Intact mass analysis and kinetic models for ranking stabilizers of quaternary structure during drug development, and application to IALS; Wensheng Yang1; Md. Amin Hossain1; Christopher Singleton2; Brandon C. Miller1; Yifan Liu1; Roman Manesch1; Jeffrey N. Agar3; 1Northeastern University, Boston, MA

TP 201 Towards Integrative Global, Phosphoprotein- and Metabolomic Profiling of Low-input Preparations of Spheroid-like Cells for Drug Discovery: Norelle C. Wildburger1; Cristina Di Poto2; Jana Zech1; Mahder Abate1; 1Silke Reischl3; Erik Allman1; Lisa H. Cazes4; Bilica Bilada1; Sonja Hess5; 1AstraZenea R&D, Gaithersburg, Maryland; 2University of Maryland College Park, College Park, MD; 3AstraZeneca, Molndal, Sweden

TP 202 Feasibility of nanoflow LC/MS/MS monitoring and screening through high pressure? Wenyi Hua1; Xiadong Feng1; 1Pfizer Inc., Groton, CT

TP 203 Mass Spectrometry-based Barcoding and Screening Platform Designed for Quantitative Macromolecular Drug Delivery; Ning Wang1; Nicole A. McNeer1; Alex Kentsis1; 1Memorial Sloan Kettering Cancer Center, New York, New York; 2Weill Medical College of Cornell University, New York, New York

TP 204 Characterization of proteins in influenza virus vaccines by LC-MS/MS and CGE; Xiaoxia Zhang1; Yang Song1; Ji Luo2; Hongxu Chen2; 1SCIEX, China, Shanghai, China; 2SCIEX, China, Beijing, China

TP 205 Deep proteomic screening and validation for systematic discovery of molecular glue compounds and novel degrader targets; Uli Ohmayer1; Martin Steger2; Bjorn Schwab1; Anastasia Bednarz1; Sophie Machata3; Jutta Fritz1; Henrik Daub1; 1NEOsphere Biotechnologies GmbH, Planegg, Germany; 2NEOsphere Biotechnologies GmbH, Planegg, Germany

TP 207 DRAFT: A Dose-Response Activity Finder Tool for drug target deconvolution in chemical proteomics experiments; Praveen Kumar1; Heng Zhao2; Aarti Kawatkar3; Steven Novick3; 1AstraZeneca, Waltham, MA

TP 208 Strategy for Bioanalysis of Liposomal Drugs in Support of Bioequivalence Studies; Yuhua Ji1; Jinghui Liu1; Min Meng1; Xueyuan Zhang2; Chunlei Li3; 1Chongqing Denali Medpharma Co., Ltd, Chongqing, China; 2CSPC Pharmaceutical Group Ltd, Shijiazhuang, China; 3The Scripps Research Institute, La Jolla, CA

TP 209 A novel online tool for interactive analysis of proteomics and phospho-proteomics data: Serhan Yilmaz1; Filipa Blasco Tavares Pereira Lopes2; Marzieh Ayati1; Mark Chance3; Mehmet Koyuturk4; 1Case Western Reserve University, Cleveland, OH; 2The University of Texas Rio Grande Valley, Edinburg, Texas

TP 210 Determination of BTK inhibitor concentration in patients with hematological diseases by HPLC-MS/MS; Wenli Sun1; Hongxing Liu2; Jinyan Guo3; Ran Xiao4; Lei Wang5; 1Beijing University of Traditional Chinese Medicine, Beijing, China; 2Nanjing University of Traditional Chinese Medicine, Nanjing, China; 3Beijing University of Traditional Chinese Medicine, Beijing, China

TP 211 Affinity selection mass spectrometry for high throughput drug screening of membrane proteins including GPCRs and solute carriers; Kundan Sharma1; Reda Assal1; Shahid Rehan1; Katharina Duerer2; Laia Malet Sanz1; Adam Sanderson3; Jonathan Hopper4; Steven Chariton5; Ali Jazayeri6; Idlir Liko7; 1OMass Therapeutics, Oxford, United Kingdom; 2The Scripps Research Institute, La Jolla, CA

TP 212 Unbiased validation of degrader drug neosubstrates by high-sensitivity pS-AF-MS/MS-identified global ubiquitonomics; Martin Steger1; Uli Ohmayer1; Bjorn Schwab1; 1The Scripps Research Institute, La Jolla, CA
| TP 224 | Mechanical Engineering, Institute of Chemical and Environmental Engineering, Neubiberg, Germany; Photonion GmbH, Schwerin, Germany |
| TP 225 | High Resolution-MS uncovers new halocyclopentadiene disinfection by-products in drinking water; Susan Richardson1; Jiafu Li1; Md. Tareq Aziz2; Caroline Granger3; University of South Carolina, Columbia, SC; Soochow University, Suzhou, China |
| TP 226 | Evaluating detectability as LoD from the predicted ionization efficiency values for ESI+ and ESI-; Amina Souili1; Jonathan Martin2; Anneli Krueve1; Department of Environmental and Materials Chemistry, Stockholm University, Stockholm, Sweden; Department of Environmental Science, Stockholm University, Stockholm, Sweden |
| TP 227 | LC-MS/MS combined with complimentary methods to quantify total PFAS concentration in contaminated water; Leif Abrell1; Osmar Luiz Moreira P Menezes1; Kartika Srivastava1; Barriette Renieres1; Jon Chorover1; Reyes Sierra Alvarez2; University of Arizona, Tucson, AZ |
| TP 228 | Functional group analysis of gas-phase oxidation products of α-pinene using high resolution collision-induced dissociation mass spectrometry; Daisuke Fukuyama1; Kanako Sekimoto1; Yokohama City University, Yokohama-shi, Japan |
| TP 229 | Environmental Spectrometry tools for confident discrimination of different qualities of poplar feedstocks; Hania A. Khouz-Hollins1; Bryan Keifer2; Rachel J Sanig3; Waters Corporation, Milislow, United Kingdom; Waters Corporation, Milislow, United Kingdom |
| TP 230 | An ultra-high sensitivity analysis approach for detecting PFAS compounds in water sources; Jianru Stahl-Zeng1; Bertram Nieland2; Abdessamad Charboun3; SCIEX, Darmstadt, Germany; SCIEX, Darmstadt, Germany; SCIEX, Macclesfield, United Kingdom; Het Water Lab, J.W. Lucasweg 2 2031 BE Haarlem, Netherlands |
| TP 231 | Comprehensive Analytical Workflow of PFAS Analysis in Aqueous Environmental Samples; Ying Long1; Ana Ramos1; James Smalley2; Lam Leung3; Chemours, NEWARK, DE |
| TP 232 | Analysis of organic chemicals in aerosol particulate matter in Mongolia using high-throughput UPLC FT-ICR MS and artificial neural network; Seungwoo Son1; Moonhee Park2; Young Hwan Kim1; Sunghwan Kim1,2,3; Kyungpook National University, Daegu, South Korea; Korea Basic Science Institute, Cheongju, South Korea; Mass Spectrometry Converging Research Center and Green-Nano Materials Research Center, Daegu, South Korea |
| TP 233 | Microplastic Analysis and Additive Screening using Thermal Desorption/Pyrolysis DART-MS; William I. Freigante1; Sam Putnam2; Kushal Modi3; Bruker Scientific, LLC, Billerica, MA |
| TP 234 | Analysis of PAHs using the Hydrogen-Optimized Source with GC-MS and GC-MS/MS in Challenging Soil Matrix; Samuel P Haddad1; Bruce D Quimby2; Anastasia A Andrianiova1; Eric L Faustett1; Agilent Technologies, Wilmington, DE |
| TP 235 | Blow flies as remote sampling devices: Detection of insensitive munitions and their degradation products in the environment using LC-MS/MS; Sarah Dowling1; Sarah Prunty1; Katie Jensen1; Christine Picard1; Nicholas Manicke1; Indiana University Purdue University Indianapolis, Indianapolis, IN |
| TP 236 | Reduction of PFAS in Drinking Water using a Filter containing Activated Carbon plus Ion Exchange Resin, measured using QSynight LC-MS/MS; Cole Strattman1; Jacob Jalalili1; Jesse Leonard2; Erasmus Cadjo3; Marc E Eile4; PerkinElmer, Shelton, CT; PerkinElmer Inc., Woodbridge, ON |
| TP 237 | Evaluating Known and Novel PFAS in Firefighter Blood with Non-Targeted Liquid Chromatography, Ion Mobility Spectrometry and Mass Spectrometry Measurements; Ashlee T Falls1; Anna Boatman1; Kaylie Kirkwood2; Heather M Stapleton2; Erin S Baker3; 1University of North Carolina at Chapel Hill, Chapel Hill, NC; 2North Carolina State University, Raleigh, NC; 3Duke University, Durham, NC | TP 247 | LC-MS/MS method for quantifying glycerol monolaurate (GML) isomers in human milk: development, validation, and relevant pilot study findings; Thomas Vennard1; Nathan A. Meredith1; Michael Gray1; Sarah Maria1; Shay Phillips1; Lauren Brink1; Ruth Simmons2; 1Mead Johnson Nutrition, Evansville, IN; 2Reckitt, Parsippany, NJ | TUESDAY POSTERS |
| TP 238 | Unravelling the biological impacts of PFAS contamination using omics-based mass spectrometry ecosurveillance techniques in wild-captured freshwater turtles; David J. Beale1; Thomas Nguyen1; Utpal Bose3; Jordi Nells1; Sally Stockwell1; James A. Broadbent1; Matthew C. Smith1; Andrew Bissett2; Gunjan Pandey1; Leon Court1; Rahul Rane1; Caltriona Walsh1; Nicholas Bourne1; Sandra Nilsson1; Viviana Gonzalez-Astdildillo1; Christoph Braun1; Brenda Baddiley1; Stephanie Shaw1; Josh Llinas2; Duncan Limpus1; Suzanne Vardy1; 1CSIRO, Dutton Park, Australia; 2CSIRO, St Lucia, Australia; 3CSIRO, Hobart, Australia; 4CSIRO, Canberra, Australia; 5CSIRO, Parkville, Australia; 6The University of Queensland, Woolloongabba, Australia; 7The University of Queensland, Gatton, Australia; 8Queensland Department of Environment and Science, Dutton Park, Australia; 9Unusual Pets Veterinarian, Brisbane, Australia | TP 248 | Quality Discrimination of Jasmine Tea using LC-Q/TOF Combined with Sensory Evaluation and Statistical Method; Xinyue Peng1; Jason Li1; Nolia Yu1; 1APTC, The Coca-Cola Company, Shanghai, China | |
| TP 239 | PY-GCMS analysis of microplastics in environmental samples using nitrogen as an alternative carrier gas; Andy Sandy1; Evelyn Wang1; Ruth Marfil2; Luis Figueroa3; Chia-Mi Okamoto3; 1Shimadzu Scientific Instruments, Columbia, MD; 2Shimadzu Scientific Instrument, Columbia, Maryland | TP 250 | Proteomics of Western Honeybees to Assess Colony Health; Vincentian deamidation sites | |
| TP 240 | Identification of a Serine-containing Microcystin by Thiol Derivatization and Specific MS/MS Neutral Losses; Sanduni H Premathilake1; Johanna A Birbeck2; Judy A Westrick1; Dragin Isalovic1; 1University of Toledo, Toledo, OH; 2Wayne State University, Detroit, MI | TP 251 | Optimization of extraction method to determine 12 novel brominated flame retardants in squid using gas chromatography–mass spectrometry (GC–MS); Banub Bag2; Sun Koung Joung1; Hamin Choi1; Sang Beom Han1; 1Chung-Ang University, Seoul, South Korea | |
| TP 241 | Characterizing the Isomeric Forms of PFASs in Biological Samples with UHPLC and Ion Mobility Mass Spectrometry; Carrie A McDonough1; David Dukes1; Jennifer Marciano1; Emily Parry1; David A Weil1; Sheher Banu Mohsin1; 1Carnegie Mellon University, Pittsburgh, PA; 2Stony Brook University, Stony Brook, NY; 3Agilent Technologies, Santa Clara, CA | TP 252 | High-resolution mass spectrometry (HRMS) method for determining 43 per- and polyfluoroalkyl substances (PFAS) in vegetables; Gui-Ru Xie1; HONG-JHANG Chen1; 1Institute of Food Science and Technology, National Taiwan University, Taipei, Taiwan | |
| TP 242 | Accurate mass library for PFAS analysis in environmental samples using high resolution GC-Q/TOF; Sofia Nieto1; Matthew Giardina1; Luann Won2; Gabrielle Black1; Thomas Young1; 1Agilent Technologies, Inc., Santa Clara, CA; 2Department of Civil and Environmental Engineering, UC Davis, Davis, CA | TP 253 | Determination of chemically induced deamidation sites of gluten peptides using ion mobility or ultra-high resolution mass spectrometry; Matthew E Daly1; Qianying Xu1; Si Cheng1; Lisa Reid1; Lee A Gethings1; Emma Marsden-Edwards1; 1EC Mills2, 4; 1Waters Corporation, Milnrow, United Kingdom; 2University of Manchester, Manchester, United Kingdom; 3Waters Corporation, Costa Mesa, CA; 4University of Surrey, Guildford, United Kingdom | |
| TP 243 | Suspect Screening of Organic Contaminants in Nutraceuticals with Ultra-High Performance Liquid Chromatography/Quadrupole Time-of-Flight Mass Spectrometry; Hung-Ju Shih1; Chia-Yann Chen1; 1Institute of Food Safety and Health, College of Public Health, National Taiwan University, Taipei City, Taiwan | TP 254 | Application Of Liquid Chromatography–Mass Spectrometry And Species And Tissue Specific Peptide Biomarkers To Food Authentication And Detection Of Adulterations; Emilia Fernal1; Anna Stachniuk1; Magdalena Montowska1; Agata Sumara1; Alicja Tzpli1; 1Medical University of Lublin, Lublin, Poland; 2University of Life Sciences, Poznan, Poland | |
| TP 244 | Integrated and Quantitative Multi-omic Method for analyzing the macronutrients of Food using Rapid-Throughput LC-MS; Chinterns Chiang1; Cheng-Yu Weng1; Garret Couture1; Carlito B. Lebrilla1; 1University of California, Davis, Davis, CA | TP 255 | Quantitative Determination of Cannabidiol (CBD) Derivatives in Hemp Containing Products by Nano LC-MS/MS; Md Mdotofa Al Amin Bhuiyan1; Cristian D. Gutierrez Reyes1; Wazah Purba1; Andrew Bennett1; Sherifdeen Onigbinde1; Adeniyi Myinouluwa1; Yehia Mechef1; 1Texas Tech University, Lubbock, Texas | |
| TP 245 | Quantitative Analysis of Anthocyanins in Plant Materials by LC-DAD-MS with Molar Relative Response Factors (MRRFs); Wen Dong1; Xin Yang1; Ning Zhang2; Pei Chen1; Jianghao Sun1; James Hanly1; Mengliang Zhang1; 1Middle Tennessee State University, Murfreesboro, TN; 2Fisk University, Nashville, TN; 3USDA-ARS, Beltsville, MD; 4MTSU, Murfreesboro, TN | TP 256 | Development of LC-MS method for quantification of Aflatoxin M1 in human urine samples; Gabriela Ávila-Villarreal1,2; Candy Andreina Montaño-Pérez2; Guadalupe Yáñez-Ibarra1; Jorge-Luis Figueroa-Cordova1,2; Cyndia-Azcuenaga González-Arias3; 1Unidad Especializada en I+D+i Calidad de Alimentos y Productos Naturales, Centro Nutiva, Guatemala; 2University of Lublin, Lublin, Poland; 3University of Life Sciences, Poznan, Poland | |
| TP 246 | Intact mass characterization reveals novel post-translationally cleaved allergenic proteins from peanut; Justin Marsh1; Danijela Apostolovic1; Govardus De Jong1; Stel J Koppelman1; Philip Johnson1; 1University of Nebraska Lincoln, Lincoln, NE; 2Karolinska Institute, Solna, Sweden; 3Wageningen University, Wageningen, Netherlands | TP 257 | Characterization of Unsatuated Fatty Acids in Negative OAD-MS/MS using LCMS-9050; Hidenori Takahashi1; Mami Okamoto1; Youmi Miyazaki1; Yohei Arao1; Natsuyo Asano1; 1Shimadzu Corporation, Kyoto, Japan |
Applications of LC-MS to analyze food-derived bioactive peptides: from food processing to simulated gastrointestinal digestion; Yu-Ping Huang1; Fernanda Furlan Goncalves Dias1; Juliana Maria Leite Nobrega De Moura Bell1; Daniela Barle1; 1University of California Davis, Davis, CA

Use of Visualized Rayleigh Limit to Aid in Charge landing neuropeptide in the presence of copper ion; Saketh Chemuru1; Jessica Prenni; Jones1; 1California Institute of Technology, Pasadena, CA; 2University of California, San Diego, CA; 3University of Michigan Ann Arbor, Ann Arbor, MI

Analysis of fatty acid content in rice by GC; Guoqun Sui1; Jun Zhang1; Jun Wang2; 1Beijing Longji Foodstuffs Group Co., Ltd, Shanghai, China; 2Institute of Oil Crops, Chinese Academy of Agriculture Sciences, Beijing, China

Bismuth-Mediated Capture of the Cysteine-Rich Dark Proteome in Mycobacteria; Hannah A. Marietta1; C. Bruce Mousseau1; Matthew M. Champion1; 1University of Notre Dame, Notre Dame, IN

Structural studies on somatostatin and octreotide in the presence of copper ions by means of FRET and ion mobility spectrometry; Lukas Rafael Benzengen1; Pi Wu2; Despoina Svingou1; Renato Zenobi1; ETH Zurich, Zurich, Switzerland

Microdropel Mass Spectrometry-based Method for Detecting Hemoglobin Adducts; Hung-Hsiang Jen1; Kang-Yu Liu1; Shu-Hui Chen; Chin-Ming Kuo1; Fung-Yu Chen1; 1National Cheng Kung University, Tainan, Taiwan

Isotopologues of Oxyanions: A Journey from Ice Cores to Humans; Caijetan Neubauer1; Kristyna Kammerova1; Sebastien Kopf1; Andreas Hilker1; 1University of Colorado Boulder, Boulder, CO; 2Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany

Dissecting the formation of protein corona on nanoparticles allows reconstructing deep plasma protein concentrations and discovering novel proteoforms; Alexey Stukalov1; Shadi Ferdosi1; Yingxiang Huang1; Moaraj Hasan1; Brittany Lee1; Asim Siddiqui1; Serafim Batzoglou1; Daniel Horburg1; 1Seer Inc., Redwood City, CA

High-efficiency survey of analytes enabled by modulated ion transfer and MS/MS analysis; Xiaomin Fan1; Zheng Ouyang1; 1Department of Precision Instrument, Tsinghua University, Beijing, China

Advances in molecular analysis at the nanoscale; Thanh Loan Lai1; Dmitry S. Verkhoturov1; Michael J. Eller2; Serge Della Negra2; Stanislav V. Verkhoturov1; Emile A. Schweikert1; 1Department of Chemistry, Texas A&M University, College Station, TX; 2Department of Chemistry and Biochemistry, California State University Northridge, Northridge, CA; 3University of Paris-Saclay, CNRS/IN2P3, UCLab, Orsay, France

Mucinase SmE enables improved glycoproteomic mapping of mucin-domain glycoproteins; Alexandra Steigmeyer1; Joann Chongsartsinuos1; Keira E. Mahoney1; Taryn M. Lucas1; Deniz Ince1; Alexandra Battison1; Marie A. Hollenhorst1; D. Judy Shontz1; Victor Atta1; Catherine Kwon1; Carolyn R. Bertozi1; Stacy A. Malaker1; 1Yale University, New Haven, CT; 2Stanford University, Stanford, CA

Exposing the molecular heterogeneity of glycosylated biotherapeutics; Luis F Schachner1; Christopher Mullenh1; Wilson Phung1; Joshua Hinkle1; Michelle Irwin Beardsley1; Tracy Bentley1; Peter Day1; Christina Tsai1; Siddharth Sukumaran1; Tomasz Baginski1; Danielle Dicara1; Nicholas Agard1; Matthieu Masereel1; Joshua Gober1; Adel Elsohly1; John E.P. Syka1; Romain Huguet1; Michael T Marty1; Wendy Sandoval1; 1Genentech Inc, South San Francisco, CA; 2Thermo Fisher Scientific, San Jose, California; 3University of Arizona, Tucson, AZ

Glycan-dependent Affinity Purification Mass Spectrometry (GAP-MS) provides novel insights into glycoprotein interaction network; Yixuan (axe) Xie1; Xingyu Liu1; Siyu Chen2; Zongtao Lin1; Carito B. Lebrilla1; Benjamin A Garcia1; 1Washington University School of Medicine, St. Louis, MO; 2University of California, Davis, Davis, CA

All in One: Direct Site-specific Detailed Glycan Characterization by Higher Energy Electron Activated Dissociation Tandem Mass Spectrometry; Ruiling Li1; Chaohuang Xia1; Haowei Wang1; Catherine University-Department of Chemistry and Biochemistry, Columbus, OH

Factors Controlling Ion Yields in Droplet Assisted Ionization; Jim Walker1; Kelvin Risty1; Oli Boswell1; Amanan Yanna1; Joshua Harrison1; Bryan R Bzdik1; 1University of Bristol, Bristol, United Kingdom

Dissecting the formation of protein corona on nanoparticles allows reconstructing deep plasma protein concentrations and discovering novel proteoforms; Alexey Stukalov1; Shadi Ferdosi1; Yingxiang Huang1; Moaraj Hasan1; Brittany Lee1; Asim Siddiqui1; Serafim Batzoglou1; Daniel Horburg1; 1Seer Inc., Redwood City, CA

High-efficiency survey of analytes enabled by modulated ion transfer and MS/MS analysis; Xiaomin Fan1; Zheng Ouyang1; 1Department of Precision Instrument, Tsinghua University, Beijing, China

Advances in molecular analysis at the nanoscale; Thanh Loan Lai1; Dmitry S. Verkhoturov1; Michael J. Eller2; Serge Della Negra2; Stanislav V. Verkhoturov1; Emile A. Schweikert1; 1Department of Chemistry, Texas A&M University, College Station, TX; 2Department of Chemistry and Biochemistry, California State University Northridge, Northridge, CA; 3University of Paris-Saclay, CNRS/IN2P3, UCLab, Orsay, France

Mucinase SmE enables improved glycoproteomic mapping of mucin-domain glycoproteins; Alexandra Steigmeyer1; Joann Chongsartsinuos1; Keira E. Mahoney1; Taryn M. Lucas1; Deniz Ince1; Alexandra Battison1; Marie A. Hollenhorst1; D. Judy Shontz1; Victor Atta1; Catherine Kwon1; Carolyn R. Bertozi1; Stacy A. Malaker1; 1Yale University, New Haven, CT; 2Stanford University, Stanford, CA

Exposing the molecular heterogeneity of glycosylated biotherapeutics; Luis F Schachner1; Christopher Mullenh1; Wilson Phung1; Joshua Hinkle1; Michelle Irwin Beardsley1; Tracy Bentley1; Peter Day1; Christina Tsai1; Siddharth Sukumaran1; Tomasz Baginski1; Danielle Dicara1; Nicholas Agard1; Matthieu Masereel1; Joshua Gober1; Adel Elsohly1; John E.P. Syka1; Romain Huguet1; Michael T Marty1; Wendy Sandoval1; 1Genentech Inc, South San Francisco, CA; 2Thermo Fisher Scientific, San Jose, California; 3University of Arizona, Tucson, AZ
TP 284  Large-scale and Site-specific Mapping of the Murine Brain O-Glycopeome with IMPa: Suttirong Suttithumyakul1, Yasuyuki Matsumoto1, Rajendra P. Ayyal1; Richard D. Cummings2; 1Department of Surgery, Beth Israel Deaconess Medical Center, Harvard Medical School, Boston, MA

TP 285  Correlating glycoform and structural heterogeneity of the intact SARS-CoV-2 receptor binding domain with ultraviolet photodissociation and collision cross section analysis; Virginia K. James1; Kate Lyn S. Zuercher1; Jennifer S. Brodbelt1; 1University of Texas at Austin, Austin, TX

TP 286  Optimization of Methods for Building Glycopeptide Libraries; Yi Liu1; Megan C. Burke1; Zachary C. Goecker1; Sergey L. Sheettlin1; Guanghui Wang1; Yuxue Liang1; Zheng Zhang1; Yuri A. Mirokhin1; Xiaoyu Yi1; Dmitri V. Tchekhovskoi1; Stephen E. Stein1; 1NIST, Gaithersburg, MD

TP 287  N-Glycosylation Profile of EpCAM in Epithelial and Breast Cancer Cells; Nicole M. Jenkinson1; Lauren R. Devine2,3; Caitlin M. Tressler1; Robert N. Cole1,3; Kristine Giunde1,3,4; 1Russell H. Morgan Department of Radiology and Radiological Science, Division of Cancer Imaging Research, Johns Hopkins University School of Medicine, Baltimore, MD; 2Mass Spectrometry and Proteomics Facility, Johns Hopkins University School of Medicine, Baltimore, MD; 3Department of Biological Chemistry, Johns Hopkins University School of Medicine, Baltimore, MD; 4Sidney Kimmel Comprehensive Cancer Center, Johns Hopkins University School of Medicine, Baltimore, MD

TP 288  Variation of Site-Specific Glycosylation Profiles for Influenza Glycoproteins from Different Vaccines and Reombinant Sources; Zachary C Goecker1; Meghan C. Burke1; Concepcion A. Remorozoa1; Yi Liu1; Yuri A. Mirokhin1; Sergey L. Sheettlin1; Dmitri V. Tchekhovskoi1; Xiaoyu Yang1; Stephen E. Stein1; 1National Institute of Standards and Technology, Gaithersburg, MD; 2National Institute for Standards and Technology, Gaithersburg, MD

TP 289  In-depth O-glycanization characterization and comparison of commercially available etanecot products using the ZenoTOF 7600 system. Wang Wentao1; Song Hexing2; Luo Ji1; Chen Hongxu2; Guo Lihai2; sciex, guangzhou, China; 1SCIX, Beijing, China; 2SCIX, Shanghai, China; 3SCIX, Beijing, China

TP 290  One-step preparation of boric acid-rich hydrothermal spheres for N-glycopeptide analysis in preeclampsia serum; Yinghua Yan1; Chuan-Fan Ding1; 1Ningbo University, Ningbo, China

TP 291  Characterizing Reproducibility of Glycoform Distributions for SARS-CoV-2 Spike Protein-Derived Glycopeptides Across Recombinant Protein Sources Using Automated, Mass Spectral Library-Based Methods; Meghan C. Burke1; Yi Liu1; Concepcion A. Remorozoa1; Yuri A. Mirokhin1; Sergey L. Sheettlin1; Dmitri V. Tchekhovskoi1; Guanghui Wang1; Xiaoyu Yang1; Stephen E. Stein1; 1National Institute of Standards and Technology, Gaithersburg, MD

TP 292  Introducing the GlycoPeaSR prototype for real-time N-glycopeptide identification on the PeaSR platform. Gad Armory1; Sven Brehmer1; Tharan Srikanth1; Lennard Pfenning1; Fokke Zijlstra1; Dennis Trede2; Gary Kruppa3; Dirk Lefeber4; Alain Van Goor5; Hans Wessels1; 1Translational Metabolic Laboratory, Department of Laboratory Medicine, Radboud Institute for Molecular Life Sciences, RadboudUMC, Nijmegen, Netherlands; 2Bruker Daltonics, Bremen, Germany; 3Bruker Ltd, Milton, ON; 4Translational Metabolic Laboratory, Department of Genetics, Radboud Institute for Molecular Life Sciences, RadboudUMC, Nijmegen, Netherlands; 5Bruker S.R.O., Brno, Czech Republic; 6Department of Neurology, Donders Institute for Brain, Cognition and Behavior, RadboudUMC, Nijmegen, Netherlands

TP 293  Mass spectrometry characterization of N-glycosylation and disulfide bonds of the spike protein from SARS-CoV-2 Omicron variant: Dongxia Wang1; Jakub Baudys1; Sarah H. Osman2; John R. Barr2; 1Centers for Disease Control and Prevention (CDC), Atlanta, GA; 2Centers for Disease Control and Prevention, Atlanta, GA

TP 294  Characterization of the site specific N- and O-glycosylation of proteins using LC-MS/MS analysis and the iTRAQ platform; Ju Yeon Lee1; Jin-Woong Choi2; Sanghyeon Bae1; Heeyoun Han2; Young Ho Juon3; Jin Young Kim4; 1Korea Basic Science Institute, Cheongju, South Korea; 2Korea Research Institute of Bioscience and Biotechnology, Yuseong-gu, South Korea; 3Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, South Korea; 4Korea university, Seoul, South Korea

TP 295  High-resolution, high-throughput glycoproteomics analysis of esophageal cancer lines reveal potential link between estrogen signaling and esophageal cancer; Chao Peng1; Jingzhi Zhao1; Ping Wu1; Gunagming Chen1; Lukang Sun1; Jing Huang1; Jun Ma1; Wenting Li1; Baozhen Shan1; 1BaizhenBio Inc., shanghai, China

TP 296  Fragment ion triggered Parallel Accumulation SERRation Fragmentation strategy for enrichment of glycopeptides data acquisition and beyond; Gad Armory1; Michael Krause2; Pierre-Olivier Schmitt3; Dennis Trede2; Gary Kruppa3; Dirk Lefeber4; Alain Van Goor5; Hans Wessels1; 1Translational Metabolic Laboratory, Department of Laboratory Medicine, Radboud Institute for Molecular Life Sciences, RadboudUMC, Nijmegen, Netherlands; 2Bruker Daltonics GmbH & Co.KG, Bremen, Germany; 3Bruker Daltonics S.A., Wissembourg, France; 4Bruker S.R.O., Brno, Czech Republic; 5Department of Neurology, Donders Institute for Brain, Cognition and Behavior, RadboudUMC, Nijmegen, Netherlands

TP 297  Regulation of Protein N-linked Glycosylation Site Occupancy.; Mariam Khaleque1; Amanda S. Nouwens1; Benjamin L. Schütz2; 1The University of Queensland, Brisbane, Australia

TP 298  Quantitative glycoproteome analysis using a novel nanoparticle-based plasma proteomics workflow; Shadi Ferdoosi1; Moajar Hasan1; Iman Mohtashemi1; Evan O’Brien2; Hongwei Wang2; Jian Wang2; Khatereh Motamedchaboki1; Harendra Guturu1; Daniel Horning1; 1Sequencing Inc., Redwood City, CA

TP 299  Correlating LC-MS/MS glycomic, glycoproteomic, and transcriptomic data to determine glycosylation pathways in lung cancer; Michael Russell S Alvarez2; Patrick Moreno3; Armin Oloumi1; Ryan Lee Schindler4; Qiweng Zhou1; Michelle Narciso1; Sheryl Joyce B. Grijaldo1; Ruel C. Nacario1; Gladys C. Comploto1; Francisco M. Heralde III1; Carlito B. Lebrilla4; 1University of California Davis, Davis, CA; 2Lung Center of the Philippines, Quezon City, Philippines; 3University of the Philippines Los Baños, Los Baños, Philippines

TP 300  Altered N-Glycoproteome of Murine Keratinocyte-Originated Exosomes under Diabetic Conditions Compromised Resolution of Wound Inflammation; Xuqiao Zeng1; Adam J Anthony1; Anu Sharma2; Jonathan C. Trinidad1; Subhadip Ghatak1; David E. Clemmer1; 1Indiana University Bloomington, Bloomington, IN; 2Indiana University Purdue University Indianapolis, Indianapolis, IN

TP 301  Sialic acid isomer-targeted glycoprotein enrichment and proteomic characterization using bioorthogonal derivatization; Hongxia Bai1; Collin McDowell1; Richard R. Drake2; 1Medical University of South Carolina, Charleston, SC

TP 302  Mass Spectrometry Analysis of N-linked Glycosylation on Influenza A(H3N2) Hemagglutinin and
Neuraminidase from Inactivated Virus; Betlehem Mekonnen1; Irina Alymov2; Jakub Baudys3; Ian York2; Donxia Wang1; John R Barr4; 1CDC, Chambley, GA; 2CDC, Atlanta, GA

TP 303 Confident Identification of Multiply Glycosylated Peptides Using Hot Electron Capture Dissociation; Margaret Down3; Cheng Lin1; Chaoshuang Xia4; Athanasios Smyrnakis5; Dimitris Papanastassiou5; Joseph Zaia1; 1Boston University Chobanian and Avedisian School of Medicine, Boston, MA; 2Fasmattech, NCSR Demokritos, Athens, Greece

TP 304 Comparative Glycomic and Glycoproteomic Analysis of Serum Exosomes Isolated Using Ultracentrifugation and Affinity-Based Method; Mojibola O Fowowe1; Cristian D Gutierrez-Reyes2; Moijgan Atashi3; Sherifeen Onigbinde3; Rogelio Najera Gonzalez2; David M Lubman1; Yehia Mechref1; 1Texas Tech University, Lubbock, TX; 2Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX; 3Institute of Genomics for Crop Abiotic Stress Tolerance, Texas Tech University, Lubbock, TX

TP 305 O-glycoproteomic mapping of amyloid precursor protein in Alzheimer’s Disease; Alexandrina S. Battison1; Stacy A. Malaker1; 1Yale University, New Haven, CT

TP 306 Target Glycoproteomics and Proteomics Analysis with Parallel Reaction Monitoring (PRM) LC-MS/MS; Muyinoluwa A Adeniyi1; Cristian D Gutierrez-Reyes2; Moijgan Atashi3; Andrew I Bennett4; Sherifeen Onigbinde3; 1University of California San Diego, La Jolla, CA; 2Texas Tech University, Lubbock, TX; 3Texas Tech University, Lubbock, TX

TP 307 The role of N-glycosylation in SARS-CoV-2 Spike protein binding specificity and kinetics; Sarah H Oaman1; Dongxia Wang1; Theodore R. Keppel1; John R Barr4; 1CDC, Chambley, GA

TP 308 Isomeric Separation of α2.3/α2.6-linked 2-amino-benzamide (2AB)-labeled Sialylglycopeptides by C18-LC-MS/MS; PeiLing Yian1; Yifan Huang1; Cristian D Gutierrez-Reyes1; Jieqiang Zhong1; Yehia Mechref1; 1Texas Tech University, Lubbock, Texas

TP 309 Analysis of Mitochondria Glycopolymers and Glycoproteomics Isolated Using Different Enrichment Methods; Judith Lila Myers1; Oluwatosin E Daramola1; Moijgan Atashi3; Mojibola O Fowowe1; Yehia Mechref1; 1Texas Tech University, Lubbock, Texas

TP 310 LC-MS/MS Characterization of the N-glycosylation of Spike protein S1 Derived from 11 variants of SARS-CoV-2; Cristian D Gutierrez-Reyes1; Sherifeen Onigbinde3; Andrew I Bennett4; Akeem Sanni6; Peilin Jiang1; Oluwatosin E Daramola1; Moijgan Atashi3; Vishal Sandi4; Mojibola O Fowowe1; Yehia Mechref1; 1Texas Tech University, Lubbock, Texas

TP 311 Improved enrichment techniques for analysis of densely O-glycosylated domains from complex samples; Keira Erol Mahoney1; Vincent Chang1; Taryn M. Lucas1; Stacy A. Malaker1; 1Yale University, New Haven, CT

TP 312 Comparison of the Relative Quantitation of N-linked Glycopeptides Using Different Chromatographic Separation Modes; Mya M Brown1; Hoang Kim Ngan2; Thai1; Ron Orlando1; 1University of Georgia - Complex Carbohydrate Research Center, Athens, GA

TP 313 Development of an Automatic Three-Dimensional Mass Spectrometry Imaging System with Infrared Matrix-Assisted Laser Desorption Electrospray Ionization (MALDESI); Ying Xi1; Kevan Knizner1; Kenneth Garrad1; David Muddiman1; 1North Carolina State University, Raleigh, NC

TP 314 Achieving Sub Parts-Per-Million Mass Measurement Accuracy on an Orbitrap Mass Spectrometry Imaging Platform with Control; Russell R Kibbe1; David C. Muddiman1; 1North Carolina State University, Raleigh, NC

TP 315 Super-resolution Expansion Mass Spectrometry Imaging; Y. L. Winnie Hung1; Jianing Wang1; Chengyi Xie1; Zongwei Cai1; 1State Key Laboratory of Environmental and Biological Analysis, Hong Kong Baptist University, Hong Kong, China

TP 316 A simplified sample preparation strategy for high-throughput mass spectrometry imaging of spheroids; Yuan Liu1; Jillian Johnson1; Hua Zhang1; Lingjun Li1; 1University of Wisconsin-Madison, Madison, WI

TP 317 immuno-DESI-MSI Spatially Locates A Drug Target, Signaling Factors, and Enzymes on Tissue; Xiaowei Song1; Richard N. Zare3; 1Stanford University, Stanford, CA

TP 318 Quantitative Biodistributions of Polymeric Nanocarriers and their Cargo via Metal-coded Mass Tag Approach; Dheeraj K. Agrohia1; Ritabrita Goswami1; Teerapong Jantarat1; Yağız Anıl Çiçek1; Taewon Jeon2; Vincent M. Rotello1; 1University of Massachusetts, Amherst, AMHERST, MA

TP 319 Improved Quantitative Imaging of Nanomaterials by LA-ICP-MS using a Novel Tissue Mimic Approach; Teerapong Jantarat1; Joshua D Lauterbach1; Jeerapat Dousngchawee1; Richard W. Vachet1; 1University of Massachusetts Amherst, Amherst, MA

TP 320 RaMALDI imaging: a novel multimodal imaging workflow integrating Raman spectroscopic and MALDI mass spectrometry imaging of a single sample; Jeong Hee Kim1; Ethan S. Gelin1; Caitlin M Trenear1; 1Boston University Chobanian and Avedisian School of Medicine, Boston, MA; 2Boston University School of Medicine, Boston, MA

TP 321 Statistical Approach to System Suitability Testing (SST) for Mass Spectrometry Imaging by Infrared Matrix-Assisted Laser Desorption Electrospray Ionization (IR-MALDESI); Olivia Diedi1; Hongxia Bai1; Emily Hector1; Kenneth P. Garrard1; David C. Muddiman1; 1North Carolina State University, Raleigh, NC

TP 322 Combining Multimodal Single Cell Imaging with Multiplexed Enzyme-based MALDI Mass Spectrometry Imaging for Translational Studies; Jaclyn B Dunne1; Jake T. Griner1; Martin Romeo1; Carsten Krieg1; Mark Lim1; 1Anand S. Mehta1; Rui Zhao1; 1North Carolina State University, Raleigh, NC

TP 323 Visualizing the Matrix: New Methods for Imaging the Distributions of Extracellular Matrix Proteins; Akaamsha Rampal1; Ngoc Vu1; Richard W. Vachet1; Shelly R. Peyton1; 1University of Massachusetts Amherst, Amherst, MA

TP 324 High-coverage Lipid C-C Imaging in tissue using lipidome imaging in biological tissues and tumor model; Yanyan Chen1; Chengyi Xie1; Peiie Xie1; Jianing Wang1; Zongwei Cai1; 1State Key Laboratory of Environmental and Biological Analysis, Hong Kong Baptist University, China

TP 325 Tissue treatment and post-ionization for mass spectrometry imaging of lipids: gains and losses; Junhao Yang1; Austin B. Moyle1; Andrew Bowman1; Wayne Buck1; David S. Wagner1; 1AbbVie Inc., North Chicago, IL

TP 326 Robust tissue single-voxel collection and processing for spatially resolved proteomics; Reta Birhanu Kitata1; Marija Velickovic1; Zhangyang Xu2; Rui Zhao2; Rosalie K. Chu2; Marda L. Jorgensen2; David Scholten1; Tao Liu1; Huiping Liu1; Clive H. Wassermann1; Chia-Feng Tsai1; Tujin Shi1; 1Biological Sciences Division, Pacific Northwest National Laboratory, Richland, Washington 99354; 2Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, Washington 99354; 3Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, Washington; 4Department of Pathology, Immunology, and Biological Analysis, Hong Kong Baptist University, Diabetes Institute, College of Medicine, University of Florida, Gainesville, Florida 32611;
TP 330
Biofilm of pathogenic bacteria analyzed by MALDI-TOF Imaging mass spectrometry (IMS) and top-down proteomic identification: Clifton K Fagerquist1; Yanlin Shi1; Produce Safety & Microbiology, Western Regional Research Center, Agricultural Research Service, USDA, Albany, CA

TP 331
4-APEBA, a new on-tissue chemical derivatization agent for enhanced imaging of phytochemicals using MALDI-MSI: Kevin J Zemalis1; Vivian Lin1; Aimirhossein H. Ahkami1; Tanya Winkler1; Robert Stanley1; Vimal Kumar Balasubramanian1; Christopher Anderton1; Dusan Velickovic1; 1PNNL, Richland, WA

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SpatialOMx analysis allows for the specific identification of lipid species paving the way for accurate flux analysis: Sunamkala Ramachandran1; Beixi Wang1; Azad Esghii1; Erica Forsberg1; Katherine Stumpo1; 1Bruker Daltonics, Billerica, MA

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MALDI-IHC-Guided In-Depth Spatial Proteomics: Targeted and Untargeted MSI Combined: Britt S.R. Claes1; Kasper Krestensen1; Gargey Yagnik2; Andrej Grigic1; Christel Kuik1; Mark J. Lim1; Kenneth J. Rothschild4; Michiel Vandenbosch2; Ron M.A. Heeren2; Kasper Krestensen1; John F. Cahill1; Tatiana Segura1; 1Bruker Daltonics, Billerica, MA; 2Uppsala University, Uppsala, Sweden; 3AMBERGEN, Inc, Annandale, VA

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Maximizing Throughput of a Liquid Microjunction Surface Sampling Probe-Mass Spectrometry Imaging System for Microfluidic Rhizosphere-on-a-Chip Habitats: Vilmos Kertesz1; Scott T. Retterer2; Muneeba Khali1; John F. Caii1; Oak Ridge National Laboratory, Oak Ridge, TN

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Mass spectrometry imaging of regioisomeric hormonal steroids: Varun Vasnheele Sharma1; Ingela Lanekoff1; 1Uppsala University, Uppsala, Sweden; 2Uppsala University, Uppsala, Sweden

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Functionality of Sucrose as a Cryoprotectant and Permeable Matrix for Analysis of Multiple Biological Systems by IR-MALDESI Mass Spectrometry Imaging: Mary F Wang1; Alexandrina L. Sohn1; Juhi Samal2; Kevin Erning3; Tatiana Segura1; David C. Muddiman2; 1North Carolina State University, Raleigh, NC; 2Duke University, Durham, NC

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Image-wide adjacent-pixel data averaging increases sensitivity toward dosed drugs of abuse and antiretrovirals in O-Quanta Mass spectrometry Imaging: Yury N. Desyatnykov1; Austin M. Jones2; Kevin M. Radermeyer2; Mary Peace McRae2; Yury O. Tsybin3; Konstantin O. Nagornov1; Anton N. Kozhinov1; Angela D.M. Kashuba1; Elias P. Rosen4; 1UNC, Chapel Hill, NC; 2Virginia Commonwealth University, Richmond, VA; 3Spectroswiss, Lausanne, Switzerland

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Improved detection of tryptic peptides from tissue sections using Desorption electrospray ionisation mass spectrometry imaging (DESI-MSI): Heather Bottomley1; Dr Jonathan Phillips1; Dr Philippa Hart2; 1University of Exeter, Exeter, United Kingdom; 2Uppsala University, Uppsala, Sweden; 3AMBERGEN, Inc, Annandale, VA; 4Bruker Daltonics GmbH & Co KG, Billerica, MA

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Evaluation of lithium adduction in mass spectrometry imaging for sphingolipid analysis via internal standard-spiked tissue homogenate: Anh Tran1; William T. Andrews1; Eugene Moskovets2; Maureen A. Kane3; Jacob W. Jones3; 1University of Maryland, School of Pharmacy, Baltimore, MD; 2Mass Tech Inc, Columbia, Maryland

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AutoPIMS: an Integrated Mass Spectrometry Imaging Workflow for Spatial Proteome Biology: Pei Su1; John P. McGee1; Kenneth R. Durbin1; Michael A. R. Hollas2; Thomas P. Conrads3; Ryan T. Fellers2; Jeannie M. Camarillo1; Jared O. Kafader1; Neil L. Kelleher1; 1Northwestern University, Evanston, IL; 2Women's Health Integrated Research Center at Inova Health System, Annandale, VA; 3Duke University, Durham, NC

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Spatial Proteomics Reveals Localization of Membrane Proteins and Post-Translational Modifications in Ocular Lenses: Kevin L. Schey1; Lee S Cantrell2; Zhen Wang1; 1Vanderbilt University, Department of Biochemistry, Nashville, TN; 2Vanderbilt University, Nashville, TN

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Art Conservation with DESI MS Imaging: Direct Mapping of Compound Localization on Wood Samples: Luke Addington1; Michael T Marty1; Anthony J Midley1; 1University of Arizona, Tuscon, Arizona; 2Waters, Milford, MA

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Spatial molecular analysis of acute cocaine exposure: Mariya Nezhva1; Rami Yaka2; Per E. Andren3; Katy Margulis4; Erik T Jansson1; Uppsala University, Uppsala, Sweden; 2Hebrew University, Jerusalem, Israel

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Evolution from Shotgun to Machine-gun - Capillary LC/MS with 1,000 Samples/Day Facilitates Proteomic MS Imaging: Ayana Tomioka1; Ryota Tomioka1; Koseke Ogata1; Issei Mori1; Makoto Arita2; Koshi Iimmwi2; Naoyuki Sugiyama3; Yasushi Ishihama2; Kyoto University, Kyoto, Japan; 2RIKEN Center for Integrative Medical Sciences, Yokohama, Japan; 3Keio University, Minato-ku, Japan; 4National Institutes of Biomedical Innovation, Health and Nutrition, Ibaraki, Japan

TP 345
Evaluation of an improved feature algorithm for QTOF and ion mobility imaging data in spatial lipidomics and metabolomics: Jacob Truong1, 2, 3, Sören-Oliver Deininger1; Andrea Pascale-Henke1; Konstantin Schwarzze1; Lisa M. Butler1, 2, 3; Paul J. Trim1, 2, 3; Martin F. Snel1; Heiko Neuweger1; University of Adelaide Medical School and Freemasons Centre for Male Health and Wellbeing, Adelaide, Australia; South Australian Immunogenomics Cancer Institute, Adelaide, Australia; 2South Australian Health and Medical Research Institute, Adelaide, Australia; 3Bruker Daltonics GmbH & Co KG, Bremen, Germany

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Exudate Dynamics of the Rhizosphere Visualized Using MALDI-MSI: Fiona M Ellsworth1; Joshua L Fischer1; Ethan Yang1; Kasia Janota2; Richard E. Marinos2; 1University of Buffalo, Buffalo, NY; 2Bruker Daltonics, Billerica, MA

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Exploring the Potential of Mass Spectrometry Imaging: Opportunities and Challenges: Michaela Schwaiger-Haber1; Ethan Stancliff1; Dhanalakshmi S. Anbukumar2; Blake E. Sells1; Jia Yi1; KevinCho1; Kayla Adkins-Travis1; Leah P. Shriver1; 1Washington University in St. Louis, St. Louis, MO

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2D (phospho)-proteome mapping of human spleen tissue at 200 μm spatial resolution: Marija Velikovic1; Reta Birhanu Kitata1; Zhangyang Xu1; Rui Zhao1; Rosalie K. Chu1; Marda L. Jorgensen1; David Scholten1; Sarah M Williams1; Ying Zhu1; Daniel J Orton1; Tao Liu1; Huiping Liu1; Clive H. Waterfall1; Chia-Feng Tsai1; Tujin Shi1; 1PNNL, Richland, WA; 2University of Florida, Gainesville, FL; 3Department of Pharmacology, Feinberg School of Medicine, Northwestern University, Chicago, Illinois 60611
TP 349 Using Native MS, Top-Down, and Bottom-Up Proteomics to Profile Regio-specific Protein Interactions on Tissue; Sarah C Beno 1, Raul A Villacob 1, Neda Feizi Gilarghi 1, Touradj Solouki 1, Baylor University, Waco, TX

TP 350 Spatial Multi-Omics Investigation of Prostate Cancer Heterogeneity using integrated spatially resolved lipidomics and transcriptomics; Wanjui Zhang 1, 2, Xander Spottebon 1, Tassiani Sarretto 1, Fabio Socciarello 1, Sebastiaan Vanuyten 4, José Ignacio Alvaria Larzigitza 9, 10, Sam Kint 11, David Wouters 12, 13, Gabriele Partel 14, Maria Mantas 15, Thomas Gevaert 16, Wout Devlies 14, 15, Katy Vandereyken 14, Steven Joniaux 14, 15, Massimo Loda 15, Bart De Moor 16, Thierry Voet 17, Alejandro Sifrim 11, Shane Ellis 5, 18, Marc Claesen 13, Nico Verbeek 12, Johannes Swinnen 20, 21, STADIUS Center for Dynamical Systems, Signal Processing and Data Analytics, Department of Electrical Engineering (ESAT), KU Leuven, Leuven, Belgium; 1Molecular Horizons and School of Chemistry and Molecular Bioscience, University of Wollongong, Wollongong, Australia; 2Illawarra Health and Medical Research Institute, Wollongong, Australia; 3Department of Pathology, Weill Cornell Medical College, New York, NY; 4Laboratory of Reproductive Genomics, Department of Human Genetics, KU Leuven, Leuven, Belgium; 5KU Leuven Institute for Single Cell Omics (LISCO), KU Leuven, Leuven, Belgium; 6KU Leuven Institute for Single Cell Omics (LISCO), KU Leuven, Leuven, Belgium; 7KU Leuven Institute for Single Cell Omics (LISCO), KU Leuven, Leuven, Belgium; 8Laboratory of Multi-omic Integrative Bioinformatics, Department of Human Genetics, KU Leuven, Leuven, Belgium; 9Laboratory of Multi-omic Integrative Bioinformatics, Department of Human Genetics, KU Leuven, Leuven, Belgium; 10Department of Urology, University Hospitals Leuven, Leuven, Belgium; 11Department of Urology, University Hospitals Leuven, Leuven, Belgium; 12Department of Development and Regeneration, KU Leuven, Leuven, Belgium; 13Department of Development and Regeneration, KU Leuven, Leuven, Belgium; 14Department of Pathology, Weill Cornell Medical College, New York, New York; 15STADIUS Center for Dynamical Systems, Signal Processing and Data Analytics, Department of Electrical Engineering (ESAT), KU Leuven, Leuven, Belgium; 16Molecular Horizons and School of Chemistry and Molecular Bioscience, University of Wollongong, Wollongong, Australia; 17Laboratory of Lipid Metabolism and Cancer, KU Leuven and Leuven Cancer Institute (LKI), Leuven, Belgium; 18Department of Urology, University Hospitals Leuven, Leuven, Belgium; 19Department of Urology, University Hospitals Leuven, Leuven, Belgium; 20Department of Development and Regeneration, KU Leuven, Leuven, Belgium; 21Department of Development and Regeneration, KU Leuven, Leuven, Belgium; 22Department of Pathology, Weill Cornell Medical College, New York, New York; 23Department of Electrical Engineering (ESAT), KU Leuven, Leuven, Belgium; 24Molecular Horizons and School of Chemistry and Molecular Bioscience, University of Wollongong, Wollongong, Australia; 25Laboratory of Lipid Metabolism and Cancer, KU Leuven and Leuven Cancer Institute (LKI), Leuven, Belgium

TP 351 Lipid Annotation for MALDI Imaging using Isotope Pattern, Spectral Pattern and Co-Localization Information; Jeff Dahl 1, Md Amir Hossen 2, Shimadzu, Columbia, MD; 3Shimadzu Scientific Instrument, Columbia, Maryland

TP 352 Development of Robust Spatial N-Glycomics and Proteomics Techniques for Human Tissue Analysis; Jessica K Lukowski 1, 2, Connor West 1, Katherine A. Stumpo 2, Young Ah Goo 1, 2, Mass Spectrometry Technology Access Center (MTAG@MGI), St Louis, MO; 3Washington University School of Medicine, St Louis, MO; 4Bruker Daltonics GmbH & Co.KG, Bremen, Germany

TP 353 Single-voxel spatial proteomics for resolving 14 ROIs across the whole mouse brain tissue section; Zhanxiang Xu 1, Reta Birhanu Kitata 1, Rosalie K. Chu 1, Rui Zhao 1, Le Z. Day 1, Matthew J Gaffrey 1, Tao Liu 1, Song-Lin Ding 1, Tong Zhang 1, Tujuan Shi 1, Biological Sciences Division, Pacific Northwest National Laboratory, Richland, Washington 99354; 2Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, Washington 99354; 3Allen Institute for Brain Science, Seattle, Washington 99354

TP 354 Characterizing Molecular Alterations to Glomeruli in Diabetic Nephropathy using MALDI IMS, Immunohistochemistry; Angela RS Kruse 1, 2, Melissa A Farrow 1, 2, Nathan Heath Patterson 1, 2, Madeline Colley 1, 2, Jamie L Allen 1, 2, Roy Larderobbie 1, Lukasz G Migas 1, 2, Morad Maleki 1, 2, Haichun Yang 1, 2, Agnes B Foge 1, 2, Raf Van De Plas 1, 2, 4, Joana P Gonçalves 1, 2, Richard M Caprioli 1, 2, 9, 10, 11, Jeffrey M Spragings 1, 2, 5, 11, Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; 2Department of Biochemistry, Vanderbilt University, Nashville, TN; 3Department of Intelligent Systems, Delft University of Technology, Delft, South Holland; 4Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; 5Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; 6Department of Pathology, Microbiology and Immunology, Vanderbilt University, Nashville, TN; 7Department of Pediatrics, Vanderbilt University Medical Center, Nashville, TN; 8Division of Nephrology, Department of Medicine, Vanderbilt University Medical Center, Nashville, TN; 9Department of Medicine, Vanderbilt University, Nashville, TN; 10Department of Pharmacology, Vanderbilt University, Nashville, TN; 11Department of Chemistry, Vanderbilt University, Nashville, TN

TP 355 Maximizing Data Coverage with Sequential Imaging of a Single Tissue Section; Erin H Sweeney 1, Edwin Escobar 1, Jennifer S Brodbelt 1, University of Texas at Austin, Austin, TX

TP 356 Bridging the Spatial Gap: A Method Enabling Spatial Transcriptomics and Lipidomics Within the Same Tissue Section; Morad C Maleki 1, 2, Martin Dufresne 1, 3, Angela RS Kruse 1, 2, Christopher J Good 1, 4, Roy Larderobbie 1, 2, Lukasz G Migas 1, 2, Katerina V Djambazova 1, 4, Jamie L Allen 1, 2, Raf Van De Plas 1, 2, 4, Joana P Gonçalves 1, 2, Jeffrey M Spragings 1, 2, 4, 5, 11, Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; 2Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; 3Department of Pediatrics, Vanderbilt University Medical Center, Nashville, TN; 4Department of Biochemistry, Vanderbilt University, Nashville, TN; 5Department of Chemistry, Vanderbilt University, Nashville, TN; 6Department of Intelligent Systems, Delft University of Technology, Delft, Netherlands; 7Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands

Spatial metabolomics via MALDI-MSI identifies pharmacodynamic biomarkers for diabetic kidney disease; Leila Hejazi 1, 2, Guanshi Zhang 1, Shoba Sharma 1, Aaron Ruiz 1, Fabio B. Tucci 1, Kumar Sharma 1, SygnaMap Inc, San Antonio, TX; 2Department of Precision Medicine, UT Health San Antonio, San Antonio, Texas; 3Epigen Biosciences, San Diego, CA

In-situ N-glycosylation signatures of ovarian cancer deciphered by combination of multimodal MS imaging and LC-MS/MS; Pengshuan Huang 1, Hua Zhang 1, Manish Patankar 1, Lingjun Li 4, 5, Department 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; 4School of Pharmacy, University of Wisconsin-Madison, Madison, WI; 5Department of Biological Chemistry, Case Western Reserve University, Cleveland, OH; 6University of California, Santa Cruz, Santa Cruz, CA; 7Department of Biophysics and Chemistry, Case Western Reserve University, Cleveland, OH; 8University of California, Santa Cruz, Santa Cruz, CA

The development of Expansion Mass Spectrometry (ExMS) towards studying spatial single cell metabolomics; Sarah E Levy 1, Vignesh Venkataramani 1, Laura Sanchez 1, Lydia Kisy 1, University of California Santa Cruz, Santa Cruz, CA; 2Department of Biophysics and Chemistry, Case Western Reserve University, Cleveland, OH; 3University of California, Santa Cruz, Santa Cruz, CA

Updates to FragPipe computational platform: new capabilities, tools, and workflows; Fengchao Yu 1, Daniel Polasky 1, Guo C Tu 1, Felipe Da Veiga Leprevrand 1, Kai Li 1, Kevin L Yang 1, Yi Hsiao 1, Ginny Xiaohe Li 1, Carolina Rojas Ramirez 1, Sarah Haynes 1, Daniel J Geiszler 1, Hui-Yin

TP 357 Spatial metabolomics via MALDI-MSI identifies pharmacodynamic biomarkers for diabetic kidney disease; Leila Hejazi 1, 2, Guanshi Zhang 1, Shoba Sharma 1, Aaron Ruiz 1, Fabio B. Tucci 1, Kumar Sharma 1, SygnaMap Inc, San Antonio, TX; 2Department of Precision Medicine, UT Health San Antonio, San Antonio, Texas; 3Epigen Biosciences, San Diego, CA
TP 361  Localized Microsampling of Formalin Fixed Paraffin Embedded Tissue for Proteomics: Blessing Chisom Ebenebougou; Kermit K. Murray; 1Louisiana State University, Baton Rouge, LA

TP 362  Development of an Easy-to-use Python Script for Visualizing Deconvoluted Top-Down Mass Spectrometric Data: A Histone Case Study: Megan Bindra; Udayan Das; James Pesavento; 1Saint Mary’s College, Moraga, CA

TP 363  Characterization of prostate post-translational modifications by top-down and bottom-up mass spectrometry and UniProt annotations: Wenrong Chen1; Yong Zang2; Xiaowen Liu3,4; 1Department of BioHealth Informatics, Indiana University-Purdue University Indianapolis, Indianapolis, IN; 4Department of Biostatistics and Health Data Sciences, Indiana University School of Medicine, Indianapolis, IN; 2Department of Medicine, Tulane University, New Orleans, LA; 3Tulane Center for Biomedical Informatics and Genomics, Tulane University, New Orleans, LA

TP 364  TMT complementary ion-interference removal enables accurate quantification for 18-plex proteomics: Yinque Fu1; Huan Sun1; Zhiting Wu1; Zhen Wang; Suresh Poudel1; Zuo-Fei Yuan1; Kartik Varadhan1; Xusheng Wang4; Jumin Peng1; 1St. Jude Children’s Research Hospital, Memphis, TN

TP 365  Optimization of DIA proteomics workflows using ground truth data simulated with Synthetia: Michael G Leeming1; Ching-Seng Ang1; Shuai Nie1; Swati Varshney3; Nicholas A Williamson2; 1The University of Melbourne, Melbourne, Australia

TP 366  Highly sensitive and scalable timsTOF Pro data analysis with MaxDIA 2.0: Juan L. Restrepo-López2; Dmitry Alexeev2; Carlo De Nart1; Juergen Cox2; 1Max Planck Institute of Biochemistry, Martinsried, Germany

TP 367  FilterFASTA: a Tool for Generating Keyword Based Bespoke Cross-Organism FASTA’s for Proteomics: John Chystek1; Jonathan Le1; Jonathan Katz1,2; 1Lawrence J. Ellison Institute for Transformative Medicine, Los Angeles, CA; 2USC, Los Angeles, CA

TP 368  An adaptive model for the protein inference problem: Emile Benoist1; Guillaume Fertin1; Géraldine Jean1; LS2N, Nantes Université, Nantes Cedex 3, France

TP 369  Bayesian Confidence Intervals for Absolute Protein Quantification: Chirag K Kumar1; Meera Gupta1; Donovan Cassidy-Nolan1; Anju Subramanian1; Vyas Pujari1; Martin Wuehr1; Lewis-Sigler Institute for Integrative Genomics, Princeton University, Princeton, NJ

TP 370  The Challenge of Plant Identification in Complex Mixtures: Closely Related Families, Large Proteomes, and Unsequenced Genomes: Melissa A. McFarland1; Sara M. Hardy1; Elizabeth Hunter2; Christine H. Parker1; Ann M. Knolhoff1; FDA-CFSAN, College Park, MD

TP 371  A Streamlined Data Analysis Workflow for Enhanced New Peak Detection (NPD) in the Multi-Attribute Method (MAM): Maurizio Bronzetti1; Aude Tartiere1; Stephen Kok1; Amy Claydon1; Arnd Brandenburg1; 1Genedata Inc., San Francisco, CA; 2Genedata Ltd, Cambridge, United Kingdom; 3Genedata AG, Basel, Switzerland

TP 372  PyC2MC: an open-source software solution for visualization and treatment of high-resolution mass spectrometry data: Maxime Sueur1; Julien Maillard2,3; Oscar LACROIX-ANDRIVET1,4,5; Christopher Rueger2,5; Pierre Giusti1,2,3; Hélène Lavannat1; Carlos Afonso1,4; 1Normandie Univ, UNIROUEN, INSA Rouen, CNRS, COBRA, 76000 Rouen, France, 2MONT SAINT AIGNAN, France; 3International Joint Laboratory - I2CMC: Complex Matrices Molecular Characterization, TRTG, Harfleur, France; 4TotalEnergies OneTech R&D, TotalEnergies Research & Technology, Gonfreville, France; 5TotalEnergies Marketing Services, Research Center, Solaize, France; 6Joint Mass Spectrometry Centre, Chair of Analytical Chemistry, University of Rostock, Rostock, Germany

TP 373  MS-based identification of the mutated peptides in HCT116 cell line through searching against a SNVs dataset derived from integrated transcriptomes: Xia Zhang1,2; Jiawei Liu; Yabing Zhu1; Zhe Ren1; Siqi Liu1,2; 1College of Life Science, University of Chinese Academy of Sciences, Beijing, China; 2Center of Proteomic Analysis, BGI Life Science Research Institute, Shenzhen, China; 3BGI Genomics, Shenzhen, China

TP 374  Fast Component Identification & Automated Well-to-Data Connectivity for High Throughput Workflows: Richard Lee1; Nikki Dare1; Rostislav Pol1; Sofya Chudova1; Nikolay Malashchenko1; 1ACD/Labs, Toronto, ON

TP 375  Streamlining Metadatum Capture for Mass Spectrometry Experiments: towards FAIR Omics metadata across R&D; Benjamin Patil3,4; Ronald C. Woodbury; 1Genedata Ltd, Cambridge, United Kingdom; 2AstraZeneca, Gaithersburg, MD; 3AstraZeneca, Cambridge, United Kingdom

TP 376  Creating a data analysis pipeline for producing high-quality glycoprotein mass spectral libraries: Dmitry Avtonomov1; Raghouthama Chaerkady1; Jana Zecha1; Sri Vishnu Vardhan Deevi; 1Lisa H Cazares1; Sonja Hess1; Stewart MacArthur1; Sebastian Wasilewski1; 1AstraZeneca, Gaithersburg, MD

TP 377  Proximit 8.0: MS2-based quantitative workflow to improve sensitivity and quantitative accuracy of proximity-dependent biotinylation experiments: Shubham Gupta1; Gomin Liu1; Brett Larsen1; Geoffrey Hesketh2; Payman Samavarchi Tehrani3; 1Hala Abdouni1; Anne-Claude Gingras3,4; Hannes Röst1,2; 1University of Toronto, Toronto, ON; 2Donnelly Centre for Cellular and Biomolecular Research, Toronto, ON; 3Lunenfeld-Tanenbaum Research Institute at Mount Sinai Hospital, Toronto, ON; 4Dalhousie University, Halifax, NS

TP 378  Workflows:Facilitate the “Get Bake Off” of Computational Workflows for the Analysis of Mass Spectrometry Data: Vedran Kasalica1; Nauman Ahmed1; Rob J Marissen1; Saskia Hillelmann1; Prat J Jagtap1; Melanie Föll1; Hervé Ménager1; 1Université, Nantes Cedex 3, France

TP 379  MassKit: A Flexible and High Performance API for Mass Spectrometry: Douglas Slotta1; Lewis Y. Geer1; 1NIST, Gaithersburg, MD

TP 380  Chimera server:: deploying the power of the cloud in your basement: Markus Schneider1; Tobias Schmidt1; Daniel P. Zolg1; Siegfried Gessulat1; Florian Seefried1; Samia Ben Fried1; Martin Heinrich Frejno1; 1MSAID GmbH, Garching b.München, Germany

TP 381  Data - Information - Knowledge effortlessly: Combining timsTOF data with PASER Information and Mass Dynamics knowledge to accelerate proteomic discoveries: Tharan Srikumar1; 1Mark Rocco Condina2;
Jonathan Krieger; Giuseppe Infusini; Brad Green; Paula Burton Ngo; Aaron Triantafyllidis; Saima Ahmed; Arthur Virolle; Patrick Van Zalm; Sven Brehmer; Dennis Trede; Christopher Adams; Judith Steen; Shibami S. Mukiwa; Hanno Steen; Andrew Ian Webb; Brucker Ltd., Milton, ON; Mass Dynamics, Melbourne, Australia; Boston Childrens Hospital, Boston, MA; Harvard Medical School, Boston, MA; Brucker Daltonics GmbH & Co. KG, Bremen, Germany; Brucker Scientific, San Jose, CA

Biology, Seattle, WA; University of California San Diego, San Diego, CA; Forschungszentrum Jülich, Jülich, Germany; Thermo Fisher Scientific, San Jose, California; National Center for Protein Sciences (The PHOENIX Center, Beijing), Beijing, China; Masaryk University, Brno, Czech Republic; European Molecular Biology Laboratory, Heidelberg, Germany

ADAP informatics for untargeted mass spectrometry-based metabolomics and exoproteomics big data; Alekandr Smirnov; Joel Hall; Toan Nguyen; Yunfei Liao; Daisy Brumit; Yuanjuan Li; Blake Rushing; Susan McRitchie; Radha Krishna Balaji; Komal Madamwar; Vanur Suresh; Shanmukh Gore; Anantnaval Galikwad; Steffy Roselena Eidnjudson; Susan Sumner; Xiaxia Du; University of North Carolina at Charlotte, Charlotte, North Carolina; University of North Carolina at Charlotte, Charlotte, NC; University of North Carolina at Chapel Hill, Chapel Hill, NC

Automated and Scalable-Based Computational Pipeline for Label-free Unbiased Plasma Proteomics Study; Joon-Yong Lee; Jinjuyong Choi; Sara Nouri Golmaei; Yuntao Hu; Sai Ramaswamy; Dijana Vlko; Wan-Fang Chou; Megan Morá; Jessica Chani; Mark Marisini; Benjamin Ta; Peter Spiro; Hoda Malekpour; Ajinkya Kakate; Robert Zawada; Bruce Wilcox; Philip Ma; Chinnay Benthangady; Manway Liu; PrognomiQ Inc, San Mateo, CA

A custom web-based bioinformatic tool for the assessment of potential molecular glucose screened by quantitative discovery proteomics; Daryl N Bulloch; Han-Yin Yang; Aman Makaju; Ishwar N Kohale; Bradford Gibson; Angen, South San Francisco, CA; Angen, Thousand Oaks, CA

Evaluation of a portable GC-MS for Drug Screening of Products Seized During a Simultaneous Nationwide Mail Blitz; Lisa M. Lorenz; Michael D. Thatcher; Megan E. Sterling; Food and Drug Administration, Office of Regulatory Affairs, Forensic Chemistry Center, Cincinnati, OH

Portable MALDI-TOF Mass Spectrometer for Bioaerosol Detection; Vadym Bercou; Stuart Case, Carmon; Scott Ezelberger; Max Cetta; Lara Moore; Caroline Haddaway; Wayne Bryden; Mike McLaughlin; Zeteo Tech, Inc., Sykesville, MD

Technology Advancements for the Extraterrestrial Molecular Indicators of Life Investigation (EMIL) Capillary Electrophoresis Electrospray Ionization Mass Spectrometer; Desmond A. Kaplan; Maria Fernanda Mora; Tomas Drewnas; Melanie C. Castellini; Ryan M. Danelli; Jacob D Graham; Friso Van Amerom; Xian Li; Andrej Grubic; Bethany P Theiling; Aaron C Noell; Antonio J Ricco; William B Brinkerhoff; Peter A Willis; National Aeronautics and Space Administration Goddard Space Flight Center, Greenbelt, MD; KapsScience LLC, Tewksbury, MA; Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA, Aerodyne, Cape Canaveral, FL; Danelli Consulting, Winterville, NC; Mini-Mass Consulting, Inc, Hyattsville, MD; National Aeronautics and Space Administration Jet Propulsion Laboratory, Pasadena, CA; National Aeronautics and Space Administration AMES, Mountain View, CA

MOMA Testbed Instrument Characterization under Mars Conditions and Engineering Test Unit Sample Database Generation; Friso H. W. Van Amerom; Xiang Li; Marco E. Castillio; Desmond A. Kaplan; Andrej Grubic; William B. Brinkerhoff; And The Moma Team; Mini-Mass Consulting, Inc, Hyattsville, MD; NASA Goddard Space Flight Center, Greenbelt, MD; ASES, Beltsville, MD; Danelli Consulting, Winterville, NC; KapsScience LLC, Tewksbury, MA; Max-Planck-Institut für Sonnensystemforschung, Göttingen, Germany
Amino Acid Quantitation of Cell Culture Media Matrices via an Integrated CE-MS Analyzer; Ji Young L Anderson; William Morgan-Evans; Bethany Kerr; Kenion H Blakeman; Milia Neffling; Graziazi Piras; "908 Devices, Inc., Boston, MA; CPI Innovation Services Ltd., Darlington, United Kingdom

Prototype Development of a Digital Linear Ion Trap based Portable GCMS for VOCs Analysis; Chenzhang Zhu; Lin Liu; Hongbing Cheng; Yulei Hu; XinFeng Zhou; Wenjian Sun; "Shimadzu Research Laboratory, Shanghai, China

Interfacing and Characterizing Portable HPLC Interfaced with Miniature Ion Trap Mass Spectrometer; Vladimir M Doroshenko; Victor Laiko; Venkateswara Panchagnula; Matthew Morse; John Stimus; "MassTech, Inc., Columbia, MD; AxcelLCC, Provo, UT

Intelligent Miniature Mass Spectrometry System for Point-of-Care Analysis; Bin Jiao; Yikun Liu; Xinwei Liu; Jiejun Bu; Wenping Zhang; Zheng Ouyang; "Tsinghua University, Beijing, China; PURSPEC Technology (Beijing) Ltd., Beijing, China

Portable Mass Spectrometer for air born particle detection; Chunchuan Chen; Chun-Hen Hsiao-Hsiang; Ju-Yao Chang; Jung-Lee Lin; Abdil Oezdemir; "National Sun Yat-Sen University, Kaohsiung City, Taiwan; Academia Sinica, Taipei, Taiwan; Sakarya University, Sakarya, Turkey

Modification of a Thermo LTQ-XL to Enable Automatic Gain Control and On-Demand 2D-MS/MS; Eric T Dziekonski; R. Graham Cooks; "Purdue University, WEST LAFAYETTE, IN

Theory and Performance of a Novel High-Resolution Mass Analyzer; Harshish Stewart; Christian Hock; Dmitry Grinfield; Matthias Biel; Philipp Cochems; Alexander Wagner; Wilko Balshuch; Alexander Makarov; "Thermo Fisher Scientific, Bremen, Germany

In Search of the Perfect Notch: a Novel Approach to the Optimization of Dipole Excitation Waveforms in Quadrupole Mass Filters; Keith Richardson; Martin Green; David Langridge; "Waters Corporation, Wilmslow, United Kingdom

Analysis of Megadalton ions using a novel dual sector Charge Detection Mass Spectrometer (CDMS); John B Hoyes; Dimitri Papanastasiou; Alexandros Lekkas; Yury Tsybin; Anton Kozhinov; Igor Filipov; "TrueMass, Rowarth, United Kingdom; Fasmatech, NCSR Demokritos, Athens, Greece; Spectroscrisys, Lausanne, Switzerland; ISCUBE Ltd, Auckland, New Zealand

 Mimicking the effects of pre-post-filters by duty cycle manipulation on a single digitally operated mass filter; Sumeet S Chakravorty; Elizabeth Groetschma; Fatima Olayemi Obe; "Washington State University, Pullman, WA; 2GAA Custom Electronics, LLC, Benton City, WA; 2GAA Custom Electronics, LLC, Benton City, WA

Using a branched RF-ion trap to combine EAD, ultraviolet-photoionization (UVPD) and CID photodissociation (UVPD); Vladimir M Doroshenko; Peter T. A. Reilly; "GAA Custom Electronics, LLC, Benton City, WA; 2GAA Custom Electronics, LLC, Benton City, WA

Improving the Efficiency of Isolation of Native Protein Complexes by a Digital Mass Filter; Robert Schrader; David Russell; "Texas A&M University, College Station, TX

Application of the Digital Tandem Mass Filter in Native Spray Analysis of Proteins; Fatima Olayemi Obe; Sumeet S Chakravorty; Elizabeth Groetschma; Gordon A. Anderson; Peter T. A. Reilly; "Washington State University, Pullman, WA; 2GAA Custom Electronics, LLC, Benton City, WA; 2GAA Custom Electronics, LLC, Benton City, WA

Real-Time Optimization of Ultra-High Resolution in Charge Detection Mass Spectrometry; David Reitenbach; Daniel Y Botamanenko; Martin F. Jarrold; "Indiana University, Bloomington, IN; Indiana University, Bloomington, IN

Impact of high temperature ion source gas; thermal protein denaturation and liner structural details at lower collisional induced unfolding energies; Mack Shih; Patrick J Faustino; Thomas O Connor; Xiaomini Xu; Jinhui Zhang; "Food and Drug Administration, Silver Spring, MD

Trapped Ion Mobility Spectrometry (tims) Facilitates Lipid and Metabolite Identification in MALDI Mass Spectrometry Imaging; Min Liu; Carolina Cruz Cepeda; John M Koomen; "Moffitt Cancer Center, Tampa, FL

Developing tandem mass spectrometry file structures for ion mobility spectrometry workflows; Bryson Gribbons; Sarah Sow; Ruwan T Kurulagama; Lauren Royer; Daniel Debord; John C Fieldsted; Richard D. Smith; Alveet Bilbao; "Pacific Northwest National Laboratory, Richland, WA; "Apient Technologies, Santa Clara, CA; "MOBILion Systems, Inc., Chadds Ford, PA; "Thermo Fisher Scientific, San Jose, California; "Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; "GAA Custom Electronics, LLC, Benton City, WA; "Thermo Fisher Scientific, Boston, MA; "Thermo Fisher Scientific, San Jose, CA

Development and Application of The Shimadzu QTOF40 Quad as an Atmospheric Monitoring Real-Time High-Definition Mass Spectrometer (30-40THD-MS); Karl K Weitz; Byron Gibbons; Rosalie K. Chu; James J Moran; Liliana Pasa-Tolic; Amirhossein H. Ahkami; Kirsten S. Hofmockel; Janet K. Janssen; Mary S Lipton; "Ballistic Pacific Northwest National Laboratories, Richland, WA; "Michigan State University, East Lansing, MI

A Novel Digital Waveform Generator for Creating High Resolution, Low Jitter, Rectangular Waveforms; Gordon Anderson; Sumeet Chakravorty; Fatima Obe; Elizabeth Groetschma; Peter T. A. Reilly; "GAA Custom Electronics, LLC, Benton City, WA; "Washington State University, Pullman, WA

Conquering Waveform-to-Waveform Reproducibility to Improve Digital Waveform Mass Analysis at High Mass in Higher Stability Zones; Peter T. A. Reilly; Sumeet S Chakravorty; Fatima Olayemi Obe; Elizabeth Groetschma; Gordon Anderson; "Washington State University, Pullman, WA; 2GAA Custom Electronics, LLC, Benton City, WA

Characterization of mass spectrometer; Abdelhak Bensaoaula; Patrick Sturm; Jais Metzger; Carsten Stoemer; Cha-Yu Tsou; Georgios Papadopoulos; Caroline Hain; Thomas Niles; Jonathan Thomet; "Tolwer AG, Thun, Switzerland; "Berner Fachhochschule BFH, Biel, Switzerland; "Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland; "Austrian Agency for Technical Cooperation, Vienna, Austria; "Rikkyo University, Tokyo, Japan

Application of the Digital Tandem Mass Filter in Native Spray Analysis of Proteins; Fatima Olayemi Obe; Sumeet S Chakravorty; Elizabeth Groetschma; Gordon A. Anderson; Peter T. A. Reilly; "Washington State University, Pullman, WA; 2GAA Custom Electronics, LLC, Benton City, WA; 2GAA Custom Electronics, LLC, Benton City, WA

Real-Time Optimization of Ultra-High Resolution in Charge Detection Mass Spectrometry; David Reitenbach; Daniel Y Botamanenko; Martin F. Jarrold; "Indiana University, Bloomington, IN; Indiana University, Bloomington, IN

Implementation of a SLIM-based High Resolution Ion Mobility Prototype with an Orbitrap Mass Spectrometer; Alan A McKenzie-Coe; Liuliu Deng; Brian Adamson; Kyle L. Fort; Elyor R Wouters; Gordon A Anderson; Lee Earley; Jean-Jacques Dunyach; Daniel Debord; Alexander A Makarov; "MOBILion Systems, Inc., Chadds Ford, PA; "MOBILion Systems, Inc., Chadds Ford, PA; "Thermo Fisher Scientific, San Jose, California; "Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; "GAA Custom Electronics, LLC, Benton City, WA; "Thermo Fisher Scientific, Boston, MA; "Thermo Fisher Scientific, San Jose, CA

Configuration and Deployment of The Shimadzu QTOF40 Triple Quad as an Atmospheric Monitoring Real-Time High-Definition Mass Spectrometer (30-40THD-MS); Karl K Weitz; Byron Gibbons; Rosalie K. Chu; James J Moran; Liliana Pasa-Tolic; Amirhossein H. Ahkami; Kirsten S. Hofmockel; Janet K. Janssen; Mary S Lipton; "Ballistic Pacific Northwest National Laboratories, Richland, WA; "Michigan State University, East Lansing, MI


**TP 423**

**Development of Top Down Protein Analysis using Trapped Ion Mobility with Two-Dimensional Mass Spectrometry with UPD and IRMPD:** Yuhong Li; Zhirong Qi; A. Michael Bowers; Julian E. Rose; Thomas O. Metz; Michael Z. Kamrath; Alexander V. Shafranetzki; Thomas C. Dang; Keya P. Runison; Brian H. Clowers; Washington State University, Pullman, WA

**TP 424**

**Differentiation and Visualization of Chiral Amino Acids Using Ion Mobility Mass Spectrometry:** Chengyi Xie; Yangyan Chen; Xiaokiao Wang; Yuling Shen; Yuanyuan Song; Xiniao Diao; Lin Zhu; Jianing Wang; Zongwei Cai; State Key Laboratory of Environmental and Biological Analysis, Hong Kong Baptist University, Hong Kong, China; Department of Chemistry, Hong Kong Baptist University, Hong Kong, China

**TP 425**

**Reproducibility of drift gas modifier effects in atmospheric pressure drift tube ion mobility spectrometry of small molecules:** Matthew Carlo; Amanda Patrick; University of Mississippi, State, MS

**TP 426**

**A Dual-Gated Structures for Lossless Manipulations Ion Mobility Orbitrap Mass Spectrometry Platform for Simultaneously Acquiring High-Resolution IM-MS-HCD Data Sets:** Adam L. Luther; Hollebach; Yehia M. Ibrahim; Vanessa M. Mora; Randolph V. Norheim; Adam P. Huntley; Washington State University, Pullman, WA

**TP 427**

**An interplatform study of three ion mobility techniques to determine lipid collision cross sections:** Anaí G. Georgie; Isabelle Schmitz; Vincent Marie; Benoit Colsch; Florent Rouvière; Sandra Alves; Sabine Heinisch; François Fenaille; Carlos Alonso; Corinne Loutelier-Bourhis; Laboratoire COBRA, UMR 6014, Université de Rouen, INSIA de Rouen, CNRS, IRCOF, Mont Saint Aignan, France; Université Paris-Saclay, CEA, INRAE, Département Médicaments et Technologies pour la Santé (DMTS), MetabolHub, F-91191 Gif sur Yvette, France; Université de Lyon, Institut des Sciences Analytiques, UMR 5280 CNRS, 5 rue de la Doua, 69100 Villeurbanne, France; Sorbonne Université, Faculté des Sciences et de l’Ingénierie, Institut Parisien de Chimie Moléculaire (IPCM), Paris, France

**TP 428**

**A Comprehensive TWIM Calibration Method for Obtaining High-Throughput Multi-Omic Collision Cross Section Values:** Hannah M. Hynde; Jana M. Carpenter; Kelly M. Hines; University of Georgia, Athens, GA

**TP 429**

**Development of a high-resolution U-shaped mobility analyzer (UMA) and its applications:** Xiaojing Zhong; Kuofeng Tseng; Kang Guo; Yangyu Miao; Lin Liu; Xinfeng Zhou; Wenjian Sun; Shimuza Research Laboratory, Shanghai, China

**TP 430**

**TW-SLIM Separations Using Asymmetric Radio-Frequency Trapping Fields:** Cullen Greer; Zackary R. Kinlein; Brian H. Clowers; Washington State University, Pullman, WA

**TP 431**

**Novel concept of sliding ion mobility windows to increase the resolution in trapped ion mobility-mass spectrometry hyphenated with gas chromatography:** Hugo Muller; Georges Scholl; Johann Far; Edwin De Pauw; Gauthier Eppe; University of Liége, Liége, Belgium

**TP 432**

**Experimental and theoretical determination of the collision cross sections of phosphoric acid clusters: anions compared to cations:** Hélène Lavanant; Valentina Calabrese; Frédéric Rosu; Valérie Gabelica; Carlos Alonso; University of Bordeaux, INRAE, INSA Rouen, CNRS, COBRA, Rouen, France; University of Lyon, University Claude Bernard 1 of Lyon, France; Institute of Analytical Sciences, CNRS UMR 5280, Villeurbanne, France; CNRS, UMS 3033, Institut Européen de Chimie et Biologie (IECB), Pessac, France; University of Bordeaux, INSERM and CNRS, ARNA Laboratory, IECB site, Pessac, France

**TP 433**

**Millions and Millions of Ions: An Improved Guard Design and Giant Ion Trap to Enhance SLIM Sensitivity and Duty Cycle:** Joshua K McBee; Lulin Deng; Adam Engelson; Zongyuan Chen; Daniel Debord; MOBI Lyons Systems, Inc, Chadds Ford, PA

**TP 434**

**Nonlinear Fourier Transform Sweeps in Conjunction with Reduced-Pressure Ion Mobility Mass Spectrometry:** Nathan W. Buzil; Elvin R. Cabrera; Brian H. Clowers; Washington State University, Pullman, WA

**TP 435**

**Real-time monitoring of dynamic isomer populations with CI-SLIM IMS-MS:** Sonia Kleef; Felipe Lopez-Hilliker; Matthieu Riva; Sebastian Gerber; Urs Rohner; Stephan Graf; Michael Z. Kamrath; TOFWERK, Thun, Switzerland; Univ. Lyon, Université Claude Bernard Lyon 1, Villeurbanne, France

**TP 436**

**Large-scale inference of Peptide Collisional Cross-Sections in an Orbitrap mass analyzer:** Ulises Hernandez Guzman; Konstantin Ayzikov; Kyle L. Fort; Martin Rykaer; Jeppe Madsen; Ana Martinez Del Val; Alexander A Makarov; Jesper V. Olsen; Nov Nordisk Foundation Center for Protein Research, Copenhagen, Denmark; Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; Rikshospitalet, Oslo, Norway; University of Lyon, Université Claude Bernard Lyon 1, Villeurbanne, France

**TP 437**

**A new TIMS-MRMS instrument for structural and in-situ analysis of biomolecules:** Anna L. Simmonds; Anthony Devlin; Alina Thenes; Gregory Brabec; Carlos Schat; Christopher A. Wootton; Josephine Bunch; Zoltan Takats; Rosalind Franklin Institute, Didcot, United Kingdom; Rosalind Franklin Institute, Hanwell, Didcot, United Kingdom; Bruker Daltonics GmbH & Co.KG, Bremen, Germany; National Physical Laboratory, Teddington, United Kingdom; Imperial College London, London, United Kingdom

**TP 438**

**CIUSuite 3: Next-generation CCS Calibration and Automated Data Analysis tool for Gas-Phase Protein Unfolding:** Chae Kyung Jeon; Carolina Rosas Ramirez; Ruwan T. Kuruligama; Brandon T. Ruotolo; University of Michigan, Ann Arbor, MI; Agilent Technologies, Santa Clara, CA

**TP 439**

**Exploring the structures and the energy landscapes of proteins in the gas phase through chemical modification and ion mobility:** Thomas Timlant; Johann Far; Edwin De Paue; Loic Quinton; MSLab ULiege, Liege, Belgium

**TP 440**

**20 mM Ammonium Carbonate Improves the Detection of Tricarboxylic Acid Cycle Intermediates:** Jarrod A Roach; Laura-Isabel McCall; University of Oklahoma, Norman, OK; University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK

**TP 441**

**Online 2D high and low-pH reversed-phase nano-LC-MS/MS system for deep proteome analysis:** Chao-Jung Chen; Yu-Ching Liu; China Medical University, Taichung, Taiwan

**TP 442**

**RP-LC gradient method development and gradient elution modelling to optimize complex mixture analysis by high-resolution mass spectrometry:** Leila Aalaei; Steffen Waldner; University of Vienna, Mass Spectrometry Core Facility - CS, Vienna, Austria; University of Vienna/
TP 445 High-throughput analysis with improved proteome coverage using new designed micro pillar array column (μPAC); Kuei Sun1, Yuan Lin2,3, Jeff Op De Beeck4; Brandon H. Robson1; Joshua A Silveira2; Paul Jacobs2; Shanhua Lin1; Theresa Fisher Scientific, Sunnyvale, CA; 2Thermo Fisher Scientific, Ghent, Belgium; 3Thermo Fisher Scientific, San Jose, CA
TP 446 Increasing Efficiency of Peptide Separations by Decreasing Particle Size and Column Dimension; Peter Pellegrini1; Benjamin Libert1; Stephanie Schuster1; Conner McHale1; Advanced Materials Technology, Wilmington, DE
TP 447 Coupling normal phase chromatographic separation with electron ionization in low and high-resolution mass spectrometry via liquid electron impact interface: Genny Grasselli1; Adriana Arigò2; Michele D'Orsi1; Giorgio Famiglini1; Marcella Terranegra1; 1Laboratoire de sciences des matériaux et de la mécanique, Université de Lorraine, Nancy, France; 2Department of Chemistry, University of Virginia, Charlottesville, VA
TP 449 Improved Biopolymer LCMS Using a New Mixed-Mode Chromatographic Stationary Phase; Benjamin Libert1; Barry E Boyes1; Chuping Luo1; Marc Goldfinger1; Mark Haynes1; Advanced Materials Technology, Wilmington, DE
TP 450 Robust profiling of crude and undepleted human plasma using μPAC-based high resolution DIA-MS workflow; Jeff Op De Beeck1; Natalie Van Landuyt1; Delphi Van Haver1; Ari Staes1,2; Francis Impens1,2,3; Xuefei Sun1,4; Yuan Lin2; Paul Jacobs2; 1Thermo Fisher Scientific, Zwijnaarde, Belgium; 2VIB Proteomics Core, Ghent, Belgium; 3Department of Biomolecular Medicine, Ghent University, Ghent, Belgium; 4Thermo Fisher Scientific, Sunnyvale, CA
TP 451 The Development of a Virtual Liquid Chromatography Method Development Tool; Melinda D Unich1; Jamie York1; John Garrey1; Chris Nelson1; Justin Steimling1; Tina Yosca1; Restek Corporation, Bellefonte, PA; 2Analytical Innovations, Inc., Dayton, OH
TP 452 Optimizing LCMS Method Development for Oligonucleotide Separations: Advantages of Bio Compatible UHPLC Systems; Patrick Cronan; Agilent, Lexington, MA
TP 453 Simultaneous determination of 85 fentanyl analogues using liquid chromatography–tandem mass spectrometry (LC-MS/MS) with serially coupled columns; Jiyou Kim1, Sang Boom Han1; 1Dept of Pharmaceutical Analysis, College of Pharmacy, Chung-Ang University, Seoul, South Korea
TP 454 Very Weak Anion Exchange (VWAX) Chromatography for Glycopeptide Enrichment and Separation; Dangning Wang1; Peng-Kai Liu1; Ting-Jia Gu1; Bin Wang1; Andrew J. Alpert2; Lingjun Li1,2,3; 1Department of Chemistry, University of Wisconsin-Madison, Madison, WI; 2Biophysics Graduate Program, University of Wisconsin-Madison, Madison, WI; 3School of Pharmacy, University of Wisconsin-Madison, Madison, WI; 4PolyLC Inc., Columbia, MD
TP 455 Hydrophilic Interaction Chromatography for Improved LC-MS/MS Analysis of Lipid Oxidation Products; Kosa P. Leyden1; Donald F. Hunt1,2, Jeffrey Shabanowitz2; 1Department of Chemistry, University of Virginia, Charlottesville, VA; 2Department of Pathology, University of Virginia, Charlottesville, VA
TP 456 Sample dilution in microLC sample loops: solving solvent/matrix peak shape artifacts during high-load liquid microchromatography/triple-quadrupole mass spectrometry of Fmoc-amino acids; John J Thoden1; Texas A&M University – Center for Translational Research in Aging and Longevity, College Station, TX
TP 457 Filtering utility for grouping untargeted mass spectrometry datasets (FUGU-MS): an open-source software tool for metabolomics; R. Aburashed1; Thomas Rydza2; Saad Luqman1; Ian A Lewis4; 1University of Calgary, Calgary, AB; 2University of Manitoba, Winnipeg, MB; 3University of Illinois at Chicago, Chicago, IL; 4University of Virginia, Charlottesville, VA
TP 458 Intense Reflex Fast Screening for Drugs in Urine: data-dependent reionization logic for screening and confirmation of presumptive positives; Patrick Batoon1; Lee Bertram2; Linfeng Wu3; 1Agilent Technologies Inc., Santa Clara, CA; 2Agilent Technologies, Santa Clara, CA; 3FidelityCheck™ Software; 4GenNext Technologies, Half Moon Bay, CA
TP 459 Time Modeling for Modified and Variant Peptide Identification; Tyler Fletcher1; Jiana Duan1; Emily Chea1; Robert Egan1; Ron Orlando2,3; 1Scitegic, Inc., Bethesda, MD; 2Sadtching Technologies, Cincinnati, OH; 3Sadtching Technologies, Austin, TX
TP 460 Tackling Cannabinoids Ion Suppression Issues in Biological Matrices Using Chromatographic Tools; Cynthia Savaria2; Georgia Savaria3; Giorgio Famiglini1; Marc R Elie4; 1Laboratoire de sciences des matériaux et de la mécanique, Université de Lorraine, Nancy, France; 2Department of Chemistry, University of Virginia, Charlottesville, VA; 3Department of Chemistry, University of Virginia, Charlottesville, VA; 4University of Manitoba, Winnipeg, MB
TP 461 Rapid fractionation of human proteome with acidic HILIC Proteome Selective Isolation Chromatography (P-SILCY) for TMT-based quantitation; Darien Yeung1; Ying Lao1,2; Victor Spicer1; Helene Perreault1,2; Oleg V. Krokhin1; 1University of Manitoba, Winnipeg, MB; 2University of Calgary, Calgary, AB
TP 462 To study the in vivo and in vitro effects of Bergamottin and Diosmetin on amoxicillin metabolism using LC-MS/MS and LC/HR-MS/MS; Sashin Dattam Pawar1; Dr.pramod Kumar1; 1National Institute of Pharmaceutical Education and Research Guwahati (NIPER-G), Guwahati, India
TP 463 Fast and Targeted Analysis of Cell Culture Media Components using QSight LC/MS/MS; Marc R Elie1; Cole Stratman1; Jacob Jalali1; Jesse Leonard2; Erasmus Cudjoe3; 1Perkin Elmer, Shelton, CT; 2PerkinElmer, Shelton, CT; 3PerkinElmer Inc., Woodbridge, ON
TP 464 The investigation of tryptophan metabolites and vitamin B in human and murine tissue via high-resolution mass spectrometry; Sandy Abujiras1; Kumari Uthayasekeran2; Jonas Bergquist1; Uppsala University, Uppsala, Sweden
TP 465 Analysis of short-chain fatty acids (SCFAs) by LC-MS/MS coupled with chemical derivatization; Hanpeng Jiang1; Zhimin Long1; Lihai Guo1; 1SCiEX, China, Shanghai, China
TP 466 Rapid analysis of 11 energy-rich phosphate compounds using the SCIEX Triple Quad 6500+ system; Junming Chen1; Dandan Si1; Zhimin Long1; 1SCiEX, Beijing, China
TP 467 Simultaneous analysis of polar metabolome and lipidome by unified-hydrophilic interaction/anion-exchange liquid chromatography tandem mass spectrometry (unified-HILIC/AEX/MS/MS); Kohta Nakatani1; Kazuki Ikeda1; Masanori Takahashi2; Takeshi Bamba1; Yoshishiro Izumi1; 1Medical Institute of Bioregulation, Fukuoka, Japan; 2Center for Translational Research in Aging and Longevity, College Station, TX
TP 478 Determination of Flux into the Tryptophan-Kynurenine Pathway in Biological Samples using Liquid Chromatography Tandem Mass Spectrometry; Jaeman Byun1; Subramaniam Pennathur1; Anna Mathew1
1University of Michigan, Ann Arbor, MI

TP 479 Multiple Reaction Monitoring (MRM) Method Development for Quantiﬁcation of Spermidine in Whole Blood; Jerich Mill1; Cameron Kaminisky1; Thomas Rafle2; Lingjun Li1,2,3;1University of Wisconsin-Madison, Department of Chemistry, Madison, WI; 2University of Wisconsin School of Medicine and Public Health, Department of Pathology and Laboratory Medicine, Madison, WI; 3University of Wisconsin-Madison, School of Pharmacy, Madison, WI

TP 480 High-throughput UHPLC-MS/MSRMRM amino acid and acylcarnitine proﬁling in early infancy predicts later obesity risk; Susanne I. Wudy1; Verena K. Mittermeier-Kleßinger1; Saphia Sharma2; Andreas Dunkel2; Karin Kiegrewel1; Regina Emeracz1; Corinne Dawid1; Thomas F. Hoppe2; 1Chair of Food Chemistry at the University of Konstanz, Konstanz, Germany; 2Molecular Sensory Science, Technical University of Munich, Freising, Germany; 3Leibniz-Institute for Food Systems Biology at the Technical University of Munich, Freising, Germany; 4Bavarian Center for Biomedical Mass Spectrometry, Technical University of Munich, Freising, Germany; 5Institute for Medical Information Processing, Biometry, and Epidemiology (IBE), Ludwig-Maximilians-Universität München, Munich, Germany; 6Division of Pediatric Cardiology and Intensive Care, University Hospital, Ludwig-Maximilians-Universität München, Munich, Germany; 7Institute of Child Nutrition, Max Rubner-Institut, Federal Research Institute of Nutrition and Food, Karlsruhe, Karlsruhe, Germany

TP 481 Targeted metaboanalysis of polyamine synthesis and metabolism by LC-MS/MS; Katelyn G. McMurray1; Jun Han1, 1, 2; Junjong Yang1; Molly McCormack1; Gillian Leach1; Kiara Kumar1; Dave Schibli1; 2; David R. Goodlett1; 3; Genome BC Proteomics Centre, University of Victoria, Victoria, BC; 2Department of Medical Sciences, University of Victoria, Victoria, BC; 3Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC

TP 482 Targeted quantitation of 400 polar metabolites of primary metabolism and energy homeostasis by LC-MS/MS; Jun Han1, 1, 2; Junjong Yang1; Molly McCormack1; Kiara Kumar1; Katelyn G. McMurray1; Gillian Leach1; Dave Schibli1; 2; David R. Goodlett1; 3; Genome BC Proteomics Centre, University of Victoria, Victoria, BC; 2Department of Medical Sciences, University of Victoria, Victoria, BC; 3Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC

TP 483 A High-Efficiency Method for simultaneous Quantification of Seven Classes of Phytohormones; Lingyun Chen1; Yun Zhao1; Qidan Li1, 1; Jin Zi1; 2; BGI-Shenzhen, Shenzhen, China

TP 484 Analysis of Polyamine Metabolism by Liquid Chromatography-High Resolution Mass Spectrometry; Bao Tran1; Lin Tan1; Thomas D Horvath1; Sara A Martinez1; John Weinstein1; Philip Lorenzo1; University of Texas MD Anderson Cancer Center, Houston, TX; 2MD Anderson Cancer Center, Houston, TX; 3Baylor College of Medicine, Houston, Texas

TP 485 Reliable quantification of adenylate nucleotides using ultra-performance liquid chromatography-tandem mass spectrometry (UPLC-MS/MS); Maleesha De Silva1; Kyle Fulghum1; David Hoekel1; Bradford G Hill2; Pawel K Lorkiewicz1; 1University of Louisville, Louisville, KY

TP 486 Analysis of Polyamine Metabolism by Liquid Chromatography-High Resolution Mass Spectrometry; Bao Tran1; Lin Tan1; Thomas D Horvath1; Sara A Martinez1; John Weinstein1; Philip Lorenzo1; University of Texas MD Anderson Cancer Center, Houston, TX; 2MD Anderson Cancer Center, Houston, TX; 3Baylor College of Medicine, Houston, Texas

TP 487 Development and Optimization of Lipidic Studies Utilizing the SICRIT® LC-Module; Ciara Conway1; Jan-Christoph Wolf1; Christoph Haisch1; 1TUNC Charlotte, CHARLOTTE, NC; 2Plasmion GmbH, Augsburg, Germany; 3Technical University of Munich, Freising, Germany

TP 488 Analysis of biological samples by fast HILIC separations of nucleotides, and RPLC separation of 3-NPH derivatized carboxylic acids with LC-MS; Ondrej Hodek1, 1; Thomas Moritz2; 1Department of Forest Genetics and Plant Physiology, Swedish University of Agricultural Sciences, Umeå, Sweden; 2Swedish Metabolomics Centre, Umeå, Sweden; 3Novo Nordisk Foundation Center for Basic Metabolic Research, Faculty of Health and Medical Sciences, University of Copenhagen, Copenhagen, Denmark

TP 489 Determination of ATP, ADP, AMP, and Adenosine Levels by Microchip Capillary Electrophoresis Coupled with High Resolution Mass Spectrometry; Kevin Kun; Xianjun Shao; 1Corvetta Agriscience, Indianapolis, IN

TP 487 High Resolution LC-MS Method for Detecting and Quantiﬁying Sterols and Sterol Adducts in Plant Matrices; Suresh Annangudi1; Scott Greenwald2; Jeffrey Simpson1; 1Corvetta Agriscience, Indianapolis, IN
TP 490  Comparing Targeted LC-MS/MS and Untargeted GC-MS for the analysis of Kynurenine Pathway in Plasma Samples; Luis M Valdevieza; Uri Keshetb; Oliver Fiehnb;  
West Coast Metabolomics Center, Davis, CA

TP 491  Quantitative analysis of antimicrobial compounds from Pseudomonas protogen: Samantha J Balboaa; Shilu Dahalb; Clemencia M. Rojasb; Leslie M. Hicsb;  
University of North Carolina at Chapel Hill, Chapel Hill, NC; University of Nebraska-Lincoln, Lincoln, NE

TP 492  Quantitative Analysis of Polar Metabolites with Comprehensive Plasma and Cell Targeted Metabolomics Workflow; Karen E Yarnellc; Cate Simmermакer; Genevieve C Van de Bittner;  
Agilent Technologies, Santa Clara, CA

TP 493  Absolute quantitation of metabolites using machine learning and “standard candies” as universal calibrators - the second generation model; Jennifer M Campbell; Timothy Kassa; Sara Costa; Jeff Pruyne; Luke Ferrob; Joshua D Lauterbach; Steven Hooper; Jack Howlandd; Gabriel Asherb; Mmoum Cadosch Deltarm; J. M. Geremia1;  
"Matterworks, Somerville, MA

TP 494  Tracking metabolism in real time: an LC-MS enabled workflow that allows seconds-level resolution of metabolic fluxes in cell culture; Ryan A Groves; Thomas Rydzak; Rafael Aburashed; Stephanie L Bishopb; Maryam Maparb; Carly C Y Chan; Ian A Lewis1;  
University of Calgary, Calgary, AB

TP 495  Absolute quantification of cellular metabolites in bioprocessing samples using machine learning; Luke S Ferrob; Jack Howland; Timothy Kassa; Ana S.H. Costab; Jeff Pruyne; Steven Hooper; Joshua D Lauterbach; Gabriel Asherb; Mmoum Cadosch Deltarm; J. M. Geremia1; Jennifer M Campbell; "Matterworks, Somerville, MA

TP 496  High-Throughput Scheduled Parallel Reaction Monitoring Mass Spectrometry of Tryptophan-Indole Metabolites in Culture Supernatant of Human Bacterial Isolates; Hudi Tiah; Elizabeth Fleming; Lisa Kozhaya; Rachel Hardy; Derya Unutmaz; Julia Oh; Xudong Yao;  
"University of Connecticut, Storrs, CT; "The Jackson Laboratory, Farmington, CT

TP 497  Delineating the natural product composition of Ashwagandha extracts by combining electrophore trapping with untargeted chemical fingerprinting and GNPS networking; Md. Nure Alam; Armando Alcazara Maganac; Jaawo Choi; Luke Marney; Paul Cheong; Mikah Brandesc; Cody Neffb; Amala Soumyanathc; Jan F. Stevens; Claudia Macker; "Oregon State University, Corvallis, OR; "Oregon Health & Science University, Portland, Oregon

TP 498  Analysis for Erinacines and Hericenones in Lion’s Mane Mushrooms using HRMS and Ion Mobility; Gordon T. Fuimotod; Sarah E. Dowd; Lindsay E. Hatch; Emily R. Britton;  
Waters Corporation, Milford, Milford, MA

TP 499  Traditiona...
oligonucleotide samples and their impurities; Youzong Liu¹; Pirot Prostko²; Dirk Valkenberg³; Jennifer L Lippens¹; Ronald De Vries¹; Thomas De Vrijer³; ¹Janssen Pharmaceutical NV, Beerse, Belgium; ²Hasselt University, Hasselt, Belgium; ³Competitive Transcription and Adduct Bypass Assay for Examining Transcriptional Perturbations and Repair of 02-Alkylthymidine Lesions; Chen Wang¹; Xiaomei He¹; Yinan Wang¹; Yunsheng Wang¹; ¹UCR, Riverside, CA

TP 516

Direct chemical characterization of double-stranded oligonucleotides crosslinked by the microbiome-derived genotoxic colibactin by high-resolution mass spectrometry: Chiara Lecchi¹; Erik S. Carlson²; Peter W. Villalta³; Emily P. Baltkus²; Silvia Baibo³, ¹, ², ³; ¹Masonic Cancer Center, University of Minnesota, Minneapolis, MN; ²Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA; ³School of Public Health, University of Minnesota, Minneapolis, MN

TP 517

Microflow liquid chromatography – nanoelectrospray mass spectrometry of oligonucleotides crosslinked by the microbiome-derived genotoxic colibactin by high-resolution mass spectrometry: Chiara Lecchi¹; Erik S. Carlson²; Peter W. Villalta³; Emily P. Baltkus²; Silvia Baibo³, ¹, ², ³; ¹Masonic Cancer Center, University of Minnesota, Minneapolis, MN; ²Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA; ³School of Public Health, University of Minnesota, Minneapolis, MN

TP 518

Tandem mass spectrometry quantification of Oligonucleotides using an isobaric internal standard: Christopher Gawlik¹; Gungör Hanci¹; Michael Ruehl¹; ¹BioSpring Gesellschaft für Biotechnologie mbH, Frankfurt am Main, Germany; ²Research Center for Biochemistry, Columbus, OH; ³Center for RNA Biology, The Ohio State University, Columbus, OH; ⁴Resource for Native Mass Spectrometry Guided Structural Biology, Columbus, OH; ⁵The Center for Retrosilical Research, The Ohio State University, Columbus, OH

TP 519

Localization of phosphorothioate linkages in partially phosphorothioated oligonucleotides: Samuel P Wein¹; Trenton M Peters-Clarke²; Oliver Kohlbacher³; ¹University of Tübingen, Tübingen, Germany; ²University of Wisconsin, Madison, WI; ³University of Tübingen, Tübingen, Germany

TP 520

Fast acquisition of DDA-MS/MS of oligonucleotides and the novel spectral merging algorithm for better assignment of sequence information: Kosuke Uchiyama¹; Yoshihiro Kinumira¹; Simon Ashton²; Richard Price²; Helen Jose¹; Atsuko Toyama¹; Neil Loftus²; ¹SHIMADZU Corporation, Kyoto, Japan; ²Shimadzu, Manchester, UK; ³University of Tübingen, Tübingen, Germany

TP 521

Profiling small oligonucleotide synthesis impurities and large mRNA sequence confirmation, including poly A tail and capping using a single LC-HRMS platform: Guert Van Raemdonck¹; Kristina Wich¹; Jessika Wynendaele¹; Eddy Ruijters¹; Koen Iterbeke¹; ¹AnaBioTec, Evergem, Belgium

TP 522

Concerted application of ion mobility and tandem mass spectrometry to differentiate isomeric/isobaric oligonucleotides produced by nuclease digestion of large RNAs: Daniele Rollo¹; Daniele Fabris²; ¹University of Connecticut, Storrs, CT; ²RiboDynamics LLC, Manchester, Connecticut

TP 523

Extending the Concept of Spectral Accuracy to the Deconvolution of Multiply Charged Large Molecules: Yongdong Wang¹; Stacey Simonoff¹; Don Kuehl¹; Nan Zhang¹; Qingfei Zheng¹; ¹Cerno Bioscience, Las Vegas, NV; ²Department of Radiation Oncology, College of Medicine, Columbus, Ohio

TP 524

Characterization of Nucleic Acid Fragment Ions by Isotopic Distributions, Michael Lanzillotti¹; Jessica G Pauling¹; Jennifer S Brodbelt¹; ¹University of Texas at Austin, Austin, TX

TP 525

LC-MS Method for Detection of Metabolites and Impurities of 1st, 2nd and 3rd Generation Oligonucleotide Therapeutics: Irina Slobdchikova¹; ¹Pharma Alliance, Marlvern, PA

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The use of liquid chromatography, ion mobility, and mass spectrometry to thoroughly characterize the diastereomer composition in oligonucleotide therapeutics: Anh Tran¹; Steven Fletcher¹; Jake W Jones¹; ¹University of Maryland, School of Pharmacy, Baltimore, MD

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High Temperature Fluoroalcohol-free Liquid Chromatography-Electron Detachment Dissociation Tandem Mass Spectrometry of DNA; Carson W Szot¹; Kristina Hakansson¹; ¹University of Michigan, Ann Arbor, MI; ²University of Michigan, Ann Arbor, Michigan

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An oligonucleotide impurity analysis workflow with the new software that calculates percentage impurity based on summed XIC peak area: Noriko Kato¹; Kosuke Uchiyama¹; Hiro/yuki Yasuda¹; Simon Ashton²; Richard Price²; Helen Jose¹; Neil Loftus²; Kiyoshi Kakiya¹; Atsuko Toyama¹; ¹SHIMADZU Corporation, Kyoto, Japan; ²Shimadzu Corporation, Manchester, United Kingdom; ³Peptistar Inc., Ssetsu, Japan

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Optimized Fragmentation of Oligonucleotides Suppresses Undesired Fragmentation Products and Enables Confident Sequence Assignment: Joshua Hinkle¹; William M. McGee²; Joshua P. Salem³; Robert L Ross⁴; Christopher Muller⁵; Scott Kronewitter⁶; John E.P. Syka¹; James L. Stephenson¹; ¹Thermo Fisher Scientific, San Jose, California; ²Thermo Fisher Scientific, Lexington, Massachusetts; ³University of Michigan Ann Arbor, Ann Arbor, MI; ⁴Thermo Fisher Scientific, Franklin, MA

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Investigating the role of HIV-1 genomic RNA transcriptional start site differences on Gag binding using native mass spectrometry: Kaylee Grabarkewitz¹, ²; Vicki H Wysocki¹, ², ³; Karin Musier-Forsyth¹, ², ³; ¹The Ohio State University; ²Department of Chemistry, The Ohio State University, Columbus, OH; ³Center for RNA Biology, The Ohio State University, Columbus, OH

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Continuing the investigation of microchip capillary electrophoresis coupled with mass spectrometry in the bottom-up characterization of progressively larger RNAs: Daniele Rollo¹; Adi Kulkarni¹; Kate Yu¹; Hamps Engstroem⁴; Guillaume Treminont⁵; Daniele Fabris⁶; ¹University of Connecticut, Storrs, CT; ²908 Devices, Boston, MA; ³Bruker Scientific LLC, San Jose, CA

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An algorithm for automated characterization of ribonuclease-digested messenger RNA using data-independent tandem mass spectrometry: Yuki Matsuura¹; Yasuto Yokoi¹; Jonathan Fox²; Maissa Gaye²; Joe Fredette²; Matthew A Lauber²; Guillaume Bechade²; Masami Koike³; Yuko Nobe³; Masato Taoka³; Hiroshi Nakayama³; ¹Mitsubishi, Minato, Japan; ²Waters S.A.S, Saint-Quentin, France; ³Waters Corporation, milford, MA; ⁴RIKEN Center for Sustainable Resource Science, Wako, Japan; ⁵Tokyo Metropolitan University, Hachioji, Japan

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Metabolite Profiling and Identification of Oligonucleotide in In Vitro Metabolic System; Gengyao Qin¹; Qiandian Miao¹; Liq Shí¹; Zhiyu Li¹; Weiqun Cao¹; Yi Tao¹; Liang Shen¹; WuXi AppTec, Shanghai, China

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Multiple binding and binding specificity: Lessons learned from native top-down MS of aminoglycoside/RNA complexes with different secondary structure motifs; Sarah Viola Heel¹; Kathrin Breuker¹; ¹Institute of Organic Chemistry and Center for Molecular Biosciences Innsbruck (CMBI), University of Innsbruck, Innsbruck, Austria; ²Institute of Organic Chemistry and Center for Molecular Biosciences Innsbruck (CMBI), University of Innsbruck, Innsbruck, Austria

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Importance of fragmentation data for the identification of phosphoramide impurities: Sven Hackbusch¹; Gary Held¹; Kenton Chodara¹; Syed K Raza²; Yi Zhang¹; Min Du²; ¹Thermo Fisher Scientific, San Jose, CA; ²Thermo Fisher Scientific, Milwaukee, WI; ³Thermo Fisher Scientific, Franklin, MA

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Fractionation of complex RNA mixtures for LC-MS/MS: Jennifer Kist¹; Cassandra Herbert¹; Patrick Limbach¹; ¹University of Cincinnati, Cincinnati, OH
TP 538  High-Resolution Accurate Mass Orbitrap mRNA Analysis: Poly-A Tail, Capping Analysis, and Bottom-up Sequence Mapping; Alice Guo1; Kevin Kun Guo2; 1Avice Laboratories, Acton, Massachusetts

TP 539  A method for predicting the monoisotopic mass in high-resolution mass spectra of oligonucleotides; Piotr Prostok1; Youzhong Liu2; Thomas De Viljder3; Tatiana Khamiakova4; Dirk Valkenborg5; 1Hasselt University, Hasselt, Belgium; 2Janssen Pharmaceuticals NV, Beersel, Belgium

TP 540  A software package for sequence confirmation and impurity characterisation of synthetic oligonucleotides using MS/MS and MS/MS. Evaluation of Protein Expression Levels Across Tissues and Species; Sebastian Urzinger1; Corongiu2; Pr Ciccimaro3; by PRM4; Lukas Reiter5; 1Waters Corporation, Newbury, UK; 2Waters Corporation, Milpslow, United Kingdom; 3Waters Corporation, Milpslow, United Kingdom; 4Waters Corporation, Milpslow, United Kingdom; 5Waters, Wilmslow, UK

TP 541  A workflow of liquid chromatography-tandem mass spectrometry data analysis for the characterization of mRNA therapeutics; Hiroshi Nakayama1; Masami Koike2; Yoko Nobe2; Masato Taoka3; 1RIKEN Center for Sustainable Resource Science, Wako, Japan; 2Tokyo Metropolitan University, Hachioji, Japan

TP 542  Targeted Profiling of F-Box proteome for biology and translational research; Viyaa Pandey1; Adarsh K Mayank2; James A Wohlshleger3; 1UCLA, LOS ANGELES, CA; 2UCLA, Los Angeles, CA; 3UCLA, Los Angeles, CA

TP 543  Assessment and prediction of the human proteotypic peptide stability for proteomics quantification; Cristina Chiva1,2; Zahra Elhamraouli3,2; Amanda Solé2,3; Marc Serreti1,2; Matthias Wilhelm1; Eduard Sabidó4,2; 1Universitat Pompeu Fabra, Barcelona, Spain; 2Center for Genomics Regulation, Barcelona Institute of Science and Technology (BIST), Barcelona, Spain; 3Technical University of Munich, Munich, Germany

TP 544  Fast screening and characterization of therapeutic peptide by online capillary electrophoresis - mass spectrometry (CE-MS); Fuxing Xu1; Ling Ling2; Chuhan-Fan Ding3; Liang Wang4; Kate Yu4; Ninaung University, Ningbo, China; 908 Devices, Shanghai, China; 908 Devices, Boston, MA

TP 545  An Ultra-Sensitive and High-Throughput Assay to Quantify Novel Bispecific Peptide by SPE–UPLC-MS/MS in Human Plasma Tre; Andy (hongfang) Xue1; Pengliang Ren2; Yu Yang3; Ruiling Wang4; Aihua Liu5; 1Pharma Alliance, Malvern, PA; 2Ashaani Micot Technology, Xi’an New Area, China

TP 546  Integrated calibration curve-based absolute quantification of biomarkers in SpectroDive; Veronique Laforto1; Maik Möll2; Magdalena Domítrz3; Tejas Gandhi4; Lukas Reiter5; 1Biognoys AG, Schlieren, Switzerland

TP 547  A Robust Protein Normalization Strategy for Comparing Protein Expression Levels Across Tissues and Species by PRM; Joshua Nicklay1; Jingjing Deng1; Eugene Cicimaro2; Petra Shkipova2; Bristol-Myers Squibb, Princeton, NJ

TP 548  The Proteomes that Feed the World; Gian Luca Corongiu1; Sarah Brjakovic1; Patrick Roehrl1; Andreas Pillier1; Sebastian Urzinger1; Lukas Wuerst1; Paula Andrade2; Galan2; Guido Giordano2; Veronica Ramirez2; Ezgi Aydin2; Genc Hafitli3; Mario Picciani4; Qussai Abbas4; Cemil Can Sayliar1; Armin Soleymannia1; Jiuyue Pan1; Sophia Hein1; Corinna Dawid1; Stephanie Heinzimier1; Claus Schwichheimer1; Chris Schoen1; Viktoriya Avramova1; Josch Paulung1; Christina Ludwig1; Dmitri Frisman1; Mathias Wilhelm1; Caroline Gutjahr1; Ralph Huchelhoven1; Brigitte Poppenberger1; Bernhard Kuster1; 1Elite Network of Bavaria, School of Life Sciences, Technical University of Munich, Freising, Germany

TP 549  Quantitative Target Occupancy in FFPE Tissues using mass-affinity Capture 2D-LC-MS/MS; Alving Yu1; Lingyao Meng1; Jintang He1; Surinder Kaur1; Keyang Xu1; 1Genentech Inc., South San Francisco, CA

TP 550  Building high-throughput analytical methods for monitoring peptide biomarkers in equine athletes; Cecily R Wood1; Abigail Burrows Franco2; Alison Porter2; Scott M Petersen1; Scott D Stanley1; 1University of Kentucky, Lexington, KY; 2Thermo Fisher Scientific, San Jose, CA

TP 551  A Robust Method for Simultaneous Detection Glycopeptide Compounds in Rat Plasma Containing Human IgG; Li Gao1; Na Li1; Yantu Ren1; Zhiyu Li3; Lili Xing3; Yi Tao4; Liang Shen5; WuXi AppTec Suzhou, China; 6WuXi AppTec Shanghai, China

TP 552  Optimizing lower limits of quantification and detection by choosing transitions in Skyline; Nicholas Shulman1; Lilian Heil1; Philip M Remes1; Michael J. MacCoss1; 1Department of Genome Sciences, University of Washington, Seattle, WA; 2Thermo Fisher Scientific, San Jose, CA

TP 553  Comparison of Endogenous Peptide Quantitation Strategies; Elena V Romanova1; David C Platt2,3; Joseph M. Williams4; David L. Ceder0,5; Ricardo Vallego6; Jonathan V. Svedeler1; 1University of Illinois at Urbana-Champaign, Urbana, IL; 2University of Illinois at Urbana-Champaign, Urbana, IL; 3SGX Medical, Bloomington, IL; 4University of Illinois at Urbana-Champaign, Urbana, IL

TP 554  N-Rich: A Tailored pyridine carboxaldehyde enrichment for high coverage and specificity N-terminal proteomics; Alexandra C. Turmon1; Andrew Palmer1; Alexander W. Sun1; Lisa Boatner1; Kerriann M. Backus1; 1University of California, Los Angeles, Los Angeles, CA

TP 555  Systematic Evaluation and Optimization of PRM Assays for the Quantification of Very Low Abundant Proteins Within Complex Samples; Danilo Ritz1; Christian Schorn1; Emmanuelle Lezan2; Alexander Schmidt2; 1Proteomics Core Facility, University of Basel, Basel, Switzerland; 2Roche Innovation Center Basel, Basel, Switzerland

TP 556  Targeted proteogenomics for detection of disease-associated protein isoforms - a case study of TPM2and bone mineral density; Michael Lehe1; Erin Jeffery2; Abdullah Aboud3; Charles Farber4; Victoria Shemykhn4; 1University of Virginia, Charlottesville, VA

TP 557  Discovery and targeted proteomic evaluation of biological responses to an MDM2 degrader in a lymphoblastic leukemia cell line; Sarah A. Martinez1; Eric Kuhn1; Susanne B. Breitkopf2; Yogesh Chutake3; Jessica Filiatroul1; Min Yuan1; Yatao Shi1; Dirk M. Walther1; Dapeng Chen1; Brad Enerson1; Stefanie Schraml1; Joyoti Dey1; Alice McDonald1; Matt Weiss1; Juliet Williams1; Chris De Savi1; Kirti Sharma; Kymera Therapeutics, Inc, Watertown, MA

TP 558  Multiplexed, Atomile-Level Detection of Proteotypic Peptides Associated with Retinoid Metabolism and Signaling, Using a Custom Internal-Standard Triggered SureQuantTM assay; Robert N. O’Meally1; Peter M. Abadir1; Robert N. Cole2; Brian Foster2; 1Johns Hopkins School of Medicine, Baltimore, MD

TP 559  Quality profiling of Tetracosactide injections using HPLC-HRMS; Janes Ilia1; Alexsandra Bracko1; 2Faculty of Pharmacy University of Ljubljana, Ljubljana, Slovenia; 3Maribor University Medical Centre, Maribor, Slovenia

TP 560  Development of a PRM Assay for Bone Fide Substrates of Protein Kinase CK2; Daniel Menyhart1; Lilia M. Williams1; Hilde Hespenheide1; Alexander Schmidt1; 1Proteomics Core Facility, University of Basel, Basel, Switzerland; 2Roche Innovation Center Basel, Basel, Switzerland

TP 561  Ocular tissue distribution and systemic pharmacokinetics of a biotherapeutic protein; Emily Werth1; Lin-Zhi Chen2; 1Boehringer Ingelheim, Ridgefield, CT

TP 562  A novel approach for generation of retention time - molecular mass chromatograms for improving molecular mass chromatograms for improving
TP 563

Assessment of Therapeutic Humanized IgG2 Antibody Concentrations in Human Plasma Using LC/PRM-MS and ELISA: A Comparative Study; Pradyum Maheshwar1; Robert Popp1; Christoph H. Borchers1, 2, 3, 4, 6; 1RMH Proteomics Inc., Montreal, QC; 2Gerald Bronfman Department of Oncology, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; 3Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; 4Division of Experimental Medicine, McGill University; 5Department of Pathology, McGill University, Montreal, QC.

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Development of an Immunocapture LC-MS/MS Assay for Semi-quantitation of ADA Isotypes of a Drug in Human Serum; Yulina Feng1; David Wali1; Jennifer Cantiff1; Manisha Saxena2; Charlie G. Knutson1; Robert Dodge3; Elena Fernandez2; 1Novartis Institutes for Biomedical Research, Inc., Cambridge, MA; 2Novartis Pharma AG, Basel, Switzerland; 3Novartis Pharmaceuticals, East hanover, New Jersey; 4Molecular Partners AG, CH-8952, Switzerland.

TP 565

Quantification of anti-inflimab antibodies in human serum using capillary electrophoresis – tandem mass spectrometry; Tessa Reinert1, 2; Pascal Houé3, 3; Oscar Hernandez Alba4; Sarah Cianferani5; Rabah Gahoual5; Yannis Nicolas Francois1; 1Laboratoire de Spectrométrie de Masse des Interactions et des Systèmes (LSMIS) UMR 7140 (Unistra-CNRS), Université de Strasbourg, France; 2Unité de Technologies Chimiques et Biologiques pour la Santé (UTCBS), CNRS UMR5658, Inserm U9327, Université de Strasbourg, France; 3Laboratoire de Toxicologie Biologique, Hôpital Lariboisière, Assistance Publique – Hôpitaux de Paris (AP-HP), France; 4Laboratoire de Spectrométrie de Masse BioOrganique (LSMBO) IPHC UMR 7178, Université de Strasbourg, France; 5Laboratoire de Spectrométrie de Masse des Interactions et des Systèmes (LSMIS) UMR 7140 (Unistra-CNRS), Université de Strasbourg, Strasbourg, France.

TP 566

High throughput quantification of biologics PTM state by peptide mapping using refocussing chromatography and ZenoTOF mass spectrometry; Montiz Heusel1; Stephen Lock2; Nick Morrice2; Sibylle Heidelberger2; Jakob Bunkenborg1; Michael Barrett Anderson1; Nicolai Bache1; Eversep BioSystems, Odense, Denmark; 1SCIEX, Macclesfield, United Kingdom.

TP 567

Advances in Intact Protein Quantitation Using Gabor Transform-Based Tools in iFAMS; Kayl D. Meldrum1; Andrew K. Swansig1; Meghan M. Daniels1; Crystal Kirmiz Cody2; Wendi A. Hale2; David L. Wong3; Michael D. Kniemen1; Xi Qi1; John Susen1; James S. Prell1; 1University of Oregon, Department of Chemistry, Eugene, OR; 2Agilent Technologies, Inc., Santa Clara, CA; 3Materials Science Institute, University of Oregon, Eugene, OR.

TP 568

Development of Quantitative cGMP Impurity Protein Assays Supporting Diverse Modalities, Part II: Analysis; Chelsea M Desbiens1; Gustavo H M F Souza2; Michael J. Nold3; 1KBI Biopharma, Durham, NC; 2Inovial, Rockford, IL; 3KBI Biopharma, Durham, NC.

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Development of Quantitative cGMP Impurity Protein Assays Supporting Diverse Modalities, Part I: Discovery; Gustavo H M F Souza1; Chelsea M Desbiens2; Michael J. Nold3; 1KBI Biopharma, Durham, NC; 2Inovial, Rockford, IL; 3KBI Biopharma, Durham, NC.

TP 570

Investigating Intra- and Extra-Cellular Protein Expression to Troubleshoot Low Expression of a Challenging Biotherapeutic using Mass Spectrometry Assays; Lisa Gorg1; Lauren M Kraft1; Chris Sauer2; Alexander N Barnakov2; Andrew Mahan3; Thomas Kelly4; Harsh Nanda5; Partha Chowdhury6; 1Janssen Research and Development, Spring House, PA; 2Johnson & Johnson, Spring House, PA.

TP 571

New USP Standards and Tools to Support Mass Spectrometry Based Multi-Attribute Method (MAM) for Therapeutics Proteins: Li Jing1; Jingzhong Guo1; Kevin Carrick1; Diane McCarthy1; 1USP, Rockville, MD.

TP 572

Host Cell Proteins (HCPs) Results Analyzed using the Orbitrap Experior 240 and Compared to Results from Gold-Standard ELISA Method; Rodney Bannwart1; 1Neelanjani Bose1; 1Emery Pharma, Alameda, CA.

TP 573

Multiplex quantitation of critical host cell proteins(HCPs) using a SureQuant mass spectrometry assay peptide panel; Jie Chol1; Bhavin Patel1; Terry Hicks2; Matthew Daniels2; Sarah Baron3; Km Shams Ud Doha3; Paul Guilde4; Scott M Peterman4; Nikki Jarrett1; Kay Opperman1; Ryan Bomgardner1; 1Thermo Fisher Scientific, Rockford, IL; 2Thermo Fisher Scientific, St Louis, MO; 3Thermo Fisher Scientific, Grand Island, NY; 4Thermo Fisher Scientific, Waltham, MA.

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Size Exclusion Chromatography Coupled to Multitangle Light Scattering and High-Resolution Mass Spectrometry for the Characterization of Therapeutic Monoclonal Antibodies; Roxana Eggleston-Rangel1; Zeshan G Ageel2; 1Phenomenex, Torrance, CA.

TP 575

Automated Data Analysis Workflow Leveraging PASEF Data Acceleration with Confident Detection of Abundance HCPs; Amy Claydon1; Guillaume Tremintin1; Juergen Kastler1; Stuart Pengeley2; Jonathan Krieger1; Arn Brandenburg1; 1Genedata Ltd, Cambridge, United Kingdom; 2Bruker, San Jose, CA; 3Genedata AG, Basel, Switzerland; 4Bruker Daltonics, Bremen, Germany.

TP 576

Peptide Characterization and Monitoring Workflow for Biosimilar mAb Drug Products using a Compliance Ready LC-MS and Informatics Platform; Yinchao Yu1; Kellen Delaney1; 1Chimique des Protéines Membranaires, CNRS, 1 Université de Strasbourg, 2 Université de Strasbourg, CNRS, IPHC, UMR 7178, Strasbourg, France; 2Laboratoire de Spectrométrie de Masse (LSMIS) UMR 7140 (Unistra-CNRS), Université de Strasbourg, Strasbourg, France.

TP 577

Structural MS of G protein-coupled receptors (GPCRs): Can HDX-MS provide sufficient information to identify ligand binding sites?; Krysztof Okrasa1; Jana Broecker2; Aneta Cooper2; Anna Dębicka2; Maria Serrano-Vega2; Nicole Solcan1; Stacey Southall2; 1Sosei Heptares, Cambridge, United Kingdom.

TP 578

Combining native mass spectrometry and mass photometry for the pentameric bacterial ligand-gated ion channel Glic; Jérôme Castel1, 2; Marie Prevost1; Nathalie Barlone1; Karontin Le Mouël1; Manuela Zoonens2; Pierre-Jean Corringer1; Sarah Cianferani3, 4; 1Laboratoire de Spectrométrie de Masse BioOrganique (LSMBO) IPHC UMR 7178, Université de Strasbourg, CNRS, IPHC, UMR 7178, Strasbourg, France; 2Infrastucture Nationale de Protéomique ProFI, FR2048 CNRS CEA, Strasbourg, France; 3Channel-Receptors Unit, Institut Pasteur, CNRS, UMR 3571, Paris, France; 4Laboratoire de Biologie Physico-Chimique des Protéines Membranaires, CNRS, UMR 7093, Université Paris-7, Institut de Biologie Physico-Chimique, Paris, France.

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Capillary Zone Electrophoresis Mass Spectrometry for Characterization of Membrane Proteins; Qianjie Wang1; Peter K Lundquist2; Liangliang Sun1; 1Michigan State University, EAST LANSING; 2Michigan State University, East Lansing, MI.

TP 580

Direct determination of membrane protein-lipid organization using lipid vesicle native mass spectrometry platform and its application in synaptic vesicle fusion; Aniruddha Panda1, 2; Kalil Gupta1, 2; 1Nanobiology Institute, Yale University, West Haven, Connecticut; 2Department of Cell Biology, Yale University School of Medicine, New Haven, Connecticut.

TP 581

Analysis of lipid transport mechanisms via native mass spectrometry; Tobias Pith1; René Zangl1; Nils Hellwig1;
TP 582  Deciphering multi drug resistance protein1 lipid trafficking using native mass spectrometry top-down approach; Maya Miller1; Tarick El-Baba1; Carol V Robinson1; 2; Oxford University, Oxford, United Kingdom

TP 583  Native mass spectrometry of extracellular vesicles to enhance understanding of molecular mechanisms in the brain; Hannah M. Brit1; 2; Tarick El-Baba1; 2; Corinne A. Lutomski1; 2; Josh Hinkle1; Christopher Mullen2; John E.P. Syka2; Carol V. Robinson2; 3; Physical and Theoretical Chemistry Laboratory, Department of Chemistry, University of Oxford, Oxford, United Kingdom; 2; Kavli Institute for Nanoscience Discovery, University of Oxford, Oxford, United Kingdom; 3; Thermo Fisher Scientific, San Jose, California

TP 584  Using Native Mass Spectrometry to Probe Mechanisms of Lipid Modulation of Ion Channel Function; Susanne M. Mesey1; Mehitab S Hayre1; Karin E J Rödström1; 2; Stockholm University, Stockholm, Sweden; 1; VU University, Amsterdam, The Netherlands

TP 585  Determining the membrane recruitment mechanisms of peripheral membrane proteins through direct top-down nativeMS analysis from a tunable lipid bilayer; Rachel A McAllister1; 2; Wonhyeok Jung1; Ky won Jeong1; Jared Shaw1; Colm O’Farrell1; 2; Yale School of Medicine, Department of Cell Biology, New Haven, CT, USA; 2; Yale School of Medicine, Department of Pharmacology, New Haven, CT, USA; 3; Department of Applied Bioinformatics, University of Tübingen, Tübingen, Germany; 4; eMSci-incy, Corvallis, OR

TP 586  Development of a quantitative targeted proteomics method for the investigation of proteins in the blood-brain barrier; Michelle Robinson1; Carmen Fernandez-Metzler2; Serge Zemero2; Richard King2; Tanvi Desai3; Michael Lyman4; Jessica Peters4; Christopher Gibson1; Weixun Wang1; 1; Merck Research Labs, West Point, PA, USA; 2; PharmacoCendence Analytical Services, LLC, Hattieville, PA, USA; 3; University of Connecticut, Storrs, CT, USA; 4; University of New Mexico, Albuquerque, NM, USA

TP 587  Integrating mass spectrometry with molecular dynamics simulations for modeling IRMPD fragmentation of membrane proteins; Neha V. Kalman1; 2; Corinne Lutomski1; 2; Tarick El-Baba1; 2; Joshua D Hinkle1; Idilir Iko1; Jack L Bennett1; 2; Andrew Dolan1; 2; Christopher Mullen2; John E.P. Syka2; Carol V Robinson1; 2; 1; Physical and Theoretical Chemistry Laboratory, Department of Chemistry, University of Oxford, Oxford, United Kingdom; 2; Kavli Institute for Nanoscience Discovery, University of Oxford, Oxford, United Kingdom; 3; Thermo Fisher Scientific, San Jose, California; 4; OMass Therapeutics, Oxford, United Kingdom

TP 588  A comparative analysis of different sample preparation methods for human plasma proteomics by LC-MS/MS; Carina Lima1; Maggy Lepine1; Lekha Sieno1; 1; University of Quebec in Montreal, Montreal, QC, Canada

TP 589  Mag-Net: Bead based capture of membrane particles from plasma enables liquid biopsy measurements for >4,500 proteins; Christine C Wu1; Jea Park1; Gennifer Merrnhew1; Kristine Tsantillas1; IreshynGovender1; Sindsiwe Buthelezi2; Justin Jordaan2; Stoyan Sto ychev2; Michael J. MacCoss1; 1; University of Washington, Seattle, WA, USA; 2; Pacific Biosciences, Pretoria, South Africa

TP 590  Electron Capture Charge Reduction Allows for Selection of Individual Nanodisc Species; Philip Lacey1; Marius M. Kostelic1; Sophie R. Harvey1; 2; Vicki H. Wysocki2; 1; The Ohio State University, Columbus, OH, USA; 2; Campus Chemical Instrumentation Center, The Ohio State University, OH, United States, Columbus, OH, USA; 3; Campus Chemical Instrumentation Center, The Ohio State University, Columbus, OH

TP 591  Biochemical Implications of the TMEM97/ Histatin-1 Interaction; Dominick Pierre-Jacques1; Kyung-No Son1; Dhara Shah1; Sang Min Lee2; Vinay Kumar Aakalu3; Stephanie M Cologna1; 1; University of Illinois at Chicago, Chicago, IL, USA; 2; University of Michigan, Ann Arbor, Michigan; 3; University of Oxford, Oxford, United Kingdom

TP 592  Detection of Membrane Proteome Variants by Data-independent Acquisition Mass Spectrometry Approach; Yu-Teng Jheng1; San-Yuan Wang1; Ya-Hsuan Chang1; Hsuan-Yu Chen1; Chia-Li Han1; 1; National Taiwan University, Taipei, Taiwan; 2; Taipei Medical University, Taipei, Taiwan; 3; Academia Sinica, Taipei, Taiwan

Quantitative proteomics for mapping active splice isoforms of mTOR induced changes to TFEB PTMs; Jim Hwang1; 2; 2; University of Pittsburgh, Pittsburgh, PA, USA; 3; Pacific Glycomics Reference Site, College of Medicine, Columbus, OH, USA; 4; The Ohio State University, Columbus, OH, USA; 5; Chemical Instrumentation Center, The Ohio State University, Columbus, OH, USA

TP 593  Electrophilic covalent modification of SARS-CoV-2 proteome by isocyanate and peptide mapping; Kristen Nields1; Scott Mack1; Robert Hepler1; Andrew Mahan1; Chetan Leonc1; Mariam Elnaggar1; Maggie Ostrowski1; Hirsh Nanda1; Janssen Biopharmaceuticals, Springhouse, PA, USA; 2; SCIEX, CA, USA; 3; Janssen Pharmaceuticals, Spring House, PA

TP 594  Characterization of the post translational modifications of the transcription factor EB (TFE3) and quantitation by imaged capillary isoelectric focusing (icIEF)-UV/MS and peptide mapping; Nova and Mars McLean Department of Chemistry and Molecular Biology, Baylor College of Medicine, Houston, TX, USA; 2; Molecular and Cellular Biology, Baylor College of Medicine, Houston, TX, USA; 3; Center for Precision Environmental Health, Baylor College of Medicine, Houston, TX, USA

TP 595  Identification of Protein Modifications Induced in E. coli Strains with a Reducible xenoRBCs; Yung Jin Oh1; 2; Dongtai Yin1; 2; Jae Ho Kim1; 3; Hyun Joo An1; 3; Kallol Gupta1; 3; 1; National Taiwan University, Department of Chemical Engineering, Taipei, Taiwan; 2; Department of Chemistry, National Taiwan University, Taipei, Taiwan; 3; Chemical Instrumentation Center, The Ohio State University, Columbus, OH, USA

TP 596  Potential role of SAMT247 small molecule on the inhibition of mTOR induced changes to TFEB PTMs; Maggie N. Young1; 2; Andrew Mahan1; Chetan Leonc1; Mariam Elnaggar1; Maggie Ostrowski1; Hirsh Nanda1; Janssen Biopharmaceuticals, Springhouse, PA, USA; 2; SCIEX, CA, USA; 3; Janssen Pharmaceuticals, Spring House, PA

TP 597  Exploring the structural and functional implications of the TMEM97/ Histatin-1 interaction; Jerry C. Dinan1; 2; James Sanford1; 2; Andrew A. J. C. Liu1; 2; Lisa M. Jenkins1; Maggie Ostrowski2; 1; University of California, Santa Cruz, CA, USA; 2; University of Pittsburgh, Pittsburgh, PA, USA

TP 598  Exploration of Histone Methyltransferase Activity in the Green Alga Chlamydomonas Reinhardtii by Biochemical and Mass Spectrometric Approaches; Emily K. Wright1; Michael Hayes1; James Pesavento1; 1; Saint Mary’s College of California, Moraga, CA

TP 599  Temporal Responses of Skeletal Muscle Thiol Redox Proteome to Endurance Exercise Training in Six-month-old Rats; Rachel Nagel1; Tyler Sagendorf1; Kwan Attah1; Sue Bodine2; Joshua Adkins1; Weijun Qian1; 1; Pacific

TP 600  Deciphering multi drug resistance protein1 lipid trafficking using native mass spectrometry top-down approach; Maya Miller1; Tarick El-Baba1; Carol V Robinson1; 2; Oxford University, Oxford, United Kingdom

TP 601  Native mass spectrometry of extracellular vesicles to enhance understanding of molecular mechanisms in the brain; Hannah M. Brit1; 2; Tarick El-Baba1; 2; Corinne A. Lutomski1; 2; Josh Hinkle1; Christopher Mullen2; John E.P. Syka2; Carol V. Robinson2; 3; Physical and Theoretical Chemistry Laboratory, Department of Chemistry, University of Oxford, Oxford, United Kingdom; 2; Kavli Institute for Nanoscience Discovery, University of Oxford, Oxford, United Kingdom; 3; Thermo Fisher Scientific, San Jose, California

TP 602  Using Native Mass Spectrometry to Probe Mechanisms of Lipid Modulation of Ion Channel Function; Susanne M. Mesey1; Mehitab S Hayre1; Karin E J Rödström1; 2; Stockholm University, Stockholm, Sweden; 1; VU University, Amsterdam, The Netherlands

TP 603  Determining the membrane recruitment mechanisms of peripheral membrane proteins through direct top-down nativeMS analysis from a tunable lipid bilayer; Rachel A McAllister1; 2; Wonhyeok Jung1; Ky won Jeong1; Jared Shaw1; Colm O’Farrell1; 2; Yale School of Medicine, Department of Cell Biology, New Haven, CT, USA; 2; Yale School of Medicine, Department of Pharmacology, New Haven, CT, USA; 3; Department of Applied Bioinformatics, University of Tübingen, Tübingen, Germany; 4; eMSci-incy, Corvallis, OR

TP 604  Development of a quantitative targeted proteomics method for the investigation of proteins in the blood-brain barrier; Michelle Robinson1; Carmen Fernandez-Metzler2; Serge Zemero2; Richard King2; Tanvi Desai3; Michael Lyman4; Jessica Peters4; Christopher Gibson1; Weixun Wang1; 1; Merck Research Labs, West Point, PA, USA; 2; PharmacoCendence Analytical Services, LLC, Hattieville, PA, USA; 3; University of Connecticut, Storrs, CT, USA; 4; University of New Mexico, Albuquerque, NM, USA

TP 605  Integrating mass spectrometry with molecular dynamics simulations for modeling IRMPD fragmentation of membrane proteins; Neha V. Kalman1; 2; Corinne Lutomski1; 2; Tarick El-Baba1; 2; Joshua D Hinkle1; Idilir Iko1; Jack L Bennett1; 2; Andrew Dolan1; 2; Christopher Mullen2; John E.P. Syka2; Carol V Robinson1; 2; 1; Physical and Theoretical Chemistry Laboratory, Department of Chemistry, University of Oxford, Oxford, United Kingdom; 2; Kavli Institute for Nanoscience Discovery, University of Oxford, Oxford, United Kingdom; 3; Thermo Fisher Scientific, San Jose, California; 4; OMass Therapeutics, Oxford, United Kingdom

TP 606  A comparative analysis of different sample preparation methods for human plasma proteomics by LC-MS/MS; Carina Lima1; Maggy Lepine1; Lekha Sieno1; 1; University of Quebec in Montreal, Montreal, QC, Canada
TUESDAY POSTERS

TP 601 Optimization of a diaPASEF method for phosphoproteomics analysis of mouse brain tissues; Marie Gébelin1; Christine Schaeffer1; Jeewan Babu Rijal1; Christine Carapito1; 1Laboratoire de Spectrométrie de Masse BioOrganique, Institut Pluridisciplinaire Hubert Curien (UMR 7178), Strasbourg, France

TP 602 Application of proteomic approach to identify antibody chemical liabilities in early-stage discovery; Xiaohua Liu1; Sagar Kathuria1; Joel Bucci1; Kyle Cole1; Pierrick Rival1; Bailin Zhang2; Alessandro Masiero2; Sanofi, Cambridge, MA; 2Sanofi, Vitry-sur-Seine, France

TP 603 Investigating the post-translational regulation of tardigrade cryptobiosis; Evan R. Stair1; Abel A. Salas1; Leslie M. Hicks1; 1University of North Carolina at Chapel Hill, Chapel Hill, NC

TP 604 Acyl-Trap, a suspension trapping-based method for proteomic analysis of S-acylation; Michael T Forrester1; Aleksandra Tata1; Purushothama Rao Tata1; Matthew W Foster1, 1Duke University Medical Center, Durham, NC

TP 605 Development of a streamlined single-injection workflow for middle-down analysis of protein therapeutics using electron activated dissociation (EAD); Haichuan Liu1; Roxana McCloskey1; Zoe Zhang1; 1SCIEX, Framingham, MA

TP 606 A novel role for ERP46 in platelet function revealed by iodoTMT & LC-MS/MS; Jin Sung Zhou1; Tong Liu2; Yi Wu3; Hong Li1; David W. Essex3; 1Columbia University, New York, NY; 2Rutgers New Jersey Medical School, Newark, NJ; 3Sol Sherry Thrombosis Research Center, Temple University School of Medicine, Philadelphia, PA

TP 607 Identification of glycated peptides using similarity of MS/MS spectrum; Hyeyin Kim1; Heeyoun Hwang2; Insung Yong1; Pilnam Kim1; Jin Young Kim1; 1Department of Bio and Brain Engineering, KAIST, Daejeon, South Korea; 2Korea Basic Science Institute, Ochang, South Korea

TP 608 SP3-RAC/MAC: Towards Universal Proteomics Sample Processing for Multi-PTM Profiling; Austin Giith1; Matthew J Galfrey2; Xiaolu Li3; Bin Yang4; Wei-Jun Qian2; 1Tandem Mass Spectrometry and Optical Spectroscopy, Mannheim, Germany; 2Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA; 3Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA

TP 609 Quality Assessment of Cellular Therapies by Structure-Based N-Glycan Mapping; Sol Kim1; 1Ji Hyeon Nam2; Myungjin Oh3; Hyun Joo An4; 1Asia-Pacfic Glycomics Reference Site, Daejeon, South Korea; 2Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, South Korea

TP 610 Disulfide bonding mapping in proteins and fluorescence-assisted quantification of cysteine side chains; Sharel Cornelius1; Christine Sarai Urbina2; Jocelyn Vincent2; Saful Chowdhury1; 1University of Texas at Arlington, Arlington, TX

TP 611 Characterization of Histone Proteoforms with Capillary Electrophoresis-Tandem Mass Spectrometry using 193 nm Ultraviolet Photodissociation; Fliza M Taidin1; Amanda Helms2; Jennifer S. Brodbel1; 1University of Texas, Austin, Texas

TP 612 Proteomic and N-Glycomic Profiling of Plasma-Derived Extracellular Vesicle and Non-Membranous Particle Subpopulations Utilizing Two-Dimensional Size Exclusion Chromatography; Alan J. Zimmern1; Junfan Gao1; Anne-Lise Marie2; Jacqueline Wood3; Alexander R. Ivanov1; 1Barnett Institute of Chemical and Biological Analysis, Department of Chemistry and Chemical Biology, Northeastern University, Boston, MA

TP 613 TimsTof DDA-PASEF phosphoproteomics analysis of human dendritic cells reveals the signaling pathways modulated by the immune suppressive biogenic amine 3-hydroxy-L-kynurenamine (3HKMA); Cristina C Clement1; Rajesh K Soni2; 1Weill Cornell Medicine, New York, NY; 2Proteomics and Macromolecular Crystallography Shared Resource, Herbert Irving Comprehensive Cancer Center, Columbia University Irving Medical Center, New York, NY, United States, New York, NY

TP 614 Phosphoproteomics of MNT-1 Melanoma Cells Reveals Novel Signaling Pathways for Polyoxymethyl B-induced Skin Hyperpigmentation; Chuan Zhang1; Xiaofen Liu1; Jing Zhang1; Hailan Wu1; Yu Wang1; Yaxin Fan1; Beining Guo1; Xingchen Bian1; Xin Li1; 1Institute of Antibiotics, Huashan Hospital, Fudan University, Shanghai, China

TP 615 Label free and Isobaric labeling mass spectrometry to monitor ubiquitination dynamics upon modulation by small molecule inhibitors; Thierry Mercier1; Jean Delaplace2; Marie Gebelin1; 1Université de Lorraine, 2Université de Lorraine, France

TP 616 Effects of Cold Ischemia on Post-translational Modifications in Patient-Derived Xenograft Models of Cancer; Keith D. Rivera1; Rajan A. Burt2; Valentina Cesman1; Gerald Bronfman3; 1John H. dosage; 2Department of Oncology, Erasmus Medical Center Rotterdam, Rotterdam, Netherlands

TP 617 Precision characterization of Phosphorylations Enabled by Individual Ion Mass Spectrometry in MEK1 protein; Raveena Gupta1; Bryon Brown2; Jared O. Kalader1; 1John H. dosage; 2Northwestern University, Evanston, IL

TP 618 Tackling citrullination and deamidation challenges in proteomics using high-resolution ion mobility-mass spectrometry (HRIM-MS); Heidi Vitrac1; Jordan Stewart1; Lauren Royer1; Ashli Simone1; Jesse Meyer2; Justyna Fert-Bobert1; Jennifer Van Eyk1; 1MOBILion Systems, Chadds Ford, PA; 2Cedars-Sinai Medical Center, Los Angeles, CA

TP 619 A proximity labeling-based orthogonal trap approach for identifying the spatiotemporal posttranslational modifications-network regulated by enzymes in living cells; Guijin Zhai1; Yepei Huang1; Kai Zhang1; 1Tianjin Medical University, Tianjin, China

TP 620 Co-Translational Incorporation of Non-Canonical Proline Analouges in Bacteria: A Novel Approach to Study the Chromophorylation of Peptides in LC-MS; Alexandre J J Prefontaine1; Yiqing Lao1; Victor Spicer1; Darien Yeung1; Nediljko Budisa1; Oleg V. Krokhin1; 1University of Manitoba, Winnipeg, MB

TP 621 Orthogonal methods quantify a proteomic profile associated with AKT inhibitor response in both breast cancer cell lines and patient tumours; Constance Sobsey1; Bjoern H. C Frohlich2; Geert Staelens3; Anri Awari4; Adriana Aguilar-Mahecha2; Mark Basik5; Christoph H Borchers1, 4, 6; Gerald Batist1; 7; 1Segal Cancer Centre, Lady Davis Institute, Jewish General Hospital, Montreal, QC; 2Division of Experimental Medicine, McGill University, Montreal, QC; 3CeMOS - Center for Mass Spectrometry and Optical Spectroscopy, Mannheim, Germany; 4Gerald Brinton Department of Oncology, McGill University, Montreal, QC; 5Segal Cancer Centre, Lady Davis Institute, Jewish General Hospital, Montréal, QC; 6MRM Proteomics Inc., Montréal, QC; 7Exactis Innovation, Montreal, QC

TP 622 Comprehensive proteome landscape of low- and high-grade gliomas; Chunjun Lan; Peking union medical college, Beijing, China

TP 623 Utilization of a disposable tip-based LC system for proteomic characterization of FFPE tissues and plasma-derived extracellular vesicles from TNBC patients; Vincent R. Richard1; 2; Georgia Mitsu1; 3; Yasamin Majedi1; Josiane Lafleur1; Adriana Aguilar-Mahecha2; Rodney Ouellette1; 2; Jeremy Roy1; Mark Basik3, 4; Christoph H Borchers1, 3, 4; 1Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; 2Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; 3Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; 4Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; 5Segal Cancer Centre, Lady Davis Institute, Jewish General Hospital, Montréal, QC; 6MRM Proteomics Inc., Montréal, QC; 7Exactis Innovation, Montreal, QC
Quantification of the PD-1/PD-L1 axis in non-small cell lung cancer by immuno-multiple reaction monitoring; Vincent Lacasse 1, 2, Rene P. Zahedi 4, 5, Vincent R. Richard 1, Hangjun Wang 2, Georgia Mitsa 3, Olivier Poetz 4, Margaret Redpath 1, Andreas Papadakis 1, Mounib Eliecheby 2, Victor Cohen 1, Jason Scott Aguilera 1, Gerald Batist 1, Alain Spatz 1, 2, Christoph H. Borchers 1, 2, 3, 4. Gaygal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; 2Department of Pathology, McGill University, Montreal, QC; 3Department of Oncology, McGill University, Montreal, QC; 4Gerald Bronfman Department of Oncology, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; 5Department of Pathology, McGill University, Montreal, QC.

TUESDAY POSTERS
TP 638 Deeper plasma proteome coverage enables identification of novel biomarkers and classification of diseases. Andreas Schmidt1; Katrin Hartinger2; Zehan Hu3; Claudia Martelli4; Katharina Limm5; Xaver Wurzenberger6; Sebastian Mueller7; Nils A. Kulak8; Bruker Daltonics GmbH & Co.KG; Bremen, Germany; 2PreCisome GMBH; Planeag/Martinsried, Germany; 3Bruker Switzerland AG, Fällanden, Switzerland; 4Biognosys AG, Zurich, Switzerland

TP 646 Integrative Proteomics and Pharmacological Analysis of Colon Cancer Reveals the Classical Lipoprotein Pathway with Prognostic and Therapeutic Opportunities. Abhilash Barpanda1; Sanjeeva Srivastava2; IIT Bombay, Mumbai, India

TP 640 diaPASEF proteomic analysis of human sputum samples for the early diagnosis of lung cancer. Alejandro Fernández-Vega1; María Del Sol Arenas-De Larriva2; Bernabé Jurado-Gámez2; Ignacio Ortea3; 1Institute for Biomedical Research and Innovation of Cadiz, Cadiz, Spain; 2Pneumology Unit, Hospital Universitario Reina Sofia, IMIBIC, Córdoba, Córdoba, Spain; 3Proteomics Unit, Nanomaterials and Nanotechnology Research Center (CINN-CSIC), Health Research Institute of Asturias (ISPA), Oviedo, Spain

TP 641 Quantification of human milk protein survival across the infant gastrointestinal tract using nano LC/Orbitrap MS. Brianne Wai1; Ningjian Liang1; Bum Jin Kim2; Brian Scottoline2; David Dallas3; Oregon State University, Corvallis, OR; 2Oregon Health & Science University, Portland, Oregon

TP 646 Charge-Based Fractionation of Blood Plasma-Derived Extracellular Vesicle Subpopulations Followed by Proteomic Characterization. Xianyi Su1; Alexander R. Ivanov2; 1Barnett Institute of Chemical and Biological Analysis, Department of Chemistry and Chemical Biology, Northeastern University, Boston, MA; 2Morgridge Institute for Research, Madison, WI

TP 642 Next-generation biotyping of microorganisms for assessment of antibiotics resistance and virulence factors. Allan Stensballe1; Nicolai Bache2; Dorte Bekker-Jensen3; Mads Løse Mogensen2; 1Aalborg University, Aalborg, Denmark; 2Evoespace, Odense, Denmark; 3Danish Cancer Society, Copenhagen, Denmark

TP 643 Ultra-deep proteome profiling of Alzheimer’s disease cerebrospinal fluid by data-independent acquisition mass spectrometry using long gradients and ion mobility separation. Ellen Casavant1; Sumedh Sankhe2; Jakob Vowinckel3; Nikhil Pandya4; 1Department of Chemistry, University of Wisconsin-Madison, Madison, WI; 2Department of Medical Oncology, National Taiwan University College of Medicine, Taipei, Taiwan; 3Department of Clinical Laboratory Medicine, Graduate School of Medicine, Kyoto University, Kyoto, Japan; 4Department of Life and Medical Systems, Doshisha University, Kyotanabe, Japan

TP 644 Proteogenomic Landscape of East-Asian Breast Cancer Reveals Pathogenesis and Subtypes for Prognostic and Therapeutic opportunities. Ya-Hsuan Chang1; Yi-Ju Chen2; Zi-Jie Hong3; Yi-Jing Hsiao4; Guo-Shiou Liao5; Sheng-Fang Su6; Kuen-Tung Lin7; Wen Chen8; Yen-Shen Lu9; 1Hsuan-Yu Chen1; Sung-Liang Yü; Jyh-Cherng Yü; Yu-Ju Chen2; 1Institute of Statistical Science, Academia Sinica, Taipei, Taiwan; 2Institute of Chemistry, Academia Sinica, Taipei, Taiwan; 3Department of Surgery, Tri-Service General Hospital, National Defense Medical Center, Taipei, Taiwan; 4Department of Clinical Laboratory Sciences and Medical Biotechnology, College of Medicine, National Taiwan University, Taipei, Taiwan; 5Graduate Institute of Oncology, National Taiwan University College of Medicine, Taipei, Taiwan; 6Graduate Institute of Toxicology, National Taiwan University College of Medicine, Taipei, Taiwan; 7Department of Medical Oncology, National Taiwan University Hospital, Cancer Center Branch, Taipei, Taiwan; 8Department of Oncology, National Taiwan University Hospital, Taipei, Taiwan

TP 645 Deep plasma protein profiling with a novel fully automated multi-nanoparticle-based sample preparation and high throughput data-independent acquisition LC-MS method. William F Beimers1; Noah M Lancaster2; Evgenia Shishkova3; Sterling C Johnson4; 1Chemistry, University of Wisconsin - Madison, Madison, WI; 2Chemistry, University of Wisconsin - Madison, Madison, WI; 3Department of Chemistry, University of Wisconsin - Madison, Madison, WI; 4Department of Medicine, University of Wisconsin-Madison, Madison, WI; 5Department of Medicine, University of Wisconsin-Madison, Madison, WI; 6Wisconsin Alzheimer’s Institute, University of Wisconsin-Madison, Madison, WI; 7Wisconsin Alzheimer’s Disease Research Center, University of Wisconsin School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI; 8Morgridge Institute for Research, Madison, WI

TP 649 The Proteome in Human Periodontal Ligament and Pulpal Fibroblasts Resulting from Contact with Root Restorative and Pulp-capping Materials. Mona Goli1; Mahmoud Mona2; Firas Kobeissy3; Roberta Pieleggi4; Yehia Mecheef5; 1Texas Tech University, Lubbock, TX; 2University of Florida College of Dentistry, Gainesville, FL; 3Morehouse School of Medicine (MSM), Atlanta, Georgia

TP 650 Development of Extracellular vesicles preparation platform for clinical proteomics. Satoshi Muraoka1; Masayo Hirano1; Satoshi Nagayama2; Junko Isayama3; Mimiko Ishida2; Takeshi Tomonaga3; Jun Adachi1; 1National Institute of Biomedical Innovation, Health and Nutrition, Ibaraki, Japan; 2The Cancer Institute Hospital of the Japanese Foundation for Cancer Research, Aikaie, Japan; 3Kyoto University, Kyoto, Japan

TP 651 Blood Stream Isolates: What’s in a Proteome?; Morgan Hebbum1; 1Rioill Hill; 2Morgan Westlund; 3Annette Uitke-Lemee; 4Soren Wacker; 5Alikhan Mansuri1; 6Gopal Ramamourthy2; Thomas Rydzak3; Joshua T Smith4; 1Andriy Plakhotnyk5; Colin MacKenzie6; Maryam Mapar7; 1Bruce J Walker; 2Ashlee M Earl; Hallgrimur Benediktsson1; Daniel B Gregson2; 1Morsel Research Institute, Ariano Irpino, Italy; 2Morehouse School of Medicine (MSM), Center for Neurotrauma, Multiomics & Biomarkers, Department of Neurobiology, Atlanta, Georgia

TP 652 Early Inflammatory Protein Responses Detected in Plasma by MALDI-ToF Profiling in SARS-CoV-2 Immunization Naïve Individuals. Amanda Weaver1; Tristan Finch1; Alicia Patrick2; Laura Peek3; Gary Pestano4; 1Biodexis, Boulder, CO

TP 653 The Role of Native MS in Antibody Response Against Snake Envenoming: Inna Oganesyan1; Julian A. Harrison2; Ledsgaard Jensen Line3; Cecile Knudsen4; 1Timothy Patrick Jenkins1; 2Lexicon, Chester - Kiel4; 3Department of Biomolecular Sciences and Pharmacology, Aalborg University, Aalborg, Denmark; 4Department of Immunology, VU University Medical Center, Amsterdam, Netherlands; 5ETHZ, Zürich, Switzerland; 6ETH Zürich, Zurich, Switzerland; 7Technical University of Denmark, Kongens
| TP 654 | Capillary chromatographic separation of nanogram protein quantities on a wide-pore superficially porous particle column for top-down proteomics. Guillaume Chevreux; Laurent Lignières; Véronique Legnés; Manel Khelli; Nicolas Senecault; Matthew A. Laube; Jean-Michel Camadot; Institut Jacques Monod, PARIS, France; 2Waters Corporation, Milford, MA |
| TP 656 | Improved characterization of ApoA4 proteoforms from plasma samples by top-down mass spectrometry using ion-ion reactions and advanced spectral averaging: Amal Mohamed Kamal; Jake T. Kline; Kenneth R. Durbín; Konstantin G. Nagaevov; Yury O Tsybin; Luca Fornelli; University of Oklahoma, Norman, OK; 2Proteinaceous, Evanston, Illinois; 3Spectroswiss, Lausanne, Switzerland |
| TP 657 | FLASHDeconVQ: a software tool for proteome-wide label-free quantification of proteoforms in top-down proteomics: Ji Hyung Kim; Kywon Jeong; Konrad Winkels; Philipp T. Kaulich; Andreas Tholey; Oliver Kohlbacher; University of Tübingen, Tübingen, Germany; Christian-Albrechts-Universität zu Kiel, Kiel, Germany |
| TP 658 | A new proteomics data analysis software for top-down mass spectrometry: George Alevizos; Mariangela Kosmopolou; Athanasios Smyrakis; Dimitris Papanastasiou; Fasmathe, NCSR Demokritos, Athens, Greece |
| TP 659 | UVD photodissociation using a diffuse light source integrated in the Omnitramp platform: Athanasios Smyrakis; Mariangela Kosmopolou; Dimitris Papanastasiou; Fasmathe, NCSR Demokritos, Athens, Greece |
| TP 660 | False discovery rate estimation in spectral deconvolution in top-down proteomics: Ayesha Feroz; Kywon Jeong; Konstantin Nagaevov; Ji Hyung Kim; Timo Sachsenberg; Yury O. Tsybin; Oliver Kohlbacher; Department for Computer Science, University of Tübingen, Sand 14, 72076, Tübingen, Germany; 2Institute for Bioinformatics and Medical Informatics, University of Tübingen, Sand 14, 72076, Tübingen, Germany; 3Spectroswiss, 1015, Lausanne, Switzerland; 4Translational Bioinformatics, University Hospital Tübingen, Hoppe-Seyler-Str. 9, 72076, Tübingen, Germany |
| TP 661 | Protein Cooking: Combining Thermal CID and EAD for intact protein sequencing: Cuong Le; Patrick Pribil; Yves Le Blanc; 2SCIEX, Concord, ON; 3SCIEX, Concord, On, ON |
| TP 662 | Capillary Zone Electrophoresis-Field Asymmetric Ion Mobility Spectrometry-Mass Spectrometry (CE-FAIMS-MS) of Histone Protein Analysis for Top-down Proteomics: Qianli Wang; Fei Fang; Liangliang Sun; 1Michigan State University, East Lansing, MI |
| TP 663 | Combining Long-Read RNA Sequencing with Curated Databases to Enhance Proteoform Identification & Characterization by Top-Down Proteomics: Joseph B. Greer; Bryan P. Early; Taojunfeng Su; Ryan T. Fellers; Neil L. Kelleher; Kenneth R. Durbín; Northeastern University, Evanston, IL; 2Proteinaceous, Evanston, IL |
| TP 664 | Top-down analysis of intact NISTmAb and CA (II) by Capillary Isoelectric Focusing coupled to Electron Capture Dissociation Mass Spectrometry: Stanislav Beloborodov; Pavel Ryumin; Wen Jin; Bradley Schneider; Bill Lloyd; 2SCIEX, Concord; 3SCIEX, Concord, ON |
| TP 665 | Leveraging intrachain disulfide bonds in proteins for improved sequence coverage in EAD top-down analysis: Wen Jin; Pavel Ryumin; Lyle L. Burton; 2SCIEX, Concord, ON |
| TP 667 | Improved characterization of ApoA4 proteoforms from plasma samples by top-down mass spectrometry using ion-ion reactions and advanced spectral averaging: Amal Mohamed Kamal; Jake T. Kline; Kenneth R. Durbín; Konstantin G. Nagaevov; Yury O Tsybin; Luca Fornelli; University of Oklahoma, Norman, OK; 2Proteinaceous, Evanston, Illinois; 3Spectroswiss, Lausanne, Switzerland |
| TP 668 | FLASHDeconVQ: a software tool for proteome-wide label-free quantification of proteoforms in top-down proteomics: Ji Hyung Kim; Kywon Jeong; Konrad Winkels; Philipp T. Kaulich; Andreas Tholey; Oliver Kohlbacher; University of Tübingen, Tübingen, Germany; Christian-Albrechts-Universität zu Kiel, Kiel, Germany |
| TP 669 | Internal fragments generated by top-down mass spectrometry can be confidently assigned by cyclic ion-mobility, enhancing the extent of protein sequence information: Migration A. Zosová; Georgios Kosmopoulou; Gene Hart-Smith; Luke Carroll; Australian Proteome Analysis Facility, Macquarie University, Sydney, Australia; 2Waters Corporation, Sydney, Australia; 3Australian Proteome Analysis Facility, Macquarie University, Macquarie Park, Australia |
| TP 670 | Internal fragmentation generates progressively smaller terminal fragments in top-down mass spectrometry: Novyara Alam; Somak Ray; Jeffrey N Agar; 1Northeastern University, Boston, MA |
| TP 671 | Coupling high-field asymmetric wavefront ion mobility spectrometry with capillary zone electrophoresis-tandem mass spectrometry for top-down proteomics: Tian Xu; Liangliang Sun; 1Michigan State University, East Lansing, MI |
| TP 672 | A standardized approach for the exploration of histone proteoforms with EAD fragmentation on the Sciex ZenoTOF MS: Richard M Searfoss; Emily Zahn; Zongtao Lin; Francisca N. de Luna Vitorino; Benjamin A Garcia; 1Washington University School of Medicine, St. Louis, MO |
| TP 673 | Heavy peaks -examples of qualitative and quantitative potential of intact protein LC-MS: Waltteri Hovi; VTT Technical Research Centre of Finland, Espoo, Finland |
| TP 674 | Evaluation of Spray-Capillary-Based Capillary Electrophoresis-Mass Spectrometry for Analysis of Sub-nanogram Mass Intact Complex Lysate using Top-Down Proteomics: Zhihao Zhao; Yanting Guo; Kellye A Cupp-Sutton; Lushuang Huang; Si Wu; 1Ohio State University, Norman, OK |
| TP 675 | Assessing alternative proteinases for quantitative proteomics: Meital Kupervaser; David Morgentern; Corine Katina; Yishai Levin; De The Botton Protein Profiling institute of the Nancy and Stephen Grand Israel National Center for Personalized Medicine, Weizmann Institute of Science, Rehovot, Israel |
| TP 676 | Real-time instrument methods to resolve chimeric spectra and post-translational modifications in multiplexed proteomics: Chris McGann; William Barshop; Jesse Canterbury; Chuwei Lin; Thomas Perkins; David Bergen; Jingjing Huang; Graeme McAllister; Devin Schewepe; University of Washington, Seattle, WA; 2Thermo Fisher Scientific, San Jose, CA; 3University of Washington, Seattle, WA |
| TP 677 | directLFQ, an algorithm for ultra-fast, accurate and open proteomics quantification: Constantin Ammar; Julia Schessner; Sander Willems; André Michaelis;
TP 687 Quantitative Proteomic Analysis of Sputum Reveals Proteins Associated with Inflammatory Response to Woodsmoke Exposure: Angie L. Moore4; Christine A. Mills1; Alexis Payton2, 3, 5; Laura E. Herring1; Neil E. Alexis1; Heather Wells1; David B. Pedena1, 5; Julia Rager2, 3, 6; Ilona Jaspers2, 4, 7; 1UNC Proteomics Core Facility, Department of Pharmacology, University of North Carolina at Chapel Hill, Chapel Hill, NC; 2Department of Environmental Sciences and Engineering, Gillings School of Global Public Health, UNC Chapel Hill, Chapel Hill, NC; 3Center for Environmental Medicine and Lung Biology, School of Medicine, UNC Chapel Hill, Chapel Hill, NC; 4Department of Pediatrics, Division of Allergy & Immunology, UNC Chapel Hill, Chapel Hill, NC; 5Institute for Environmental Health Science, Gillings School of Global Public Health, UNC Chapel Hill, Chapel Hill, NC; 6Department of Microbiology and Immunology, UNC Chapel Hill, Chapel Hill, NC.

An API-independent Smart-close-out enable faster TMT RTS-SPS-MS3 assisted in-depth proteome profiling: Weixian Deng1; Aman Makaj1; Daryl Bulloch2; Bo Zhou1; 1Amgen, Thousand Oaks, CA; 2Amgen, Inc., South San Francisco, CA.

TP 689 Proteomic Analysis of Six Mammalian Cell Lines Reveals Individual Lysosomal Composition and Novel Lysosomal Proteins: Sara Bonini1; Fatema Akter1; Srigayatri Ponniyai1; Blanca Kögl-Mohrbacher1; Florian Bleibbaum1; Markus Damme1; Bernhard Y. Renard1; Dominic Winter1; 1Institute for Biochemistry and Molecular Biology, Medical Faculty, Rheinische Friedrich-Wilhelms-University of Bonn, Bonn, Germany; 2Bioinformatics Unit (MF1), Robert Koch Institute, Berlin, Germany; 3Institute for Biochemistry, Kiel, Germany.

TP 690 TMT quantitative proteomics of bortezomib treated cell line models of AL amyloidosis and multiple myeloma: Gary Bradshaw1; Cameron S. Fraser2; Marian Kalocsay1; Christopher Sarosi2, 3; 1Laboratory of Systems Pharmacology, Boston, MA; 2John B. Little Center for Radiation Sciences, Harvard TH Chan School of Public Health, Boston, MA; 3Program in Molecular and Integrative Physiological Sciences, Harvard TH Chan School of Public Health, Boston, MA; 4Department of Experimental Radiation Oncology, Division of Radiation Oncology, The University of Texas MD Anderson Cancer Center, Houston, TX.

TP 691 Light-dark dependent changes in cyanobacterium Crocosphaera sub tropica ATCC 51142 proteome: Punyatoya Panda1; Uma K. Aryal1; 1Purdue University, West Lafayette, Indiana.

TP 692 Systemized proteomics by automating the TMT global protein profiling workflow: Tayler P Ma1; Hanna G Budayeva1; Kristen Bahn1; Beatriz Ramirez1; David D. N. Dou2; 1Genentech, Inc., South San Francisco, CA; 2Genentech Inc, South San Francisco, CA; 3Thermo Fischer Scientific, San Jose, CA; 4Thermo Fisher Scientific, San Jose, CA.

Enabling high depth proteomic analysis of rat plasma through comparison of depletion strategies: Jan Munte1; Theresa Keil1; Christin Zasada1; Janine Sequeira1; Marsilio Adrian1; Krzysztof Okraska1; Hannes Hahn1; 1OMICScouts, Freising, Germany; 2Sosei Heptares, Cambridge, United Kingdom.

TP 688 Developing differential absolute quantification assays for targeted cancer proteogenomics: Yassene Mohammed1; Constantinos Bli Atsios2; Karl Makepeace3; Pallab Bhowmick1; Vincent R. Richard1; Christoph H. Borchers1, 4, 5, 6, 8; 1Center for Proteomics and Metabolomics, Leiden University, Leiden, Netherlands; 2Department of Oncology, McGill University, Montreal, QC; 3University of Victoria Genome British Columbia Proteomics Center, Victoria, BC; 4Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; 5Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; 6Center for Bioinformatics and Computational Biology, McGill University, Montreal, QC; 7Division of Experimental Medicine, McGill University, Montreal, QC; 8Department of Pathology, McGill University, Montreal, QC.

TP 689 Developing differential absolute quantification assays for targeted cancer proteogenomics: Yassene Mohammed1; Constantinos Bli Atsios2; Karl Makepeace3; Pallab Bhowmick1; Vincent R. Richard1; Christoph H. Borchers1, 4, 5, 6, 8; 1Center for Proteomics and Metabolomics, Leiden University, Leiden, Netherlands; 2Department of Oncology, McGill University, Montreal, QC; 3University of Victoria Genome British Columbia Proteomics Center, Victoria, BC; 4Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; 5Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; 6Center for Bioinformatics and Computational Biology, McGill University, Montreal, QC; 7Division of Experimental Medicine, McGill University, Montreal, QC; 8Department of Pathology, McGill University, Montreal, QC.

TP 690 Developing differential absolute quantification assays for targeted cancer proteogenomics: Yassene Mohammed1; Constantinos Bli Atsios2; Karl Makepeace3; Pallab Bhowmick1; Vincent R. Richard1; Christoph H. Borchers1, 4, 5, 6, 8; 1Center for Proteomics and Metabolomics, Leiden University, Leiden, Netherlands; 2Department of Oncology, McGill University, Montreal, QC; 3University of Victoria Genome British Columbia Proteomics Center, Victoria, BC; 4Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; 5Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; 6Center for Bioinformatics and Computational Biology, McGill University, Montreal, QC; 7Division of Experimental Medicine, McGill University, Montreal, QC; 8Department of Pathology, McGill University, Montreal, QC.

TP 685 Discovery and validation of “missing human proteins” based on analysis of gastric cancer tumor cells: Yining Cai1; Chunhui Gu1; Fuchung Hsiao1; Jennifer B. Dennison1; Jody Vykoukal1; Johannes Fahrmann1; Kim-Anh Do1; Shumei Song1; Jaffer Ajan1; Ehsan Irajizad1; Hirohito Katayama1; Sanjay A. Mordant1; St. Vincent’s College of Medicine, University of Texas MD Anderson Cancer Center, Houston, TX.

TP 686 Developing differential absolute quantification assays for targeted cancer proteogenomics: Yassene Mohammed1; Constantinos Bli Atsios2; Karl Makepeace3; Pallab Bhowmick1; Vincent R. Richard1; Christoph H. Borchers1, 4, 5, 6, 8; 1Center for Proteomics and Metabolomics, Leiden University, Leiden, Netherlands; 2Department of Oncology, McGill University, Montreal, QC; 3University of Victoria Genome British Columbia Proteomics Center, Victoria, BC; 4Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; 5Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; 6Center for Bioinformatics and Computational Biology, McGill University, Montreal, QC; 7Division of Experimental Medicine, McGill University, Montreal, QC; 8Department of Pathology, McGill University, Montreal, QC.

TP 687 Proteomics reveals specific metabolic pathways responsible for the antinociceptive effect of Flavonoids found in Cannabis sativa: Fatima Boujenoui1; Mathilde Laba1; Francis Beaudry1; Universite de Montreal, St-Hyacinthe, QC.

TP 686 Developing differential absolute quantification assays for targeted cancer proteogenomics: Yassene Mohammed1; Constantinos Bli Atsios2; Karl Makepeace3; Pallab Bhowmick1; Vincent R. Richard1; Christoph H. Borchers1, 4, 5, 6, 8; 1Center for Proteomics and Metabolomics, Leiden University, Leiden, Netherlands; 2Department of Oncology, McGill University, Montreal, QC; 3University of Victoria Genome British Columbia Proteomics Center, Victoria, BC; 4Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; 5Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; 6Center for Bioinformatics and Computational Biology, McGill University, Montreal, QC; 7Division of Experimental Medicine, McGill University, Montreal, QC; 8Department of Pathology, McGill University, Montreal, QC.

TP 687 ESI Source Comparison and Optimization on a Capillary-flow SureQuant Assay: Yi (jimmy) Zeng1; Ruby Karimjee1; Sara Nouri Gomaei1; Hao Qian1; Estelle Hoedt1; Joon-Yong Lee1; Philip Ma1; Bruce Wilcox1; PrognomiQ Inc, San Mateo, CA.

TP 688 Enabling high throughput proteomics with short gradients and ZenoSWATH DIA by utilising the speed and sensitivity of the ZenoToF 7600: Dylan Xavier1; Keith Ashman2; Peter G Hains3; Phillip J Robinson1; Procan1; children’s Medical Research Institute, Faculty of Medicine and Health, The University of Sydney, Westmead, Australia; 2SCiEX, Sydney, Australia.

TP 683 Non-invasive micro-sampling and targeted MS-based longitudinal blood proteome profiling to establish intra-individual protein reference ranges of athletes: Vincent R. Richard1; Georgina Mitsa1, 2; Darla Chaplygina1; Mario Thevis1, 2; Christoph H. Borchers1, 4, 5, 6, 8; 1Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; 2Division of Experimental Medicine, McGill University, Montreal, QC; 3Institute of Biochemistry, Center for Preventive Doping Research, German Sport University, Cologne, Germany; 4European Monitoring Center for Emerging Doping Agents (EuMoCEDA), Cologne/Bonn, Germany; 5Gerald Bronfman Department of Oncology, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; 6Department of Pathology, McGill University, Montreal, QC.

TP 684 Enhanced TMT data analysis with AI-driven workflows utilizing CHIMERYS and INFETERS algorithms: Mick Greer1; Mark Sanders2; David M Horn2; Kai Fritzmeier2; 1Thermo Fisher Scientific, Austin, TX; 2ThermoFisher Scientific, Somerset, NJ; 3ThermoFisher Scientific, San Jose, CA; 4Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany.

TP 685 Discovery and validation of “missing human proteins” based on analysis of gastric cancer tumor cells: Yining Cai1; Chunhui Gu1; Fuchung Hsiao1; Jennifer B. Dennison1; Jody Vykoukal1; Johannes Fahrmann1; Kim-Anh Do1; Shumei Song1; Jaffer Ajan1; Ehsan Irajizad1; Hirohito Katayama1; Sanjay A. Mordant1; St. Vincent’s College of Medicine, University of Texas MD Anderson Cancer Center, Houston, TX.
TUESDAY POSTERS

Federal University of Pernambuco, Recife, Brazil; São Marcos Hospital/Rede D’Or, Recife, Brazil

Deep proteome profiling of breast implant capsules with contracture shows high burden of inflammatory processes: Ole Østergaard1, Andreas Larsen2, Tim Kongsmark Welz3, Mikkel Herly3, Jesper Velgaard Olsen1; 1NFF CENTER FOR PROTEIN RESEARCH, Copenhagen, Denmark; 2Department of Plastic Surgery and Burns Treatment, Copenhagen University Hospital, Copenhagen, Denmark; 3Department of Immunology and Microbiology, University of Copenhagen, Copenhagen, Denmark

MALDI and LC-ESI-MS for amyloid-beta peptide profiling in brain of Alzheimer’s disease and Down syndrome patients: Elena Camporese1, Amal Kasiri2, Gunnar Brinkmalm3, Marie-Claude Polier4, Henrik Zetterberg5, Eleni Gkanatsiou6, Lev Stimmer7, Andre Strydom3, Yannick Vermeiren9; 1Gothenburg University, Gothenburg, Sweden; 2Institute of the Cerveau-CNRS UMR7225-Inserm U1127-UPMC, Hopital de la Pitié-Salpetrière 47, Paris, Paris, France; 3University of Gothenburg, Molndal, Sweden; 4INSERM US27, Platform for Experimental Pathology, MIRCen, Fontenay-aux-Roses, France, Paris, France; 5Department of Forensic and Neurodevelopmental Sciences, Institute of Psychiatry, Psychology and Neuroscience, King’s College London, London, United Kingdom; 6London, United Kingdom; 7Department of Immunology and Microbiology, University of Copenhagen, Copenhagen, Denmark

Comprehensive Proteomics Analysis of the Crustacean Cuticle: Vu Nang Tran1,2; Gaoyuan Lu1; Wenxin Wu1; Thao Duong1; Lingjun Li1,2; 1University of Wisconsin-Madison School of Pharmacy - Madison, WI, Madison, WI; 2Department of Chemistry, University of Wisconsin-Madison, Madison, WI

Phosphoproteomic profiling of Stk33-knockout testis reveals widespread phosphorylation changes in spermatogenesis: Wuqing Yu1; Liping Yao1; Xiangzheng Zhang1; Xuejiang Guo1; 1Nanjing Medical University, Nanjing, China

Kinase assay-linked phosphoproteomic profiling identified AKAP34 as important phosphorylation substrates of STK33 during spermiogenesis: Chenghao Situ1; Weiling Yu1; Hong Chen1; Leping Yao1; Xiangzheng Zhang1; Xuejiang Guo1; 1Nanjing Medical University, Nanjing, China

A medium-throughput DIA-MS workflow enables preclinical and clinical proteome studies in cardiac tissue: Lisa Neuenroth1,2; Jumana Jaber1,2; Verena Ebner1,2; Stephan Lehnhart1,2,3,4,5; Henning Urlaub1,2,3,4,5; Christof Lenz1,2,3,4,5; 1University Medical Center Goettingen, Goettingen, Germany; 2DFG Collaborative Research Centre 1002, Goettingen, Germany; 3DFG Collaborative Research Centre 1190, Goettingen, Germany; 4DZHK, Goettingen, Germany; 5Max Planck Institute for Multidisciplinary Sciences, Goettingen, Germany

Identification of proteins affected by increased intraocular pressure in the glaucomatous female mouse retina by label-free proteomics: Khadiza Zaman1,2; Autum B Morgan3; Dori Nguyen3; Katalin Prokai-Tatrai4; Denise M Irman2; Laszlo Prokai4; 1Department of Pharmacology and Neuroscience, The University of North Texas Health Science Center, Fort Worth, TX; 2Department of Pharmaceutical Sciences and the North Texas Eye Research Institute, The University of North Texas Health Science Center, Fort Worth, TX

Optimization of Extraction Methods to Allow Detection and Quantification of Protein Targets from Various Mammalian Tissues: Fabio N. Najjar1,2,3; M Magaña1; 1AstraZeneca, Cambridge, United Kingdom; 2AstraZeneca R&D, Gaithersburg, MD; 3AstraZeneca, Maynooth, Ireland

Comparison of Sample Preparation Methods for Genetically Variant Peptide Identification in Human Hair: Zheng Zhang1; William E. Wallace1; Guanghui Wang3; Meghan C. Burke Harris1; Yi Liu1; Sergey L. Sheetlin2; Stephen E. Stein2; 1NIST, Gaithersburg, MD

Spatially-resolved proteomics of drug-dosed tissue by use of liquid extraction surface analysis: Peter Macie1; Iain B. Styles2; Helen J. Cooper1; 1University of Birmingham, Birmingham, United Kingdom

Differential proteomics to probe molecular basis for a renal phenotype associated with GPR110 deletion: Bill Huang1; Karl Kevala1; Hee-Yong Kim1; 1NIAAA/NIH, Rockville, Maryland

Hollow Fiber Field-Flow Fractionation coupled with nano-LC/MS/MS improved the characterization of protein aggregates in whole brain lysates from B6 mice; Zohaib Khan1,2; Valentina Marassi3; Barbara Roda3; Cristina C. Clement4; 1Weill Cornell Medicine, New York, New York; 2Department of Chemistry, University of Bologna, Bologna, Italy

Survey of Estrogen-Related Endocrine Disruption in Aquatic Ecosystems by Mass Spectrometry-Based Proteomics Using Hylaeola azteca as Model Organism: Marcel L. Prokai1,2,3; Khadiza Zaman1,2; Vladimir Shulaev3; 1University of North Texas, Denton, TX; 2University of North Texas, Mayaguez, Puerto Rico; 3Maynooth University, Maynooth, Ireland

Biting into the Tooth Proteome: protein extraction, data acquisition, and data processing: Priyam Jain1; Olivier Duverger1; Marian Young1; Lee Janince1; Yan Wang1; 1NIH/NIDCR, BETHESDA, MD

SYSTEMS BIOLOGY OF Atherosclerotic Human Carotid Arteries Through Mass Spectrometry-Based Proteomics: Laszlo Prokai1,2,3; Eva Csösz2; Gergő Kálló2; Aijees Kumar2; Khadiza Zaman1,2; Uladzislau Vadadokhau3; László Poto4,5,6; Zoltán Hendrik4; Gábor Méhes4; Csaba Tóth2; Péter Gergely1; József Tőzsér2; György Balla1; József Balla1,2,3; 1University of North Texas Health Science Center, Fort Worth, TX; 2University of Debrecen, Faculty of Medicine, Debrecen, Hungary; 3University of Debrecen, ELKH-UD Vascular Pathophysiology Research Group, Debrecen, Hungary

Quantitative Target Engagement for a KRASG12C Inhibitor in FFPE Tumor Tissue: Andrew Chambers1; Steve Sweet2; Zifeng Song2; David Chain2; Claire Rooney2; Yeoun Jin Kim1; 1AstraZeneca R&D, Gaithersburg, Maryland; 2AstraZeneca, Cambridge, United Kingdom

Proteomics of adipose tissue-derived extracellular vesicles from bariatric surgery patients: Jacelyn Greenwald1; Paola Loreto Palacio1; Yongseok Kim2; Setty M Magaña3; Vicki H Wysocki1; 1The Ohio State University - Department of Chemistry and Biochemistry, Columbus, OH; 2Department of Pediatrics, Division of Neurology, Center for Clinical and Translational Research, Abigail Wexner Research Institute, Nationwide Children’s Hospital, Columbus, Ohio
TP 714 Poly[n]rotaxanes: From Synthesis To Mass Spectrometric Characterizations; Bo Song 1; James Seale 1; Yunyan Qiu 1; Fraser Stoddart 1; 1Northwestern University, Evanston, IL; 2National University of Singapore, Singapore, Singapore

TP 715 Detecting Oxygen Inhibition in Adhesive Systems Using ASAP-MS; Christopher Joseph Shaffer 1; Spencer Johnson 2; Dana Reid 3; Amanda Leone 4; Wayne Mahoney 4; Eric Nelson 5; 1,3,5,7,10,12,14-Decanatetrafuran (DTCF) as an electronic oxide sensor for detection of AMSOIL 4; 2Birmingham Young University, Provo, UT

TP 716 Dissecting Complex Polymer Mass Spectra by Fourier Transform-based Deposition and Macromolecular Mass Defect Analysis; Andrew K Swansinger 1; Christopher M. Crittenden 2; Rekha Thomas 3; James S Prell 3, 4; 1University of Oregon, Eugene, OR; 2Genentech Inc, South San Francisco, CA; 3Materials Science Institute, University of Oregon, Eugene, OR

TP 717 Investigation of fluoropolymer synthesis by Thermodesorption/Pyrolysis-DART coupled to very high-resolution mass spectrometry; Pierre Pacholski 1, 2; Frédéric Progent 1; Sébastien Schramm 2; Frédéric Aubriet 2; 1CEA, DAM, DIF, F-91297 Arpajon, France; 2Laboratoire de Chimie et Physique-Approche Multi-échelles des Milieux Complexes (LCP-A2MC), Université de Lorraine, METZ, France

TP 718 Direct analysis of brominated flame retardants in high-polymer polypropylene and acrylonitrile butadiene styrene copolymer with DIP-APCI TQ-TOF MS; Ville Nissinen 1; Krista Gronlund 1; Janne Jänis 1; Jarkko J. Saarinen 1; Mika Suvanto 1; Ilkka Ryoluto 2; Jani Pelto 3; 1University of Eastern Finland, Department of Chemistry, Joensuu, Finland; 2VT Technical Research Centre of Finland Ltd., Tampere, Finland

TP 719 Combining IMS with MS/MS for Accelerated Readout of Digital Polymers; Isaura Sergent 1; Thibault Schultz 2; Laurence Oswald 1; Jean-François Lutz 2; Laurence Charles 2; 1Aix Marseille Université, CNRS, Institut de Chimie Radiculaire, MARSEILLE, France; 2Université de Strasbourg, CNRS, UMR 7006, Institut de Science et d'Ingénierie Supramolécules, Strasbourg, France; 3Université de Strasbourg, CNRS, UPR 22, Institut Charles Sadron, Strasbourg, France

TP 720 Controlling the charge states of ultra-high molecular weight polystyrene MALDI ions through cationization reagents; Awinash Adhikrao Patil 1; Th Khanh Ly Lai 1; Wen-Ping Peng 1; National Dong Hwa University, Shoufeng, Taiwan

TP 721 >10,000 Da polymer detection using QExactiveTM UHMR: In-Source Trapping and Charge Reduction; Junho Jeon 1; Anthony Gies 1; Zoltan Szabo 1; Katie Peterson 1; 1The Dow Chemical Company, Lake Jackson, TX; 2Thermo Fisher Scientific, San Jose, CA

TP 722 Detecting and Identifying Sample-Classification Markers from Direct-HRMS Experiments: How to Manage Comparative DART-HRMS data; Luke K Ackerman 1; Kristen I. Reese 2; Jánis Rubko 2; Ingus Pērkons 2; 1FDA Center for Food Safety, College Park, MD; 2Institute of Food Safety, Animal Health and Environment “BIOR”, Riga, Latvia

TP 723 An LC-MS/MS method for the determination of a kind of polypentosyl with polysulfonic groups in SD rat tissue homogenate; Chao Li 1; Fexue Wang 1; Li Fang 1; Peiyun An 1; Jinlian Liu 1; Zhiyu Li 1; Yi Tao 1; Liang Shen 1; 1Wuxi AppTec, Shanghai, China

TP 724 Waters RADIANTM ASAP Probe: Industrial Application of a ASAP Direct Mass Detector and a UHR-MS ASAP; Janece Potter 1; Junho Jeon 1; Anthony Gies 1; Bryan Katzenmeyer 1; 1Dow, Inc., Lake Jackson, TX; 2Waters Corporation, Milford, MA

TP 725 NP-SIMS as a tool for evaluating the homogeneity of extreme-ultraviolet resists; Jander Cruz 1; Stanislav Verkhoturov 2; Emile A. Schweikert 2; Michael Eitter 2; 1California State University Northridge, Northridge, CA; 2Texas A&M University, College Station, TX

TP 726 High throughput mass spectrometry-based metabolomics reveal nanoplastics-induced mitochondrial dysfunction in normal human-derived cells; Lin Sui 1, 2, Zongwei Cai 1; Chunmiao Zhang 1; 1State Key Laboratory of Environmental and Biological Analysis, Hong Kong Baptist University, Hong Kong, Hong Kong SAR, China, Hong Kong, China; 2Department of Chemistry, Hong Kong Baptist University, Hong Kong, China; 3State Environmental Protection Key Laboratory of Integrated Surface Water-Groundwater Pollution Control, School of Environmental Science and Engineering, Southern University of Science and Technology, Shenzhen, China; 4EIT Institute for Advanced Study, Ningbo, China

TP 727 LC-MRM Analysis Reveals Improved In Vivo Stability of SMARTag® Tandem-Cleavage MMAE Antibody-Drug Conjugates as Compared to Vedotin Conjugates; Dominick Y Ye 1; Reji N Nair 1; Ayodile O Ogunkoya 1; Xiao Ca 1; Stepan Chuprakov 2; Robyn M Barfield 2; Maxine Baozun 2; Tiffany Unsalung 2; Jesus Aguilar 2; Thomas Linz 2; Jia Yang 1; Fangjiu Zhang 1; Alyssa G Occiano 1; Dhamaraj Samuel 1; Penelope M Drake 1; 1Catalent Pharma Solutions, Emeryville, CA

TP 728 Detection and quantitation of benzodiazepines in less than 3 min using Probe Electrospray Ionization mass spectrometry and isotope dilution approach; Pauline Griffeuille 1; Sylvain Dulaurent 1; Souleiman El Balkhi 2; Stephane Moreau 2; Franck Saint-Marcoux 2; 1NHIM, Limoges, Limoges, France; 2SHIMADZU Europe, Cugnaux, France

TP 729 Harmful textile chemicals - Investigation of dermal uptake and peptide modifications in reconstructed human epidermis; Jesstine Carlson 1; Pablo Pardo Menacho 1; Conny Ostman 1; Ulrika Nilsson 1; 1Stockholm University, Stockholm, Sweden

TP 730 Modeling The Effect of Staphyloccocal Enterotoxin B on Cardiac, Epidermal and Lung Cells Utilizing Organ-on-a-Chip Methodology; Conor C Jenkins 1; Elizabeth Dhummakuppu 1; Gabrielle Rizzo 1; Allison Melka 1; Dylan Fudge 1; Tyler Goralski 2; 1U.S. Army DEVCOM CBC, APG; 2U.S. Army DEVCOM Chemical Biological Center, Aberdeen Proving Ground, MD; 3EXCT Incorporated, Edgewood, MD

TP 731 Drugs of abuse in hair: high speed and sensitivity demands for LC-MS/MS; Ichiro Hirano 1; Marcos Pudenzi 2; Luis Otavio Junqueira 2; Shimadzu do Brasil Comercio Ltda, Barueri, Brazil; 2Shimadzu do Brasil Comercio Ltda, Barueri, Brazil

TP 732 An Untargeted Workflow to Comprehensively Identify Drug-Related Adducts for Bioactivation Derisking in Drug Discovery and Development; Yu Feng 1; Ili Erdemir 1; Lei Zhu 1; Matthew Kuhls 1; Wen Kang 1; Nianyu Li 1; Raymond Gonzalez 1; Kara Pearson 1; 1Merck & Co., West Point, PA

TP 733 Investigating the fate of hazardous textile pollutants in a new process for chemical recycling of post-consumer garments; Tim Åström 1; Maria Ximena Ruiz Caldas 2; Ioannis Sadiktis 3; Ulrika Nilsson 3; Aji P Mathew 2; 1Stockholm University, Stockholm, Sweden; 2Stockholm University, Stockholm, Sweden
**WP 038** An ultra-sensitive and robust assay for an antibody-drug conjugate payload (paclitaxel) in human plasma using SLE–UPLC-MS/MS; Andy (hongfang) Xue1; Emily Williamson1,2; Daniel Skrocki3; Min Meng1,4; Aihua Liu1,4
1Alliance Pharma, Malvern, PA; 2Chongqing Medpharma Co. Ltd, Chongqing, China

**WP 039** LC-MS Characterization of Multi-Specific Antibodies; Jeremy Wolff1; Vera B. Ivleva1; Yile Li1; Melissa Resto1; Jason G. Gall1; Q. Paula Lei1; NIIH, Gaithersburg, MD

**WP 040** Conformation of Native Antibody-Drug Conjugate Charge Variants Revealed by Microchip Capillary Electrophoresis Coupled with Trapped Ion Mobility; Eli U. Larson1; Adi M Kulkarni2; Hampus Engstroem1; Erin Rodden2; Kate Yu3; Yue (hongfang) Xue1; Guillaume Tremintin1;2; Bruker Daltonics, San Jose, CA

**WP 041** Rapid identification of conjugation sites in antibody drug conjugates using Microchip Capillary Electrophoresis Coupled with Mass Spectrometry; Yue Liu1; Adi M Kulkarni1; Hampus Engstroem1; Erin Rodden2; Kate Yu3; Ying Ge1,4,5; 1Department of Chemistry, University of Wisconsin-Madison, Madison, WI; 2908 Devices, Inc., Boston, MA; 3Department of Cell and Regenerative Biology, University of Wisconsin - Madison, Madison, WI; 4Humain Proteomics Program, University of Wisconsin - Madison, Madison, WI; 5Bruker Daltonics, San Jose, CA

**WP 042** Analyses of chemical modifications in therapeutic antibodies by high resolution multi-turn TOF-MS system; Yusuke Tateishi1; Hiroyuki Miura1; Hiroko Morinaga1; Koichi Kimura2; Tetsuo Iida3; Junna Nakazono3; Masaru Nishiguchi1; Osamu Furuhashi1; Daiuse Okumura1; Yuki Yamaguchi1; Susumu Uchiyama1; SHIMADZU Corporation, Kyoto, Japan; 2Osaka University, Suita, Osaka, Japan

**WP 043** Improved intact antibody characterization with a new ion source design; Kilian Mayr1; Daniel Jajcic2; Lauren Stempfl1; Christian Albers1; Dodge Baluya4; José Bonfiglio5; Rebekka Kroiter2; Annette Vogt1; Roche Diagnostics GmbH, Penzberg, Germany; 2Bruker Daltonik GmbH, Bremen, Germany; 3Bruker Scientific, San Jose, CA

**WP 044** Implementation of Multi-Attribute Method in the context of continuous biopharmaceutical manufacturing: from clone selection to analytical support in GxP runs; Mélanie Jakobczyk; Merck KGaA, Darmstadt, Germany; 2Corser-Sur-Vevey, Switzerland

**WP 045** Investigation of drug-to-antibody ratio for FORCE oligonucleotide conjugates using Microchip CE-MS; Benjamin F. Vieira1; Aditya Kulkarni2; Kate Yu3; Peiyi Shen4; Min Meng1,4; Timothy Weeden3; Dyno Therapeutics, Inc., Waltham, MA; 2908 Devices, Inc., Boston, MA

**WP 046** Structural Characterization of Biopharmaceutical Proteins using Ion-Mobility and Collision Induced Unfolding; Ine F. Parson1; Hunter Walker1; Greg Adams1; FUDJ/FILM Biosynths Biotechnologies USA, Morrisville, NC

**WP 047** Sensitive bioanalysis of galactosylphosphoglycerol (GalSPH) and glucosylphosphoglycerol (GluSPH) in cerebral spinal fluid; Kean Woodmansey1; Jack Steed2; Jessica Smith1; Freddy Gostebri1; Jianru Stahl3; Michel Zerah4; Jerome Larghero5; Jean-Marie Husa5; Stefan Segal6; Ruocci8; Hyacinthe, QC; 2University of British Columbia, Vancouver, Canada; 4German Center for Neurodegenerative Diseases (DZNE), Munich, Germany; 3Neuroproteomics, School of Medicine, Klinikum Rechts der Isar, Technische Universität München, Munich, Germany; 5Proteomics Platform Necker, Paris, France; 6Department of Pediatrics, University of Lorraine, Nancy, France; 7Department of Immunology, University of Lorraine, Nancy, France; 8Division of Experimental Medicine, Roswell Park Comprehensive Cancer Center, Buffalo, NY

**WP 048** 5-Lipoxygenase Clinical Biomarker Method Development – Overcoming Selectivity, Stability, and Reagent Resourcing Challenges; Lu Yang1; John Meissen1; Elke Franssen1; Anton I. Rosenbaum1; 1Integrated Bioanalysis, Clinical Pharmacology, Safety Sciences R&D, AstraZeneca, South San Francisco, CA, 2Translational Medicine, Respiratory & Immunology, BioPharmaceuticals R&D, AstraZeneca, Cambridge, United Kingdom

**WP 049** Improvement in quantitation targeting 270 human plasma proteins by MRM/MS with stable-isotope labelled internal standards when automated nanoparticle fractionation I; Claudia Gaither1,2; Robert Popo1; Aaron S. Gajadhar2; Paul Pease3; Lucy Williamson4; Asim Siddiqui4; Christoph H. Borchers5, 6, 7; 1MRM Proteomics Inc., Montréal, QC; 2Département de Biomédecine Vétéranire, Faculté de Médecine Vétéranire, Université de Montréal, Saint-Hyacinthe, QC; 3Seer Inc., Redwood City, CA; 4Seer, Inc., Redwood City, CA; 5Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montréal, QC; 6Gerald Bronman Department of Oncology, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; 7Division of Experimental Medicine, McGill University, Montreal, QC

**WP 050** Quantitative GI-MS Analysis of High-Density Lipoproteins in Alzheimer’s Disease using LC-MS/MS; Armin Oloumi1; Brian Hong1; Yasmine Bouchibit1; Michael Russell S. Alvarez2; Angela M. Zivkovic3; Carlito B. Lebrilla1; 1UC Davis, Davis, CA

**WP 051** A stringently controlled, LC-MS-based strategy to procure intrastitial fluid with minimal intra-cellular contamination from tissues; Min Meng1; Yue (hongfang) Xue1; Minh Trinh1; Shichen Shen1; Ming Zhang2; Jun Qiu1,2; 1University at Buffalo, Buffalo, NY; 2Roswell Park Comprehensive Cancer Center, Buffalo, NY

**WP 052** Advancements in supercritical fluid chromatography-mass spectrometry expand the horizons for the analysis of smaller molecules in complex samples; Kumari Ubhayasekera1; Jonas Bergquist1; Uppsala University, Uppsala, Sweden; 2Uppsala University, Uppsala, Sweden

**WP 053** LC-MS/MS quantification of pTau217 using sepcific immunocapture in the context of Alzheimer’s disease; Florine Leipp1; Sylvain Lehmann2; Christoph Hirtz2,3; Jerome Vialaret1; Shimadzu France, Noisiel, France; 1IRM-B-PPC, INM, CHU Montpellier, INSERM CNRS, 2IRMBB-PPC, INM, CHU Montpellier, INSERM CNRS, 3Hôpital Eurex, CHU, CHU Montpellier, INSERM CNRS

**WP 054** Proteomic analysis of amniotic fluid from Myelomeningocele fetuses unveils specific upregulation of nervous system development key proteins; Lucie Guilhaud1,2; Kevin Roger1; Andree Schmidt1; Cenna Chhuon4; Stefan Breimann5; Joanna Lipecka1; Sophie Dreux4; Mueller Stefan1,5; Michel Zerah4; Jerome Larghero5; Jean-Marie Husa5; Stefan Segal6; Chiara Guerrera1; Sorbonne University, Department of Fetal Medicine, AP-HP, Armand Trousseau Hospital, DMU ORIGYNE, National Reference Center for Rare Disease: Vertebral and Spinal Cord Anomalies (MAVEM Center), Paris, France; 2Paris University, Stem Cell Biotechnologies Unit, INSERM U376, CIC-BT CBT01, AP-HP, Saint-Louis Hospital, Paris, France; 3Proteomics Platform Necker, Paris, France; 4German Center for Neurodegenerative Diseases (DZNE), Munich, Germany; 5Neuroproteomics, School of Medicine, Klinikum Rechts der Isar, Technische Universität München, Munich, Germany; 6Proteomics Platform Necker, Paris, France; 7Proteomics Platform Necker, Paris, France; 8Paris University, Biochemistry-Endocrinology, AP-HP, Robert Debré Hospital, Paris, France; 9Paris University, Department of Pediatric Neurosurgery, AP-HP, Hôpital Necker-Enfants Malades, Paris University, Paris, France

**WP 055** The mucin selective protease StcE improves proteomic profiling of mucin containing human airway samples enhancing biomarker discovery in respiratory disease; Lisa H. Cazares1; Raghotama Chakrabarti1; Ching-Yun Chang1; Abby J. Chiang1; Helen Killick2; Jessica Holmén Larsson2; Ian Christopher Scott2; Sonja Hess1
WP 056 Absolute quantification of plasma biomarkers to validate the first blood-based diagnosis of the silent phase of Alzheimer’s Disease. Antoine Berthemy1; Maud Heuillet2; Aude Dupuy-Gayral3; Eric Haudebourg3; Catherine Pech4; Benoît Soucet5; Alkéos Michail6; Baptiste Bilior7; Jérôme Braudeau8; François Autelitano9; 1ÉVOTEC, Toulouse, France; 2Agent, Paris, France

WP 057 Development and evaluation of a rapid LC-MS/MS quantitation method for the measurement of reactive aldehydes in biological samples. Yuyan Jian1; Yulemin Han2; Anh Tran3; Jade W. Jones4; 1University of Maryland, School of Pharmacy, Baltimore, MD

WP 058 Development of biomarkers for the delayed effects of acute radiation exposure: evaluation of diagnostic, predictive, and pharmacodynamic utility. Swaminath Pandey1; Nageswara Pili2; William Temple Andrews3; Ludovic Muller4; Maureen Kane5; 1University of Maryland, School of Pharmacy, Baltimore, MD

WP 059 Enhanced LC-MS Analysis of Volatile Organic Compound Metabolites in Wastewater. David Hoekker1; Zhengxi Xie1; Pawel Lorkiewicz2; Ted Smith3; Sanjay Srivastava4; 1Christina Lee Brown Environ Institute, University of Louisville, Louisville, KY; 2Center for Healthy Air Water Soil, University of Louisville, Louisville, KY; 3Superfund Research Center, University of Louisville, Louisville, KY

WP 060 Herding PCATs: Development of a Robust, High-Throughput Method for Quantification of Native Plasma Catecholamines by LC-MS/MS. Stacy Dee1; Christopher M. Shuford1; Russell P Grant1; 1LabCorp, Burlington, NC

WP 061 Highly sensitive analysis using EVOSEP-LC/MS assay for targeted PD-L1 and PD1 expression level for predicting response to immune checkpoint inhibitors. Shane Kamik1; Matthew Hartlie1; Melodie Boute2; Richard Rue2; Corinne Ramos2; 1Pyxant Labs, Inc., Colorado Springs, CO; 2ImaBiotech, Loos, France

WP 062 Isotyping Anti-Drug Antibodies using LC-MS/MS QTOF quantification of SIL peptides. Christian I. Ruse1; Ashish Vaswani1; Carl Luongo1; Hannah Zhang1; Srijan Gandy2; Mathew Digby3; Jason Delcarpini4; Darshana Jani5; Ling Morgan6; Serenus Hua7; 1Modern Therapeutics, Cambridge, MA

WP 063 Online Enrichment of Low-Abundance Protein Biomarkers for Targeted LC-MS. Nathaniel B. Axtell1; Thuy Truong1; Alex Butters2; Jeffrey R. Whiteaker3; Lei Zhao4; Amanda G. Paulovich5; Ryan T. Kelly6; 1BYU, Provo, UT; 2Fred Hutchinson Cancer Center, Seattle, WA

WP 064 Proteomic Profiling of Irradiation-Induced Skin Fibrosis and its modulation by Low Molecular Weight Fucoidan. Pang-Hung Hsu1; National Taiwan Ocean University, Keelung, Taiwan

WP 065 Qualitative Analysis of Protein Ions Based in Isotopic Pattern Distortions. Snehin R. Momin1; Touradj Solouki1; 1University of Louisville, Louisville, KY

WP 066 The Detection and Quantitation of Stercobilin in Autism Model Fecal Extracts Using LC-MS; Erin R. Tiede1; Emily R. Sekera2; Troy D. Wood2; 1University at Buffalo, Buffalo, NY; 2The Ohio State University, Columbus, OH

WP 067 timsTOF HT improves protein identification and quantitative reproducibility for deep unbiased plasma protein biomarker discovery. Diiana Vital1; Wan-Fang Chou1; Mark Marisipi1; Sai RamaNamy1; Sara Nouri Golmaei1; Yuntao Hu1; Joong Yong-Lee1; Megan Mora1; Jessica Chan1; Guillermo Flores-Campanuzo2; John Blume1; Chinmaya Behlangdy2; Manway Liu1; Philip Ma1; Bruce Wilcox1; 1PrognomiQ, San Mateo, CA; 2Switch Therapeutics Inc., San Francisco, CA

WP 068 Using a Specific Antibody for the Immunocapture LC-MS/MS Assay of the Biomarker, Troponin Fast (TNNI2). Shane Needham1; Mitch Johnson1; Colt Cookson1; 1AstraZeneca R&D, Gaithersburg, Maryland; 2AstraZeneca, Cambridge, United Kingdom

WP 069 Mapping of the Human Cell Metabolome Identifies Novel Cancer Therapeutic Targets in MYC-amplified Group 3 Medulloblastoma. William D Gwynne1; Yuin Suki2; Jeremy K Chan3; Stefan Custers2; Cunjie Zhang4; Andrew T Quail2; Chitra Venugopala5; Sheila K. Singh1; Rafael Montenegro-Burke1; 1Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, ON; 2Center for Discovery in Cancer Research, McMaster University, Hamilton, ON

WP 070 The Identification of the HLA Class I Immunopeptide of Malignant Peripheral Nerve Sheath Tumors via Mass Spectrometry. Kyle A Richards1; Suzanne Coleman1; Jessica Liebau1; Mitchell Hruska2; Tyler Jubelival1; Reid Wagner1; Subina Mehta2; David A Largassa2; 1Timothy J Griffin1; 2Masonic Cancer Center, Department of Pediatrics, University of Minnesota, Minneapolis, MN; 3Minnesota Supercomputing Institute, University of Minnesota, Minneapolis, MN; 4Biochemistry, Mol. Biology, and Biophysics, University of Minnesota, Minneapolis, MN

WP 071 Detecting impending infections in immunocompromised cancer patients. Sara Vlontane1; Ruben J. F. Ramos1; Hannah Lees2; Emma E. Rennier2; James S. Pyke3; Andrew D. McEachen3; 1Children’s Hospital of Wisconsin, Milwaukee, WI; 2Memorial Sloan Kettering Cancer Center, New York, NY; 3Agilent Technologies, Santa Clara, CA

WP 072 Multimicroscopy approach to elucidate the role of endoplasmic reticulum-mitochondria contact sites in tumor metabolic rewiring. Brandon Chen1; Pietro Morlacchi2; Costas Lyssiotis; Yatrik Shah1; 1University of Michigan-Ann Arbor, Ann Arbor, MI; 2Agilent Technologies, Lexington, MA

WP 073 Targeted proteomics for discovery of novel biomarkers in human plasma for early breast cancer diagnosis. Margret Thorsteinsdottir1; Kristrun Yr Holm1; Kari Aarnason1; Finnur Eiriksd1; Sigrídur Klara Bodvarsdottir1; Yassene Mohammed1; 1Faculty of Pharmaceutical Sciences, University of Iceland, Reykjavik, Iceland; 2BioMedical Center, University of Iceland, Reykjavik, Iceland; 3Leiden University Medical Center, Leiden, Netherlands; 4Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC

WP 074 Quantitative proteomic analysis of MCF10A cells with PTEN knockdown reveals the regulation of EphA2 and PTEN interaction. Kyle A Richards1; Costas Lyssiotis; Yatrik Shah1; 1 University of Michigan-Ann Arbor, Ann Arbor, MI; 2Agilent Technologies, Lexington, MA

WP 075 Identification of Cholesterol and Cholesterol Derivatives in Prostate Cancer Cell Lines using LC-MS/MS. David Hoetker1; Costas Lyssiotis; Yatrik Shah1; 1University of Michigan-Ann Arbor, Ann Arbor, MI; 2Agilent Technologies, Lexington, MA

WP 076 Mass spectrometry-based proteomic profiling of CB-5083 resistant colon cancer cells. Ting Yu Wang1; Feng Wang2; Shane Li1; Chai Foong Lai1; Tian Chen2; 1California Institute of Technology, Pasadena, CA

WP 077 Quantitative proteomic analysis of MCF10A cells with PTEN knockdown reveals the regulation of EphA2 expression by PTEN. Qiong Wang1; Hongming Song1; Li Wang1; Senthos Renuse1; Kiran Mangalaparthi1; Akhielsh Pandey1; Xinyan Wu1; 1Mayo Clinic, Rochester, MN; 2Thermo Fisher Scientific, San Diego, CA

WP 078 Comparative Proteomics studies of mono and co-cultured drug-resistant and -sensitive cancer cells. Lindsey Olsen1; Yuqing Dou1; Bing Zhang2; 1Lester and Sue Smith Breast Center, Baylor College of Medicine, Houston, TX; 2Department of Molecular and Human Genetics, Baylor College of Medicine, Houston, TX

WP 079 Computational discovery of protein isoforms associated with drug response in breast cancer. Lindsey Olsen; Yuqing Dou1; Bing Zhang2; 1Lester and Sue Smith Breast Center, Baylor College of Medicine, Houston, TX; 2Department of Molecular and Human Genetics, Baylor College of Medicine, Houston, TX
reveal potential interaction targets: Zongkai Peng1; Zhibo Yang1; Ahsan Nagib1,2; 1University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK; 2Mass Spectrometry, Proteomics and Metabolomics Core Facility, Stephenson Life Sciences Research Center, The University of Oklahoma, Norman, OK.

WP 081 Integrated Omics approaches to understand Pituitary Adenomas disease biology: Arghya Banerjee1; Sanjeeva Srivastava2; 1IIT Bombay, Mumbai, India

WP 082 Role of MGA3 and “Bisecting GlcNAc” N-glycans in TGF-β1 induced epithelial-mesenchymal transition (EMT) of lung adenocarcinoma: Wei Ge1; Soochow University, Suzhou, China

WP 083 Using lipidomics analysis to determine the metabolic impact of PIKFyve inhibition in Pancreatic Ductal Adenocarcinoma: Caleb Cheng1; Pietro Morlachchi2; Li Zhang1; Pete Sajawalukit1; Jasmine Wisniewski1; Bailey Jackson1; Yuanyuan Qiao1; Costas Lyssiotis1; Arul M Chinnaiyan3; 1Graduate Program in Cell and Molecular Biology, University of Michigan, Ann Arbor, Michigan; 2Agilent Technologies, Lexington, MA; 3School of Medicine, University of Michigan, Ann Arbor, Michigan; 4Doctoral Program In Cancer Biology, University of Michigan, Ann Arbor, Michigan; 5College of LSA, University of Michigan, Ann Arbor, Michigan; 6Michigan Center for Translational Pathology, Department of Pathology, University of Michigan, Ann Arbor, Michigan; 7Department of Molecular and Integrated Physiology, Department of Internal Medicine, University of Michigan, Ann Arbor, Michigan

WP 084 Initial Results from Mass Spectrometry Imaging of Tumor Heterogeneity driving differential fluorescence of Organotypic Breast Cancer Spheroids Using LC-MS/MS: Ramisa Farinha1; Zahra Ahmed1; Jad Hamze1; Emma Rothkopf1; 1Brown University, Providence, RI

WP 085 Top down proteomics reveals histone H2A C-terminal truncations as potential modulators of DNA damage and cell proliferation in cancer: Faith Joseph1; Nicolas Leon Young2,3; 1baylor college of medicine, houston, TX; 2Verna & Mams Mclean Department of Biochemistry & Molecular Biology, Baylor College of Medicine, Houston, TX; 3Department of Molecular Cellular Biology, Baylor College of Medicine, Houston, TX

WP 086 Tumor intrinsic metabolic effects associated with inhibition of PARP7 in a lung cancer cellular model: Jennifer R Molina1; Pietro Morlachchi2; Jefferey Song3; Sonal Gera3; 1Ribon Therapeutics, Cambridge, Massachusetts; 2Agilent Technologies, Lexington, MA

WP 087 Integrated proteomics and metabolomics reveal an association between NFR2-mediated upregulation of KYNU and tumor immunosuppression and poor prognosis: Ricardo A Leon Letetier1; Ali Hussein Abdel Sater1; Yihui Chen1; Ranran Wu1; Jennifer B Dennison1; Soyoung Park1; Ehsan Irajizad1; Hiroyuki Katayama1; Jody Vykoukal1; Samir M Hanash1; Edwin J Ostrin1; Johannes Kahr1; 1MD Anderson Cancer Center, Houston, TX

WP 088 Integrative Single-Organoid Proteomics in 3D Models of Ovarian Cancer Uncovers Remodeled Mitochondria-ER Contacts and Bioenergetics: Krystal K Lum1; Oscar Pundel1; William A Hofstadter1; John Muroski2; 1University of Oklahoma, Department of Neurosurgery, University of Oklahoma, Norman, OK; 2MD Anderson Cancer Center, Houston, TX

WP 089 Regulation of the FKBP10 transcriptional locus in lung metastasis: Ryan Rivas1; Alexander B Saltzman1; Doug Chan1; Anna Malovannaya1; 1Baylor College of Medicine, Houston, Texas; 2MD Anderson, Houston, TX

WP 090 Proteomics investigation of gliomas resected after S-ALA fluorescence guided surgery reveals molecular heterogeneity driving differential fluorescence: Saicharan Ghat1; Amruth Molyadi2,4; Shridhar Epari1,4; Sanjeeva Srivastava2; 1Centre for Research in Nano Technology and Science, Indian Institute of Technology Bombay, Mumbai, India; 2Centre for BioSystems Science and Engineering, Indian Institute of Science, Bengaluru, India; 3Department of Neurosurgery, Tata Memorial Centre’s – Advanced Centre for Treatment, Research and Education in Cancer, Navi Mumbai, India; 4Homi Bhabha National Institute, Mumbai, India; 5Department of Biosciences and Bioengineering, Indian Institute of Technology Bombay, Mumbai, India

WP 091 INFLUENCE OF MDR (MULTIDRUG RESISTANCE) AND CELLCELL INTERACTIONS ON DRUG UPTAKE OF SPHEROIDS: Amit Singh1; Zongkai Peng1; Zhibo Yang1; Anthony Burgett1; 1University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK; 2The University Of Oklahoma Health Sciences Center, College of Pharmacy, Oklahoma City, OK

WP 092 Assessing the Impact of Paclitaxel Absorption by 3D Breast Cancer Spheroids Using LC-MS/MS: Ramisa Farinha1; Zahra Ahmed1; Jad Hamze1; Emma Rothkopf1; 1Brown University, Providence, RI

WP 093 Identification of metabolic pathways driven by SMARCB1 deficiency in bladder cancer: Chandra Sekhar Amara1; Abu Hena Mostafa Kamal1; Danthasinghe Waduge Badrachara Priyaratna1; Arun Sreekumar1; Msaouel Pavlos1; Nagireddy Puttur1; 1Baylor College of Medicine, Houston, Texas; 2MD Anderson, Houston, TX

WP 094 Identification of angiogenesis and mitochondrial metabolism in bladder cancer disparity: Karthik Reddy Kamreddy1; Junhyoung Park1; Vasanta Puttur1; Danthasinghe Waduge Badrachara Priyaratna1; Martha K Teriss1; Seth P Lerner1; Yair Lotan1; Benny Abraham Kapparettu1; Nagireddy Puttur1; 1Baylor College of Medicine, Houston, Texas; 2Augusta University, Augusta, Georgia; 3UT Southwestern Medical Center, Dallas, Texas

WP 095 LC-MS method to measure the D- and L- L2Hydroxyglutarate in Cerebrospinal Fluid: Satwikreddy Puttur1; Abu Hena Mostafa Kamal1; Leomar Y Ballester1; 1University of Texas MD Anderson Cancer Center, Houston, TX; 2Baylor College of Medicine, Houston, Texas; 3MD Anderson, Houston, TX

WP 096 Application of the MassSpec Pen Technology for Molecular Identification of Human Sarcomas and Surgical Margin Evaluation: Ashley E. Montgomery1; Justin E. Bird1; Douglas Fletcher2; Sharon Landers2; Sintawat Wangsiricharoen1; Wei-Lien Wang4; Wendonng Yu4; Livia S. Eberlin3; Keila E. Torres3; 1Baylor College of Medicine, Department of Student Affairs, Houston, Texas; 2MD Anderson Cancer Center, Division of Surgery, Department of Orthopedics, Houston, Texas; 3Baylor College of Medicine, Houston, Texas; 4The University of Texas MD Anderson Cancer Center, Division of Surgery, Department of Surgical Oncology, Houston, Texas; 5MD Anderson Cancer Center, Division of Pathology Lab-Medicine, Department of Pathology, Houston, Texas; 6Baylor College of Medicine, Division of Surgical Oncology, Michael E DeBakey Department of Surgery, Houston, Texas

WP 097 Probing the Biosynthetic Pathway of Heparin Sulfate Using Capillary Electrophoresis Zone Mass Spectrometry: Jandi Kim1; Neil G. Patel1,2; Ryan Joseph Weiss1,2; 1I. Jonathan Amster1; 1University of Georgia, Athens, GA; 2Complex Carbohydrate Research Center, Athens, GA

WP 098 Does The Chemistry of Glycosidic Bond Cleavage Vary? Joy Namachchivaya1; Lauren Schultz2; Lauren Davis1; Dylan Carter2; Benjamin Bythell2; 1Ohio University, Athens, OH; 2Ohio University, Athens, OH

WP 099 Combined Tandem Mass Spectrometry and Computational Chemistry for Structural Elucidation of Singly and Doubly Deprotonated Galacturonaric Acids: Ola Bataineh1; Jordan Rabus1; Rebecca Flinchbaugh1; Dylan Carter1; Lauren Davis1; Benjamin Bythell2; 1Ohio University, Athens, OH; 2Ohio University, Athens, OH
WP 101 Mass Spectrometry-based High-throughput Profiling of Porcine Notochordal-Cell Matrixglycans Using GlycanExplorer™ Software: Rupanjana Goswami¹, Kieran Joyce¹, Büşra Güney², Melanie Ng Tung Hing³,⁴, Cailtornia Walsh³, Tara Schmitz⁴, Marianna Tryfonidou⁴, Keita Ito⁴, Karthik Kollι, Abhay Pandit³, Radka Saldova¹,³,²,⁴, Arun Apte³,¹, PREMIER Biosoft, San Francisco, CA; ²CURAM, SFI Research Centre for Medical Devices, National University of Ireland, Galway, Galway, Ireland; ³GlycoScience group, National Institute for Bioprocessing Research and Training (NIBRT), Dublin, Ireland; ⁴UCD School of Medicine, College of Health and Agricultural Science, University College Dublin, Dublin, Ireland; ¹Contract Research group, National Institute for Bioprocessing Research and Training (NIBRT), Dublin, Ireland; ²Orthopaedic Biomechanics, Department of Biomedical Engineering, Eindhoven University of Technology, Eindhoven, Eindhoven, Netherlands; ³Department of Clinical Sciences, Faculty of Veterinary Medicine, Utrecht University, Utrecht, Netherlands

WP 102 Adduct Activity of Sheath Liquid CE-MS Interface Depends on the Sheath Liquid Glycan Content for Glycosaminoglycans: Jonathan Choi¹,²; I. Jonathan Amster³,⁴; Jandi Kim¹,²; University of Georgia, Athens, GA

WP 103 Characterizing degradation products from Bacteroides thetaotaomicron to understand bacterial dextran utilization in the gut: Neil Gregory Rumachik¹,²; Tian Tian¹,²; Hannah Gibson¹,²; David Boliam¹,²; Yan Liu¹,²; Fiona Cuskin¹,²; Thermo Fisher Scientific, Sunnyvale, CA; ³Newcastle University, Newcastle upon Tyne, United Kingdom; ⁴Forysth Institute, Cambridge, Massachusetts; ¹University of Pennsylvania School of Veterinary Medicine, Philadelphia, Pennsylvania

WP 104 Analysis of Chondroitin Sulfate Oligosaccharides in cartilage with mucopolysaccharidosis VII using Capillary Zone Electrophoresis–Fourier Transform Ion cyclotron Resonance Mass Spectrometry: Elijah T. Roberts¹,²; Jandi Kim¹,²; Stephanie Archer¹,²; Jonathan Amster¹,²; Zilu Ye¹,²; Walter and Eliza Hall Institute of Medical Research, Parkville, Melbourne, Australia; ¹Department of Medical Biology, University of Melbourne, Parkville, Melbourne, Australia; ²Faculty of Faculty Health and Medical Sciences, The University of Adelaide, Adelaide, Australia

WP 105 Isomeric Separation of Permethylated Glysans using LC-FAIMS-MS/MS: Md Abdul Hakim¹; Akem Adegben Sanni¹; Wazilha Purba¹; Oluwatosin Daramola¹; Yehia Mechref¹; ¹Texas Tech University, Lubbock, TX

WP 106 Isomeric separation of native N-glycans using nano ZIC-HILIC column: Oluwatosin E Daramola¹; Cristian D Gutierrez-Reyes¹; Judith Ntwalo¹; Mobijola Fowowe¹; Sherifdeen Onigbindin¹; Yehia Mechref¹; ¹Texas Tech University, Lubbock, TX

WP 107 HCD, ETD, and ETHCD Fragmentation Spectra of Co2+-Adducted Human Milk Oligosaccharides Distinguish Linkage Isomers: Sebastian N Alberti¹; Darren Gass³; Elyssia S. Gallagher¹; ¹ Baylor University, Waco, TX

WP 108 Comprehensive Characterization of Functional Polysaccharides derived from Marine Algae: Dae Sik Cha¹,²; Sol Kim¹,²; Hong Ju Kim¹,²; Nari Seo¹,²; Hyun Joo An¹,²; ¹Graduate School of Analytical Science and Technology, Chugnang National University, South Korea; ²Asia-Pacific Glycomics Reference Site, Daejeon, South Korea

WP 109 Mass spectrometry-based characterization of native and aging-modified polysaccharides for natural gums identification in complex formulations: Marie Tammine¹,²; Hanane Termoul¹; Stéphanie Flament¹; Fabrice Bray¹; Christian Rolando¹,³; ³UAR CNRS 3290 - MSAP, Villeneuve d'ascq, France; ²Lesaffre International - R&D analytical department, Marquette-Lez-Lille, France; ³Shenking Sixties - 1-3 Allée Lavoisier, Villeneuve d'Ascq, France

WP 110 Structural and compositional characterization of dissolved hemicellulose with 12-T ESI FT-ICR in positive and negative ion modes: Mikko nikunen¹; Timo Kekäläinen¹; Janne Jänis¹; ¹University of Eastern Finland, Department of Chemistry, Joensuu, Finland

WP 111 Sensitive Analysis and Differentiation of Oligosaccharides Isomers by Direct Infusion Mass Spectrometry: Enoch Amoah¹; Abraham Kwame Badu-Tawiah¹; ¹The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH; ²The Ohio State University, Columbus, OH

WP 112 Developing Novel capillary electrophoresis tandem mass spectrometry strategies for the characterization of complex mixture Heparan sulfates: Yeqing Zhang¹,²; Jonathan Amster¹; ¹University of Georgia, Department of Chemistry, Athens, GA; ²University of Georgia, Athens, GA

WP 113 Optimization of SIM LC/MS Method for glycosaminoglycan Disaccharide Profiling in C. Elegans: Lauren Heidenreich¹; Franklin E. Leach Ill¹; ¹University of Georgia, Athens, GA

WP 114 Quantitation of glycosaminoglycans expression in cancer cells by 2-aminoacridone–labeled disaccharides with LC-MS/MS analysis: Fu-An Li¹; Yu-Shing Cheng¹; ¹Institute of Biomedical Sciences, Academia Sinica, Taipei, Taiwan

WP 115 A Novel LC-MS/MS Approach for Identification and Quantification for Hexosamine-Phosphates and Differentiate GlmS Regulation Between Staphylococcus aureus and Enterococcus faecium: Nitish R. Mishra¹,²; William G. Gutheli¹; ¹University of Missouri-Kansas City, Kansas City, MO

WP 116 A window of optimisation: optimising diAPEF approaches for liquid biopsy proteomics for a large-scale clinical cohort: Samantha J Emery-Corbin¹,²; Megan Penno¹,³; Jamuna M Yousuf¹,³; Vineet Vaibhav¹,³; Helena Oakley¹; Jennifer J Couper²; Leonard C Harrison²; John M Wentworth²,³,⁴; Toby Dito²,³; Andrew I Webb³,⁴; Laura F Dagley¹,²; ¹Advanced Technology and Biology Division, The Walter and Eliza Hall Institute of Medical Research, Parkville, Melbourne, Australia; ²Department of Medical Biology, University of Melbourne, Parkville, Melbourne, Australia; ³Faculty of Faculty Health and Medical Sciences, The University of Adelaide, Adelaide, Australia; ⁴Population Health Division, The Walter and Eliza Hall Institute of Medical Research, Parkville, Melbourne, Australia

WP 117 Fast multi-shot acquisition of comprehensive proteomes by DIA using narrow isolation windows on a novel high-resolution accurate mass LC-MS platform: Ulises Hernandez Guzman¹; Ana Martinez Del Val¹; Akeem Adegben Sanni¹; Wazilha Purba¹; Oluwatosin Daramola¹; Yehia Mechref¹; ¹Texas Tech University, Lubbock, TX

WP 118 Robust, Precise and Deep Proteome Profiling Using a Small Mass Range and Narrow Window Data-Independent Acquisition Scheme: Klemens Fröhlich¹,²; Christian Schori¹;²; Regula Furrer¹;²; Alexander Schmidt¹;²; ¹Proteomics Core Facility, University of Basel, Basel, Switzerland; ²Biozentrum, University of Basel, Basel, Switzerland

WP 119 midia-PASEF maximizes information content in data-independent acquisition proteomics and uses machine learning based-deconvolution to generate DDA quality spectra: Ute Distler¹; Mateusz Krzyztof Łącki¹; Michał
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### Additional Information:

- **WP 120**
  - Benchmarking commonly used software suites and analysis workflows for DIA proteomics and phosphoproteomics: A head-to-head comparison using a high-resolution mass spectrometer for DDA-like specificity from DIA data. Authors: Piotr Startek, David Teschner, Sven Brehmer, Jens Decker, Thilo Schild, Jonathan Krieger, Florian Krohs, Oliver Raether, Andreas Hildebrandt, Stefan Tenzer.
  - Department of Immunology, University of California, Riverside, Riverside, CA; 2Department of Biochemistry, University of British Columbia, Vancouver, BC

- **WP 121**
  - Cross-lab Evaluation of Quality Control for Large-scale Data-Independent Acquisition-based quantitative proteomics. Authors: Gaozhuanhuan Gao, He Wang, Yantao Li, Zhongxian He, Boston, MA; 2Boston Children's Hospital, Harvard Medical School, Boston, MA; 3Program and Precision Vaccines Program, Boston Children's Hospital, Harvard Medical School, Boston, MA

- **WP 122**
  - The synchro-PASEF scan mode on a TIMS-qTOF mass spectrometer for DDA-like specificity from DIA data. Authors: Patricia Skowronek, Georg Wallmann, Maria Wahle, Ericka C. M. Itagaki, Polina Koval, Marvin Thielert, Florian Krohs, Markus Lubeck, Sander Willems, Oliver Raether.
  - Max Planck Institute of Biochemistry, Martinsried, Germany; 2Bruker Daltonics GmbH & Co.KG, Bremen, Germany; 3Novo Nordisk Foundation Center for Protein Research, Copenhagen, Denmark

- **WP 123**
  - Multiplexed data-independent acquisition (DIA) using a novel high-resolution accurate mass spectrometer: A rapid and efficient approach for the comprehensive analysis of complex biological samples. Authors: Sophia Steigerwald, Wen-qing Shui, Min Tian, Piotr Startek, Hanno Steen, Jonathan Krieger.
  - University of California, Riverside, Riverside, CA; 2Department of Biochemistry, University of British Columbia, Vancouver, BC

- **WP 124**

- **WP 125**
  - Department of Pathology, Boston Children’s Hospital, Harvard Medical School, Boston, MA; 2Neurobiology Program and Precision Vaccines Program, Boston Children’s Hospital, Harvard Medical School, Boston, MA

- **WP 126**
  - Rapid and integrated proteome and lipidome analysis of mouse livers using Multi-Omic Single-Shot Technology and Data Independent Acquisition. Authors: Margaret Lea Robinson, Yuchen He, Evgenia Shishkova, Katherine A Overmyer, Joshua J. Goon, University of Wisconsin, Madison, WI; 2University of Wisconsin-Madison, Madison, WI; 3Morgridge Institute for Research, Madison, WI

- **WP 127**
  - Deciphering the molecular pathway driving cell competition using DIA label-free mass spectrometry. Authors: Suniya Khatun, Riccardo Zenenzi, Chiozzi, Manasi Kelker, Guillem Lowe, Konstantinos Thalassinos, Department of Structural and Molecular Biology - UCL, London, United Kingdom; 2Department of Structural and Molecular Biology - UCL, London, United Kingdom

- **WP 128**
  - Data-independent acquisition leverages untargeted proteomics in microbes to quantify both engineered and endogenous protein abundances. Authors: John Murosk, Gabriel Navarro, Mona Elsadawi, Amyris, Emeryville, CA

- **WP 129**
  - Optimizing dia-PASEF isolation window schemes for proteomics measurements on a timsTOF instrument. Authors: Markus Lubeck, Stephanie Kaspar-Schoenfeld, Christoph Krisp, Andreas Schmidt, Florian Busch, Eduardo Carrascosa, Oliver Raether, Gary Kruppa, Bruker Daltonics GmbH & Co.KG, Bremen, Germany; 3Bruker S.R.O., Bremen, Germany

- **WP 130**
  - Integrating permethylation and Zeno SWATH method to characterize nucleic acid modifications. Authors: Yixuan (axe) Xie, Ye Chen, Francisca N De Luna Vitorino, Zongtai Lin, Xingyu Liu, Emily Zahn, Arabella Garcia, Benjamin A. Garcia, Washington University in St. Louis, St. Louis, MO

- **WP 131**

- **WP 132**
  - Data-Independent Analysis of Human Eye Lens Proteome Reveals New Sites of Aspartic Acid Isomerization. Authors: Evan E. Hubbard, Yana Lyon, Ryan R. Julian, University of California, Riverside, Riverside, CA; 2Inhibix Inc., La Jolla, 92037, 3University of California Riverside, Riverside, CA

- **WP 133**

- **WP 134**
  - Application of advanced targeted MS and long-read RNA-seq for proteogenomic discovery and expanded detection of alternative protein isoforms. Authors: Saurabh Bandyopadhyay, Eri D. Jeffery, Robert A. Schmutz, Ben Jordan, Gloria Sheynkman, Department of Molecular Physiology and Biological Physics, University of Virginia, Charlottesville, Virginia, USA, Charlottesville, VA; 2Division of Molecular Medicine, University of Virginia, Charlottesville, VA; 3Department of Cell Biology, Harvard Medical School, Boston, MA, USA, Boston, MA; 4Cancer Genomics Research Laboratory, Frederick National Laboratory for Cancer Research, Frederick, MS USA, Frederick, MD; 5Department of Biochemistry and Molecular Genetics, University of Virginia, Charlottesville, VA, USA, Charlottesville, VA; 6Center for Public Health Genomics, University of Virginia, Charlottesville, VA, USA, Charlottesville, VA; 7UVA Comprehensive Cancer Center, University of Virginia, Charlottesville, VA, USA, Charlottesville, VA

- **WP 135**
  - Optimization and evaluation of precursor isolation schemes in midiaPASEF acquisition mode. Authors: Ute Distler, Mateusz Krzysztof Łącki, Michal Piotr Starpek, David Teschner, Jonathan Krieger, Florian Krohs, Oliver Raether, Stefan Tenzer, Institute for Immunology, University Medical Center of the Johannes-Gutenberg University Mainz, Germany; 2Faculty of Medicine, Mathematics, Informatics, and Mechanics, University of Warsaw, Warsaw, Poland; 3Institute for Informatics,
WP 136  Doing More With Less: Addressing The MicroSampling Sensitivity Challenge in DMPK Studies Using Vacuum Jacketed Column UHPLC-cycloidal Ion Mobility MS; Robert Plumb1; Andrew Leightner1; Ian D Wilson2; Billy J Molly3; Russell Morttishe-Smith4; 1Waters, Milford, MA; 2Imperial College, London, United Kingdom; 3Waters Corporation, Wilmslow, United Kingdom

WP 137  Ultra-High Throughput Metabolic Stability Assay using Acoustic Ejection Mass Spectrometry; Jacob Watson McCabe1; Anuja Bhalkikar1; Han Joo Lee1; 1SCIEX, Framingham, MA

WP 138  Assessment of Chromatographic Performance in High-Throughput ADMET Screening; Carson Powell1; John Janiszewski1; Ross Wallace1; 1Lavo Oncology, Louisville, CO

WP 139  Improving the workflow of pharmacokinetic study of herbal medicines. Cudrania tricuspidata leaf extracts, using molecular networking; Jeong In Seo1;2; Hye Hyun Yoo1; Hanyang University, Ansan, South Korea; 1Brigham and Women’s Hospital, Boston, MA

WP 140  Automated workflow to study microsomal clearance and analysis of metabolites using collision-induced dissociation and electron-activated dissociation MS/MS; Bahar Rezvi1; Rahul Baghia2; Eshani Nandita3; 1Sciex, Framingham, MA; 2SCIEX, Redwood City, CA

WP 141  An efficient permeability screening flow using LC-MS/MS based PAMPA assay followed by MDCK assay of selected compounds; Yongjinyang Jiang1; Phuong Nguyen1; Quanynan Alan Xu1; Qi Wu1; Thomas Quill1; 1University of Texas MD Anderson Cancer Center, Houston, TX

WP 142  Metabolite profiling and characterization byon mobility LC-timsTOF Pro PASEF; Xuejun Peng1; Surendar Tadi1; Beiki Wang1; Erica Forsberg1; 1Bruker Daltonics Inc., San Jose, CA; 2Bruker Scientific, LLC, Billerica, MA

WP 143  Reducing Turnaround Time and Compound Consumption for ADMET Screening with Echo® Liquid Handling and Automation Enabling High Capacity. LC-MS/MS Assay; Ashley A. Rehm1; Biru Patel1; Mitchell J. Martineau1; Shantanu Roychowdhury1; 1Eurofins Panlabs, Saint Charles, MO

WP 144  Global profiling of AMG510 modified proteins identified tumor suppressor KEAP1 as an off-target; Yini Wang1; Bowen Zhong1; Caixia Xu1; Dongdong Zhang1; Yi Wang1; Jun Qin2; 1National Center for Protein Sciences (The PHOENIX Center, Beijing), Beijing, China; 2National Center for Protein Sciences (The PHOENIX Center, Beijing), Beijing, China

WP 145  LC-MS metabolic profiling of a standardized extract of PACs from Vitiss vineraseeds in healthy volunteers andin-vitrot supporting studies; Giovanni Baron1; Larissa Dela Vedova1; Francesca Gado1; Laura Fumagalli1; Marina Carini1; Cristian Del Bo1; Paolo Morazzoni1; Giancarlo Aldini1; 1Department of Pharmaceutical Sciences (DISFARM), Università degli Studi di Milano, Milan, Italy; 2Department of Food, Environmental and Nutritional Sciences, Università degli Studi di Milano, Milan, Italy; 3Divisione Nutraceutica, Distillerie Umberto Bonollo S.p.A., Mestrino, Italy

WP 146  Determination of Bicalutamide in Human and Mouse serum using PerkinElmer QSiight 420 LC-MS/MS system with Epic C18 column; Sergey Shulga-Morskoy1; Cole Strattman2; 1Perkin Elmer Health Sciences Inc, Hopkinton, MA; 2Perkin Elmer, Shelton, CT

WP 147  Open Port Interface with Electromagnetic Mixing for an Affinity Selection MS System; Thomas R. Covey1; Chang Liu1; Peter Kovarik2; Jonathan Shrimpl3; Nate Hoxie1; Michael Ronzetti2; Bolormaa Baliijnymaa1; Colin Kelly1; John Janiszewski1; Meghav Verma2; Sam Michael2; Matthew Half2; Anton Simeonov2; Richard Van Breenem2; Yuandan Liu3; Jianli Zhao4; Emmet Welch4; 1SCIEX, Concord, ON; 2National Center For Advancing Translational Sciences, Rockville, MD; 3Oregon State University, Corvallis; 4PhosphoENex, Torrance, CA

WP 148  Microliter well based MS method scheduling for highthroughput mass spectrometry; David Cox1; Chang Liu2; Bogdan Georgescu1; 1SCIEX, Concord, ON

WP 149  Investigating CYP Reaction Phenotyping using HEPATOPAC® for Low Turnover Compounds: Identifying Inhibitor for CYP2B6 and Describing Temporal CYP1A2 Activity Decline. Mark Athanasian1; Sheri Smith1; Bennett Ma1; Karsten Menzel1; 1Pharmacokinetics, Merck & Co., Inc., West Point, Pennsylvania

WP 150  Quantitative Assessment of Membrane Transporters in Rat and Human Hepatocytes for Model Informed Drug Development; Mariel R Mendroza1; Mark Athanasian1; Michelle Robinson1; Xiaoyan Chu1; Jinging Guo1; Matthew Del Mazar2; Wuxian Cheng2; 1RIKEN, Tokyo, Japan; 2Drug Metabolism, Pfizer, Groton, CT

WP 151  Mitragynine UPLC-MS/MS Method Development and Preclinical Pharmacokinetics; China Ryu1; Natalie R. Hagen1; Junfeng Huang1; Xin Xu1; Amy Q. Wang1; 1National Center for Advancing Translational Sciences, National Institutes of Health, Rockville, MD

WP 152  Improved Performance of a Milli fluidic System for Drug Absorption Studies ex vivo based on Rapid Mass Spectrometry; Chloe E Spencer1; Malcolm R. Clench1; Vikki Carolan1; Stephen Rumble2; 1BMRC, Sheffield Hallam University, Sheffield, United Kingdom; 2CRODA, New Castle, Delaware

WP 153  Metabolites of the Large Cyclic Peptide Antibiotic Cyclosporin A Characterized Using HPLC/ESI-Exact-Mass-MS/MS Data with the iHAPPE Structure Elucidation Software: Marshall M. Siegel1; Gary E Walker1; Serhiy Hnatyshyn1; 1MS MassSpec Consultants, Fair Lawn, NJ; 2BMS, Princeton, NJ

WP 154  Chemical derivatization coupled with 2D-LC-MS/MS enabling sensitive quantitation of SEP-383103 (a major metabolite of ulotaran) in Rat Plasma; Yu-Luan Chen1; Jingduan Chi1; Melissa Molfkoya1; Lei Shi1; 1Sunovion Pharmaceuticals Inc., Marlborough, MA; 2PPD, Middleton, WI

WP 155  Quantification of Sazetidine-A from Rat Brain and Plasma for the Treatment of Tinnitus; Emily M Hubecky1; Samantha A Olendorff1; Donald Caspy1; Lynne Ling1; Kevin R Tucker1; 1Southern Illinois University Edwardsville, Edwardsville, Illinois; 2Shimadzu, Columbus, MD; 3Southern Illinois University School of Medicine, Springfield, IL

WP 156  A Highly Sensitive 2D-LC/MS Method for the Quantitation of Ethynyl Estradiol and Etonogestrel in Human Plasma; Jingduan Chi1; Melissa Molfkoya1; Zhijing Huang1; 1PPD Inc, Madison, WI

WP 157  Analysis of apixaban, dabigatran and metabolites in human liquid samples employing vortex-assist ed salt-enhanced liquid-liquid microextraction coupled with UHPLC-MS/MS; Tzu-Yu Pan1; Chia-Fang Wu2; 1, 2Ming-Tsang Wu3, 4, 5, 6; 2, 5, 6Kaohsiung Medical University Research Center for Environmental Medicine, Kaohsiung city, Taiwan; 1International Master Program of Translational Medicine, National United University, Miaoli city, Taiwan; 2Kaohsiung Medical University Research Center for Environmental Medicine, Kaohsiung city, Taiwan; 2, 3Ph.D Program in Environmental and Occupational Medicine, College of Medicine, Kaohsiung Medical University, Kaohsiung city, Taiwan; 2Department of Public Health, College of Health Sciences, Kaohsiung Medical University, Kaohsiung city, Taiwan; 2Department of Family Medicine, Kaohsiung Medical University Hospital, Kaohsiung Medical University, Kaohsiung city, Taiwan

WP 158  Determination of Ethyl Glucuronide in plasma by ATLAS-LEXT NHD combined with LC-MS/MS; Chen
WP 159  Structure elucidation of a macrocyclic GSH-adduct metabolite of Rizalubrutinib, a reversible covalent BTK inhibitor; 1Cathy Muste; 1Shu-Yu Liao; 1Chungang Gu; 1Biogen, Cambridge, MA.

WP 160  Novel Application of LC-MS to Qualitatively Identify Underivatized Metropolotrol Acid in Equine Plasma to Prove Metropolotrol Administration; 1Benjamin J Burns; 2Hai Le Copley; 3Mark A Musetti; 3Deirdre E Damon; 4Ryan M Farmer; 4Soobeng Tan; 4Ohio Department of Agriculture, Reynoldsburg, OH.

WP 161  Exploring the Applicability of Multi-Reflecting Time-of-Flight Mass Spectrometry for Expedited Biotransformation Studies; 1Daniel J Weston; 3Emma Marsden-Edwards; 4Martin Palmer; 5Laura Tomlinson; 1Richard Gregory; 1Kevin Colizzi; 1Ander Mack; 4GSK, Stevenson, United Kingdom; 3Waters Corporation, Wilmslow, United Kingdom; 4GSK, Collegeville, PA; 3Waters Corporation, Wilmslow, United Kingdom.

WP 162  Pharmacokinetics of Ketamine Transfer into Human Milk; 1Palika Datta; 1Kaytlin Krutsch; 1Teresa Baker; 1Thomas Hale; 1Texas Tech University Health Sciences Center, Amarillo, TX.

WP 163  Mass spectrometry analysis of the contradiction between antiparasitic protection and immune responses in a Chagas disease nonhuman primate vaccination model; 1Zongyuan Liu; 1Priscila Silva Grijó Farani; 1John L. Vandeberg; 1Igor C. Almeida; 1Laura-Isobel McCall; 1Department of Chemistry and Biochemistry, University of Oklahoma, Norman, OK; 1Border Biomedical Research Center, University of Texas El Paso, El Paso, TX; 1Department of Human Genetics, South Texas Diabetes and Obesity Institute, Edinburg, TX.

WP 164  Development of an Ion Mobility CCS Database for Detection of Quaternary Ammonium Compounds and their Hepatic Phase I Human Metabolites; 1Ryan Nguyen; 1Ryan P Seguin; 1Liben Xu; 1University of Washington, Seattle, WA.

WP 165  Multi-Elemental Determination of Heteroatoms for Standard-Free Quantitation of Xenobiotics; 1Grace E Hahn; 1Freino A Redeker; 1Kaveh Jorabchi; 1Georgia Tech University, Atlanta, GA.

WP 166  Metabolism study of the novel cathinone derivative 3-MMC combining three in vitro approaches, LC-HRMS acquisition and molecular networking tools; 1Eilles Zarrouk; 1Alan Barnes; 1Stephane Moreau; 1Neil Loftus; 1Sylvain Dulaughter; 1Souleiman Elbalkhi; 1Franck Saint-Marcoux; 1CHU Limoges, Limoges, France; 2Shimadzu Corporation, Manchester, United Kingdom; 3Shimadzu Europa GmbH, Duisburg, Germany.

WP 167  Optimization of the Ion Source-Mass Spectrometry Parameters Using High Throughput Rapidfire Mass Spectrometry and Design of Experiments Approach; 1Timothy Schwartz; 1Hoora Shaghaghi; 1Alliance Pharma Inc, Malvern, PA.

WP 168  Improved Quantitation of Sulfated Compounds in Human Plasma and Urine through Hydrolysis with Purified Arylsulfatase; 1Amada C. McGee; 2Douglas Waites; 1L. Andrew Lee; 1Integrated Micro-chromatography Systems, Inc, Imo, SC.

WP 169  Bioanalytical Support for a Single-Arm Human Mass Balance and Absolute Bioavailability Study for Involisibul using a Stable Labeled IV Microtracer; 1Ryan Johnson; 1Xiaorong Liang; 1Brian Dean; 1Shuguang Ma; 1Sungjoo Choo; 1Genentech Inc, South San Francisco, CA.

WP 170  Enhancing Structural Elucidation of Drug-related Metabolites by Coupling Ion Mobility and Site-of-Metabolism Collision Cross-Section Prediction; 1Jarod Fincher; 1Ismael Zamora; 1Mark Cancilla; 1Merck & Co., West Point, PA; 2Lead Molecular Design, S.L., Sant Cugat del Valles, Spain.

WP 171  Investigation of fenebrutinib metabolism and bioactivation pathways via tandem-in-time fragmentation in an Ion Trap MS; 1Aishah M Alsibae; 1Ali S Abdelhamied; 1Mohamed W. Atwa; 1Adnan A Kadi; 1College of Pharmacy, King Saud University, Riyadh, SA, Riyadh, Saudi Arabia.

WP 172  Investigation of in-vitro potential toxic metabolite formation for some selected tyrosine kinase inhibitors; 1Abdulaziz Aljohari; 1Adham Bahain; 1Adnan A Kadi; 1A. F. M. Motiur Rahman; 1King Saud University, Riyadh, Saudi Arabia.

WP 173  Polymer StudioTM: a novel software for fast profiling and identifying complex pharmaceutic excipients by UHPLC-HRMS/MS technique; 1Zhe Wang; 1Jiamin Gao; 1Xinjian Li; 1Yanan Wang; 1Ning Sheng; 1Runtao Tian; 1Jinlan Zhang; 1Institute of Materia Medica, Chinese Academy of Medical Sciences & Peking Union Medical College, Beijing, China; 2Chemind Technologies Co., Ltd., Beijing, China.

WP 174  Unraveling sequences of impurities and degradants of a non-linear therapeutic peptide using a high-resolution LC-MS/MS workflow with electron-activated dissociation; 1Eva Duchoslav; 1Harini Kaluarachchi; 1Giulia Calloni; 1SCIEX, Concord, ON; 2SCIEX, Darmstadt, Germany.

WP 175  Method Translation from EI GC/HRMS to Atmospheric Pressure Ionization GC/MS/MS: Quantitative Analysis of Organochlorine Pesticides in Biota; 1Douglas Stevens; 1Lindsay Hatch; 1Sarah Dowd; 1Frank Dorman; 1Waters, Milford, MA.

WP 176  A Quick MRM Method for FASAs Analysis in Surface Water Using UHPLC-MS/MS; 1Danyang Wang; 1Yanisree Mulabagal; 1Meredith Feltman; 1Pavel Vlcek; 1Joel Hayworth; 1Auburn University, Auburn, AL.

WP 177  A Compound Discoverer workflow integrated with molecular networking enables non-targeted class-based separation of Per- and polyfluoroalkyl substances (PFAS) homologous series; 1Juan M Sanchez; 1Ralf Tautenhahn; 1ThermoFisher Scientific, Redwood City, CA; 2ThermoFisher Scientific, San Jose, CA.

WP 178  Total Fluorine Quantitation by Plasma Assisted Reaction Chemical Ionization Mass Spectrometry; 1Samuel R White; 1Kaveh Jorabchi; 1Georgia Tech University, Washington, DC.

WP 179  A Comparison of Liquid-Liquid Extraction and Stir Bar Sorptive Extraction for the Analysis of Organo-iodides using GCxGC High-Resolution Mass Spectrometry; 1Caroline O. Granger; 1Heather A. Brant; 1Haley B. Lawton; 1Stephanie N. Gamble; 1Amie C. McElroy; 1Joseph M. Mannion; 1Savannah River National Laboratory, Aiken, SC.

WP 180  Determination of reference values for PFAS in a wide variety of biotic and abiotic commercially available reference materials; 1Camden Camacho; 1John A. Bowden; 1University of Florida, Chemistry Department, Analytical Chemistry Division, Gainesville, FL.

WP 181  Online LC / 217 FT-ICR MS and ICP-MS Analysis of Dissolved Organic Matter (DOM); 1Ryan P Rodgers; 1Martha L. Chacon-Patino; 1Win Robbins; 1Deisy Giraldo; 1Joseph Frye-Jones; 1Chad Weisbrod; 1Alan G Marshall; 1Brice Bouysiere; 1Pierre Giusti; 1National High Magnetic Field Laboratory, Tallahassee, FL; 2Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL; 3International Joint Laboratory - iC2MC: Complex Matrices Molecular Characterization, TRTG, Harlequin, France; 4Universite de Pau et des Pays de l'Adour, Pau, France; 5International Joint Laboratory - iC2MC: Complex Matrices Molecular Characterization, TRTG, Harlequin, France; 6Total Energies Research & Technology, Gontreville, France.
### WP 206 Combining DART-MS and GC-EI-MS Spectral Signatures for Classifying an Unknown Seized Drug: An Exploratory Approach

**Authors:** William J Feeney; Edward Sisco; National Institute of Standards and Technology, Gaithersburg, MD

**Abstract:** Investigating the utility of hybrid similarity scores with mass spectra collected using DART-MS: A case study with PCP analogs.

**Keywords:** DART-MS, GC-EI-MS, spectral signatures, unknown drug classification

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### WP 207 Rapid GC-MS and Solid-Phase Microextraction as a Screening Method for Forensic Fire Debris Applications

**Authors:** Briana A Capistran; National Institute of Standards and Technology, Gaithersburg, MD

**Abstract:** Target compounds for mass spectrometry imaging after fingerprint enhancement techniques.

**Keywords:** GC-MS, solid-phase microextraction, forensic fire debris

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### WP 208 Detection of post-blast triacetone triperoxide (TATP) by 3D-printed cone spray, DART, and SPME-GC-MS: a comparison for forensic casework

**Authors:** Ryan M. Bain; Pat. Cr.W. Fedick; Tji Pinedo; Christopher C. McGillan; Shane Kullen; Gui-hua Lang; Douglas J. Klapc; Bureau of Alcohol, Tobacco, Firearms and Explosives, Beltsville, MD; Naval Air Warfare Center, United States Navy Naval Air Systems Command (NAVAIR), China Lake, CA; Illinois state university, Normal, IL

**Abstract:** Development of a post-blast TATP detection method using 3D-printed cone spray, DART, and SPME-GC-MS.

**Keywords:** TATP, 3D-printed cone spray, DART, SPME-GC-MS

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### WP 209 Recovery and Detection of Fentanyl Analogs and Precursors from Shipping Materials by Pressure-Sensitive Adhesive and Paper Spray-Mass Spectrometry

**Authors:** Sarah Prunty; Nicholas Manicke; Elizabeth Dhummkakupt; Dan Carmany; Indiana University-Purdue University Indianapolis, Indianapolis, IN; Indiana University-Purdue University Indianapolis, Indianapolis, IN; U.S. Army DEVCOM Chemical Biological Center, Aberdeen Proving Ground, MD; EXCEX Incorporated, Edgewood, MD

**Abstract:** Average Signal Intensities from Qualitative Large-Scale Trace-Residue Analysis of Discarded Drug Paraphernalia Provide Quantitative Information on Dynamic Illicit Drug Markets

**Keywords:** Fentanyl analogs, pressure-sensitive adhesive, paper spray-mass spectrometry

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### WP 210 Application of DART ionization in the forensic investigation of pesticide poisoning

**Authors:** Giuseppe T. Wurzler; Alexandre N. P. Aguiar; H. J. Jost; Institute for Atmospheric and Earth Research, Gaithersburg, MD

**Abstract:** Application of DART ionization in the forensic investigation of pesticide poisoning.

**Keywords:** DART ionization, pesticide poisoning, forensic analysis

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### WP 211 Application of Machine-learning to Predict Physical Activity from Endogenous Fingerprint Compounds

**Authors:** Daphne R Patten; Trevor T Forsman; Andrew E Paulson; Young Jin Lee; Janeiro, Brazil; São Paulo, Brazil

**Abstract:** Application of machine-learning to predict physical activity from endogenous fingerprint compounds.

**Keywords:** Machine-learning, physical activity, fingerprint compounds

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### WP 212 Differentiation of Hemp and Marijuana Using Ag-Ligand Ion Complexation and a Semi-Quantitative Decision-Point Assay

**Authors:** Alleigh N. Couch; Jayleey M. Lanza; Christopher M. Zall; Tji Pinedo; Indiana University-Purdue University Indianapolis, Indianapolis, IN; Indiana University-Purdue University Indianapolis, Indianapolis, IN; U.S. Army DEVCOM Chemical Biological Center, Aberdeen Proving Ground, MD

**Abstract:** Differentiation of hemp and marijuana using Ag-Ligand ion complexation.

**Keywords:** Hemp, Marijuana, Ag-Ligand ion complexation, Decision-Point Assay

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### WP 213 Over-The-Counter sex wellness products screening using a portable/field deployable MS equipped with a Direct Sampling Atmospheric Pressure source

**Authors:** Enrico Davoli; Alice Passoni; Claudio Medana; Enrica Mecarelli; Victor Laiko; Eduardo Erisman; Arun Moorthy; Indiana University-Purdue University Indianapolis, Indianapolis, IN; University of Illinois at Urbana-Champaign, Urbana, IL; Universita' degli Studi di Torino, Torino, Italy; Universita' degli Studi di Torino, Torino, Italy; University of Melbourne, Melbourne, Australia

**Abstract:** Screening of over-the-counter sex wellness products using a portable/field deployable MS equipped with a direct sampling atmospheric pressure source.

**Keywords:** Over-The-Counter sex wellness, Direct Sampling Atmospheric Pressure, MS

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### WP 214 Toward Improved Isomers Separation through Reductive Amination in Synthetic Cathinone, take 4-Methylcathinone, 4-Ethylcathinone and 4-methyl-N,N-dimethylcathinone as an example

**Authors:** Shih-Shin Liang; Kaohsiung Medical University, Kaohsiung, Taiwan

**Abstract:** Toward improved isomers separation through reductive amination in synthetic cathinones.

**Keywords:** Synthetic cathinones, reductive amination, isomers separation

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### WP 215 Differentiation of synthetic sources of an organophosphorus chemical by LC-MS-based metabolomics

**Authors:** Carla Orlandi; Grégoire Delaporte; Christine Albaret; Emmanuel Joubert; Anne Bossée; Laurent Debrouwer; Emilien L Jamín; Oxalim (Research Center in Food Toxicology), Toulouse university, INRAE, ENVT, INP-Purpan, Toulouse, France; Analytical Chemistry Department, DGA CBRN Defence, 5 rue Lavoisier, Vert-Le-Petit, France; Chemistry Division, DGA CBRN Defence, 5 rue Lavoisier, Vert-Le-Petit, France

**Abstract:** Differentiation of synthetic sources of an organophosphorus chemical by LC-MS-based metabolomics.

**Keywords:** Organophosphorus chemical, LC-MS, metabolomics

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### WP 216 Liquid Chromatographic High Resolution Accurate Mass Characterization of Polydimethylsiloxanes on Condoms and Sexual Lubricants

**Authors:** B. McKay Alford; James Adams; Joshua Little; USACIL, Forest Park, GA; ORISE - USACIL, Forest Park, GA

**Abstract:** Liquid chromatographic high resolution accurate mass characterization of polydimethylsiloxanes on condoms and sexual lubricants.

**Keywords:** Liquid chromatography, high resolution accurate mass, polydimethylsiloxanes

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### WP 217 Molecular Investigation of benzodiazepines in human blood by DART ionization and High-Resolution Mass Spectrometry

**Authors:** Cecilia A. Bhering; Anna S. Antonio; Giuseppe T. Wurzler; Adaig G. Aquiag; Diego R. Carvalhosa; Antônio C. G. Jardim; Marc Y. Chalom; Francois Espourelle; Julio C. G. Silva; Francisco R. A. Neto; Gabriela V. Costa; Universidade Federal do Rio de Janeiro, Instituto de Química, NAF – LADETEC, Rio de Janeiro, Brazil; PCEUR, SEPOL, Instituto Médico Legal Atriano Peixoto (IMLAP), Rio de Janeiro, Brazil; SENS Advanced Mass Spectrometry, São Paulo, Brazil; Consultancy, SAO PAULO, Brazil; Bruker Scientific, Billerica, MA; Nova Analítica, São Paulo, Brazil

**Abstract:** Molecular investigation of benzodiazepines in human blood by DART ionization and high-resolution mass spectrometry.

**Keywords:** Benzodiazepines, human blood, DART ionization, high-resolution mass spectrometry

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### WP 218 Application of DART ionization in the forensic investigation of pesticide poisoning

**Authors:** Giuseppe T. Wurzler; Alexandre N. P. Aguiar; H. J. Jost; Institute for Atmospheric and Earth Research, Gaithersburg, MD

**Abstract:** Application of DART ionization in the forensic investigation of pesticide poisoning.

**Keywords:** DART ionization, pesticide poisoning, forensic analysis

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### WP 219 Application of Machine-learning to Predict Physical Activity from Endogenous Fingerprint Compounds

**Authors:** Daphne R Patten; Trevor T Forsman; Andrew E Paulson; Young Jin Lee; Janeiro, Brazil; São Paulo, Brazil

**Abstract:** Application of machine-learning to predict physical activity from endogenous fingerprint compounds.

**Keywords:** Machine-learning, physical activity, fingerprint compounds

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### WP 220 Using High Resolution Mass Spectrometry to clarify ambiguous Benzodiazepine ions in the NIST EI-MS Library

**Authors:** Edward Erisman; Arun Moorthy; William E. Wallace; Stephen E. Stein; NIST, Gaithersburg, MD

**Abstract:** Using high resolution mass spectrometry to clarify ambiguous benzodiazepine ions in the NIST EI-MS library.

**Keywords:** High resolution mass spectrometry, benzodiazepine ions, NIST EI-MS library

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### WP 221 Comparing Peptide Sequence Accuracy of MRM to Peptide Spectra Searching

**Authors:** Wei Yang; Erin Butler; Iowa State University, Ames, IA; National Institute of Standards and Technology, Gaithersburg, MD

**Abstract:** Comparing peptide sequence accuracy of MRM to peptide spectra searching.

**Keywords:** Peptide sequence accuracy, MRM, peptide spectra searching

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### WP 222 Enhanced Ultra-Sensitive Detection of Explosives Through Thermal Desorption Filters Sampling and Multi-Scheme Ambient Pressure Chemical Ionization Source (MION)

**Authors:** Elie Latour; Aleksie Shcherbinin; Juha Kangasluoma; Paxton Juuti; Jussi Kontro; Joanna Mikkila; Jyri Mikkila; H. J. Jost; Research scientist/Scientific Sales Lead, Helsinki, Finland; Kansa Ltd., Helsinki, Finland; Institute for Atmospheric and Earth System Research (INAR), University of Helsinki, Helsinki, Finland

**Abstract:** Enhanced ultra-sensitive detection of explosives through thermal desorption filters sampling and multi-scheme ambient pressure chemical ionization source.

**Keywords:** Ultra-sensitive detection, explosives, thermal desorption filters, multi-scheme ambient pressure chemical ionization source

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### WP 223 Open Port Sampling Interface (OPSI) with a Compact Mass Spectrometer for Trace Contraband Detection

**Authors:** Shin Muramoto; National Institute of Standards and Technology, Gaithersburg, MD

**Abstract:** Open port sampling interface (OPSI) with a compact mass spectrometer for trace contraband detection.

**Keywords:** Open port sampling interface (OPSI), compact mass spectrometer, trace contraband detection
WP 226  Van de Graaf generators as combined sampling devices and ion sources for non-contact mass spectrometry analysis of evidentiary materials; Kenyon Evans-Nguyen; Madison Autrey; University of Tampa, Tampa, FL

WP 227  Rapid Characterization of Alkaloids using Probe ESI Q-TOF LCMS-9050 in OAD-MS/MS; Hitoderi Takahashi; Kaoru Nakagawa; Mami Okamoto; Yuta Miyazaki; Yohei Arano; Tetsuo Iida; SHIMADZU Corporation, Kyoto, Japan

WP 228  High-speed analysis of drugs of abuse in urine using Acoustic Ejection Mass Spectrometry; Anuja Bhakhkhar; Jacob Watson McCabe; Han Joo Lee; Rahul Baghila; Casey W. Burrows; Alexandre Wang; SCIEX, Framingham, MA; SCIEX, Redwood city, CA

WP 229  Generic extraction method developed for the screening of whole blood at 8 Seconds per Sample Using the LDTD-MS/MS; Sylvain Letarte; Hugues Sinnett; Serge Auger; Jean Lacourcière; Jonathan Rochon; Pierre Picard; Phytronix Technologies, Quebec, QC

WP 230  Extraction of Illicit Drugs from Wastewater using a Solid Phase Extraction Syringe-cartridge Capsule; Michael Apsokardu; Xiaohui Zhang; Guotao Lu; CDS Analytical, Oxford, PA

WP 231  An Innovative Approach to QTOF High Resolution Accurate Mass Analyte Screening Using an Improved Software Algorithm and Screener Tool; Peter Stone; Chemistry Department, Kingston, RI

WP 232  Characterization of lipoprotein subclasses using Orbitrap charge detection mass spectrometry; James D. Sanders; Kimberly N. Focke; Michael T. Marty; University of Arizona, Tucson, AZ; University of Arizona, Tucson, AZ

WP 233  Architecture of Adeno-Associated Viral Capsids with Surface-Induced Dissociation and Charge Detection Mass Spectrometry; Markus K. Kostelic; Chen Du; Vicki H Wysoczak; Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH; Resource for Native Mass Spectrometry-Guided Structural Biology, The Ohio State University, Columbus, OH

WP 234  Towards reference-free byproduct characterization of agrochemicals in raw plant extracts by ion spectroscopy; Matthias Vink; Jonathan Martens; Wybren Jan Buma; Giel Berden; Jos Oomens; FELEX Radboud University, Nijmegen, Netherlands; University of Amsterdam, Amsterdam, Netherlands

WP 235  Identification of organic dye molecules using QIT-ToF-SIMS and photodepletion spectroscopy; Chang Min Choi; Center for Scientific Instrumentation, Korea Basic Science Institute (KBSI), Cheongju-si, South Korea

WP 236  Towards routine annotation of mass spectral features with infrared ion spectroscopy; Kas J. Houthuys; Jonathan K. Martens; Giel Berden; Vasuk Gautam; David S. Wishart; Jos Oomens; Radboud University Nijmegen, Nijmegen, Netherlands; University of Alberta, Edmonton, AB

WP 237  Design of an Optical Ion Trap (OIT) Mass Analyzer; Liam Dungan; Frederick Lanni; Mark E Bier; Carnegie Mellon University, Pittsburgh, PA

WP 238  A Quadrupole Time-of-Flight Mass Spectrometer with Off-Axis Ion Trap for Infrared Ion Spectroscopy in the Hydrogen Stretching Region; Madeline Schultz; Neil A. Ellis; Maleesha T. Fernando; Miyuru M. Wellalage; Daniel A. Thomas; University of Rhode Island, Kingston, RI

WP 239  Site-Specific Gas-Phase Acidities of Isoprene and the Negative Ion Photoelectron Spectra of C5H7 Radical Anions Resulting from Isoprene Oxidation; Dushmantha N. Koku Hannadige Abeyesooriya; Kie T. Workman; Wilson Gichuhi; Department of Chemistry, Tennessee Tech University, 1 William L. Jones Dr., Cookeville, TN 38505; School of Environmental Studies, Tennessee Tech University, Cookeville, TN 38505; Department of Chemical Engineering, Tennessee Tech University, 1 William L. Jones Dr., Cookeville, TN 38505

WP 240  Action spectroscopy of triazole ions in the ultraviolet; Alexandre Giulianni; Hélöise Dossmann; Denis Duflot; Synchrotron Soleil, Gif-Sur-Yvette, France; INRAE, UMR1008, TransforT Department, Rue de la Gérardière, BP 71627, 44316 Nantes, France, Nantes, France; Sorbonne Université, Faculté des Sciences et de l’Ingeniérie, Institut Parisien de Chimie Moléculaire (IPCM), Paris, France; Université de Lille, Laboratoire de Physique des Lasers, Atomes et Molécules, Villeneuve d’Ascq, France

WP 241  Gas Phase Intramolecular Photo Crosslinking in Tetrazole-Peptide Conjugates; Jiahao Wan; Haocheng Qian; Frantisek Turcek; University of Washington, Seattle, WA

WP 242  Identifying the Structural Properties of Choline-Chloride Deep Eutectic Solvents by Mass Spectrometry and Condensed-Phase Analysis; Maleesha T Fernando; Miyuru M Wellalage; Emily M Molino; Madeline Schultz; Neil Ellis; Daniel A Thomas; University of Rhode Island, Kingston, RI

WP 243  Combining Mass Spectrometry and Condensed-Phase Analysis for the Structural Investigation of Hydrophobic Deep Eutectic Solvents; Miyuru M Madduma Wellalage; Maleesha T Fernando; Emily M Molino; Madeline Schultz; Neil Ellis; Daniel A Thomas; University of Rhode Island, Kingston, RI; University of Rhode Island, Kingston, RI

WP 244  Influence of the decavanadate oxidation state on its reactivity and structural dynamics in solution studied with 18O exchange; Daniel T Favre; Igor Kaltashov; UMARRS Amherst, Amherst, MA

WP 245  Exploring Emitters for Generating ultra-low Current Electrospray Ionization; Ian T Ferrari; Huishan Li; Nicholas Allen; Taoqing Wang; Anlyn Li; Department of Chemistry, University of New Hampshire, Durham, NH

WP 246  Ionization Efficiency of Glycans, Proteins and Subunits in femto Electrospray Modes; Huishan Li; Nicholas Allen; Taoqing Wang; Ian T Ferrari; Mengtian Li; Anlyn Li; University of New Hampshire, Durham, NH

WP 247  Elevation of the baseline in Quadrupole Mass Spectrometers: Mechanism and Solution; Markus Langner; Hendrik Kersten; Michael Benter; University of Wuppertal, Wuppertal, Germany

WP 248  Mapping Nano-Electrospray Ionization Plumes on an Orbitrap Fusion Lumos Tribrid Mass Spectrometer Equipped with FAIMS; Joshua A Silveira; Gary A Schultz; Kristina Rucker; Yuan Lin; Matt Tsal; Michael Bellford; Cornelia Boeser; Eloy R Wouters; Thermo Fisher Scientific, San Jose, CA

WP 249  Uncatalyzed N-alkylation of Primary Amines via Plasma-Droplet Fusing Reactions: Quantification of Internal Energy Deposition and Product Collection; Alexander J Groome; Abraham K. Badu-Tawiah; The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH

WP 250  Investigation of Long-Term Behavior of Large, Charged ESI Droplets Aspired into the High Vacuum Region of two Commercial MS Systems; Chris Vico Heintz; Oliver Braubach; Walter Wissdorf; Lisa Schnödewind; Thorsten Benter; University of Wuppertal, Wuppertal, Germany

WP 251  Observation of charged ESI droplets aspired into the vacuum system of a commercial QIT under varied LC conditions; Patricia Itzenhüser; Laura Lehmann; Walter Wissdorf; Ferdinand Wachter; Hendrik Kersten; Thorsten Benter; University of Wuppertal, Wuppertal, Germany

WP 252  Investigating effects of supercharging reagents on signal intensity of peptides in negative ion mode using capillary vibrating sharp-edge spray ionization; Amanda Devor; Jing Wang; Madison Pursell; Onanrewaju Awoyemi; Stephen Ting; Fang Li; West Virginia University; C. Eugene Bennett Department of Chemistry, Morgantown, WV
Gas-phase oxidation of benzaldehyde to benzoic acid under electrospray ionization mass spectrometric conditions; Shimin He; Sihang Xu; Athula Attygalle; 
1Stevens Institute of Technology, Hoboken, New Jersey

Thermal-Desorption Electrospray-Mass Spectrometry (TD-ESI-MS) for Dye Analysis; Jiarui Rachel Wu; Xinyi Su; Brian Musselman; Nelson R Vinuela; 1North Carolina State University, Raleigh, NC; 2Bruker Scientific, Billerica, MA

Design and investigation of homemade argon plasma ion sources – An overview of source development, application, and ionization mechanism; Florian Stappert; 1; Alexandr Pape; 1; Juan P. Ayala-Garibay; 1; Florian Utenschil; 2; Oliver J. Schmitz; 2; Applied Analytical Chemistry, University of Duisburg-Essen, Essen, Germany; 2Teaching and Research Center for Separation, University of Duisburg-Essen, Essen, Germany; 2Department of Analytical Chemistry, University of the Basque Country, Leioa, Spain

Measurement of Distribution of Ion Acceptance (DIA) in ESI and APCl ion sources; Adam Bulut; 1Chris Vico Heintz; 1Walter Wissdorf; 1Thorsten Benter; 1University of Wuppertal, Wuppertal, Germany

Feeding the ALPACA: Testing the Performance of Charge-Induced Atomization of Electrosprayed Particles; Cristian A. Blanco-Combariza; Jeffrey E Dick; 1Purdue University, West Lafayette, IN; 2Purdue University Department of Chemistry, West Lafayette, IN

Fast and Ultra Fast Lipids and Drugs Analysis in Whole Blood by GC-MS with Cold EI; Benjamin Neumarck; 1Oneg Elkebats; 2Aviv Amirav; 2Tel Aviv University, Tel Aviv, Israel; 2Aviv Analytical Ltd, Hod Hasharon, Israel

Solving Non-Linearity in GC-MS By Using Cold EI; Alex Yakovichuk; 1Alexander Gordin; 1Aviv Amirav; 1Tel Aviv University, Tel Aviv, Israel

Determination of six aromatic amines in the mainstream smoke of tobacco products; Huihua Ji; 1Weihua Ji; 2Weihua Ji; 2Ohio State University, Columbus, OH; 1Purdue University, West Lafayette, IN

Differential analysis of soil using GC Orbitrap MS and mainstream smoke of tobacco products; Israel; Anthony Tchekhovskoi; 1Thermo Fisher Scientific, Austin, Texas; 2Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; 1Foundation for the Promotion of Health and Biomedical Research in the Valencian Region (FISABIO-Public Health), Valencia, Spain

Operational Fundamentals and Optimization of Vacuum-Assisted Headspace Solid Phase Microextraction for Gas Chromatography Analysis of Solid Samples; Shannon L. Thomas; 1Colton Myers; 1Jason Herrington; 2Kevin A. Schug; 2University of Texas at Arlington, Arlington, TX; 1Restek Corporation, Bellefonte, PA

More than 43,400 High Quality Spectra Added to a Comprehensive Electronic Ionization (EI) Mass Spectral Library; Weihua Ji; 1Lewis Y. Geer; 1Nirina Rabe Andriamaharavo; 1Yufang Zheng; 1Edward P. Erisman; 1H. Martin Garraffo; 1James Little; 1Gary Mallard; 1Sanford P. Markay; 1Yun A. Mirokhin; 1Quan-Long Pu; 1Dmitri V. Tchebakovskii; 1Zhenyu Jin; 1University of Kentucky, Lexington, KY

Differential analysis of soil using GC Orbitrap MS and Compound Discoverer; Dominic Roberts; 1Xin Zheng; 2Lukasz Rajski; 2Nicholas Warner; 2Daniel Kutscher; 2Jason Cole; 2Thermo Fisher Scientific, Runcorn, United Kingdom; 2Thermo Fisher Scientific, Austin, Texas; 2Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany

Characterization of virgin and recycled industrial plastics using pyrolysis with soft ionization coupled to high-resolution mass spectrometry and statistical analysis; Rachel J Sanig; 1Bryan C. Katzenmeyer; 1Jeff Goshawk; 1Arianna L. Kopp; 1Nirina Rabe Andriamaharavo; 1Weihua Ji; 2William E. Wallace; 2William E. Wallace; 2John Gonzales; 2JEOL Ltd., Tokyo, Japan; 2JEOL USA, Inc., Peabody, MA

Characterization of UV-degraded Polyethylene Terephthalate by Reactive-Pyrolysis GC-TOFMS and MALDI-TOFMS; Takaya Satoh; 1Masaaki Ukubaka; 1Azusa Kubota; 1Ayumi Kubo; 2Robert A. Dipasquale; 2JEOL Ltd., Tokyo, Japan; 2JEOL USA, Inc., Peabody, MA

Untargeted screening and identification of substances in plastic food contact materials using an Orbitrap GC mass spectrometer; Dominic Roberts; 1Jason Cole; 1Lukasz Rajski; 2Xin Zheng; 2Pablo Miralles; 1Clara Coscolla; 1Thermo Fisher Scientific, Runcorn, United Kingdom; 2Thermo Fisher Scientific, Austin, Texas; 1Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; 1Foundation for the Promotion of Health and Biomedical Research in the Valencian Region (FISABIO-Public Health), Valencia, Spain

Simultaneous determination of fatty acids in commercial lipid samples by gas chromatography coupled with single quadrupole mass spectrometry (GC-SQMS); Mark Dennis Chico Retraito; 1Siyuan Oiu; 1Anna Lundquist; 1Aida Zuburovic Muratovic; 1Kumari Ubhayasekera; 1Jonas Bergquist; 1Department of Chemistry - Biomedical Center, Analytical Chemistry and Neurochemistry, Uppsala University, Uppsala, Sweden; 1Innovation and Development Department, Fresenius-Kabi, Uppsala, Sweden; 1Swedish Food Agency (Livsmedelsverket), Uppsala, Sweden

Rearrangement of the TMS ester of 4-Difluoromethoxy-N-methylbenzylamine and analogs in EI mass spectra; Quan-Long Pu; 1Yufang Zheng; 1Kirill V. Treytakov; 1William E. Wallace; 1Stephen E. Stein; 1NIST, Gaithersburg, MD

Using Hydrogen as Carrier Gas for GC/MS Analysis: GCXGC-HR-TOFMS with Multi-Mode Ion Source; George Tikhonov; 1Scott Pugh; 1Vyhacevsky Artemii; 2LECO Corporation, Saint Joseph, MI

Rearrangement of the TMS ester of 4-Difluoromethoxy-N-methylbenzylamine and analogs in EI mass spectra; Quan-Long Pu; 1Yufang Zheng; 1Kirill V. Treytakov; 1Edward P. Erisman; 1NIST, Gaithersburg, MD

Measurement and Evaluation of Plant Derived Compounds for a Comprehensive Electron Ionization MS Library; Nirina Rabe Andriamaharavo; 1Mak D. Tytus; 1Weihua Ji; 1William E. Wallace; 1Stephen E. Stein; 1NIST, Gaithersburg, MD; 1National Institute for Standards and Technology, Gaithersburg, MD; 1National Institute for Standards and Technology, Gaithersburg, MD

Full Evaporative Vacuum Extraction – A Quantitative and Green Approach for Analysis of Semivolatile Organic Compounds in Water Using GC-MS; Weier Hao; 1Dan Cardin; 1John Quintana; 1Tim Raub; 2Entech Instruments, Simi Valley, CA

Analysis of Volatile and Semivolatile Organic Compounds in Oral Rinse using Vacuum Assisted Sorbent Extraction and GC-MS; Tim Raub; 1Dan Cardin; 1Weier Hao; 1John Quintana; 2Entech Instruments, Simi Valley, CA

Helium to Hydrogen: Explosives & Pesticides & VOAs, Oh My! Successful Transition of GC/MS Analyses; Eric Fausett; 1Anastasia Andrianova; 2Bruce Quimby; 2Angiea
WP 278 Large Volume Static Headspace for Flavor/Fragrance Analysis by GC-MS Using Novel Hybrid Capillary/Packed Sorbent Traps: John Quintana1; Dan Cardin2; Weier Hao3; Tim Raub4;1Entech Instruments, Simi Valley, CA

WP 279 Analysis of Hop Oil Chemical Composition using GC/MS-SCD to Quantitate Essential Oil from 3 PPM -1 w/w%: Lupe Saldana1; Jacqueline Brummett1; Patrick Jensen1;1Yakima Chief Hops - Yakima, WA, Yakima, WA

WP 280 Bench Scale Py-GC/MS with In-Line Reactor for Predicting Arrhenius Parameters: Jeffrey Michael McGuire1; John C Carpin2;1U.S. Army DEVCOM Chemical Biological Center, Aberdeen Proving Ground, MD; EXC Incorporated, Edgewood, MD

WP 281 Internal standards for optimization of precision and accuracy of an automated liquid handler for hydrogen exchange-mass spectrometry (HX-MS): Ekaterina Deyanova1; David Weis1;1Bristol-Myers Squibb, Princeton, NJ

WP 282 An Improved Apparatus with On-Line Chromatography for Hydrogen Deuterium Exchange Mass Spectrometry Measurements from Milliseconds to Hours: Joseph Anacleto1,2; Cristina Lento1; Ayesha Maqsood1; Derek Wilson1; Emeritus, Brampton, ON; 2York University, Toronto, ON

WP 283 Development and Application of Spray-capillary to Room Temperature Hydrogen-Deuterium Exchange for Top-Down Mass Spectrometry Applications: Joel B Langford1; Mulin Fang1; Kelsey A. Cupp-Sutton1; Jack Kline1; Luca Fornelli1; Si Wu1; University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK

WP 284 HILIC separations for HDX-MS at subzero temperatures: Kyle W Anderson1; Jeffrey W Hudgens1; NIST, Rockville, MD

WP 285 GenMix_GUI: A software package for automated HDX-MS data analysis and interrogation: Hyeyun Jung1; Seunjae Na2; Eunok Paek3; Grinnell College, Grinnell, IA; 2Hanyang University, Seoul, South Korea

WP 286 Development of a PNGase Rc column for efficient online deglycosylation of complex glycoproteins during HDX-MS: Thomas Ole Tandrup Lambert1; Marius Gramlich1; Luke Smith1; Luisa Stutzke1; Dingyu Deng2; Philip Kaiser3; Alexis Escobedo4; Ellie James5; Mike Guttmann1; Justin LP Benisch6; Ulrich Rothbauer6; Maximiliane Koenig6; Cornelia Wagner6; Pavla Vankova6; Petr Pomphach6; Petr Novak6; Anne Zeck6; Kasper D. Rand6; Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark; 2NM1 Natural and Medical Sciences Institute at the University of Tübingen, Reutlingen, Germany; 3Physical and Theoretical Chemistry Laboratory, Department of Chemistry, University of Oxford, Oxford, United Kingdom; 4Department of Medicinal Chemistry, University of Washington, Seattle, Washington; 5Roche Pharma Research and Early Development, Large Molecule Research, Penzberg, Germany; 6BioCeV - Institute of Biotechnology of the CAS, Prague, Czech Republic; 7BioCeV - Institute of Microbiology of the CAS, Prumyslova, Czech Republic

WP 287 Development of a thiol-ene microfluidic chip for sub-zero temperature hydrogen/deuterium exchange mass spectrometry (HX-MS): Anton B. Hansen1; Rasmus R. Svejdal1; Jack Barrett1; Jörg P. Kutter1; Kasper D. Rand1; Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark

WP 288 Differential HX-MS of complex drug targets extracted from cells: a full solution using HX-DIA technology: František Filandř1; Vladimir Sarpe1; Shaunak Raval1; Morgan Khan1; Pauline Douglas1; Yuqi Shi2; Rosa Viner2; Stephen Coales1;2David Schrimer1; University of Calgary, Calgary, AB; 3Thermo Fisher Scientific, San Jose, CA; 4Trajan Scientific & Medical - Raleigh, Morrisville, NC

WP 289 A fully automated HX-DIA data analysis workflow for whole proteome deuterium experiments: Vladimir Sarpe1; František Filandř1; D Alex Crowder1; David C Schrimer1; University of Calgary, Calgary, AB

WP 290 Histidine hydrogen-deuterium exchange (His-HDX) mass spectrometry for identifying protein-ligand interactions: Kouhei Tanaka1; Tanoue Kishimoto2; Shinko Watanabe1; Kaori Mitsu2; Chieko Okumura1; Kouta Murasaki1; Masaru Miyagi2; Ayako Kurimoto2; Sen Ilker2; Mitsubishi Tanabe Pharma Corporation, Kanagawa, Japan; 2Case Western Reserve University, Cleveland, OH

WP 291 Nylon membrane immobilized acid protease digestion for hydrogen deuterium exchange capillary electrophoresis mass spectrometry: Jordan Aerts1; Per E. Andren1; Erik T Jansson1; Uppsala University, Uppsala, Sweden

WP 292 Millisecond hydrogen/deuterium-exchange mass spectrometry of tryptophan side chains: Jess Ramsay1; Dr Daniel Kattnig1; Dr Jonathan Phillips1; University of Exeter, Exeter, United Kingdom

WP 293 The Deuterium Exchange Mass Spectrometry of Millisecond HX-MS Using Novel Hybrid Line Reactor for through Hydrogen-Deuterium Exchange Mass Spectrometry Data Analysis: Kelly A Cupp-Sutton1; Thomas Welborn1; Mulin Fang1; Joel Langford1; Si Wu1; University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK

WP 294 Cross-Platform Standardization of Gas-Phase Hydrogen/Deuterium Exchange: Aleksi R Escobedo1; Sunjil S. Uppal1; Mike Guttmann1; University of Washington, Seattle, WA

WP 295 New tools for aid with the analysis of bimodal HDX-MS data: Miklos Gutman1; University of Washington, Seattle, WA

WP 296 Large Scale Investigation of Protein Stability and Dynamics Using High-Throughput Hydrogen-Deuterium Exchange Mass Spectrometry: Anna L. B. Ferrari1; Suygan M Dixit1; Jane M Thibeault1; Gabriel J Rocklin1; Northwestern University, Chicago, IL

WP 297 HDX-MS with in-line electrochemical reduction of disulfide bonds – state of the art: Hendrik-jan Brouwer1; Jean-Pierre Cheret1; Martin Eysberg1; Antec Scientific, Alphen a/d Rijn, Netherlands; Antec Scientific, Boston, MA 02108

WP 298 Operation at Constant Ultrahigh Resolution with µDeiution using the Dynamically Harmonised Cell: Benedict Gannon1; Diana C Palacio Lozano1; Hugh E Jones1; Mark P. Barrow1; University of Warwick, Coventry, United Kingdom

WP 299 Handling the noticeable non-linearity of mass calibration in high resolution ToF MS: Boris Kozlov1; Sergey Kirillov2; Waters, Wilmslow, United Kingdom; 2MSC-CG Ltd, Bar, Montenegro

WP 300 Increased sensitivity and throughput for native intact mass analysis using an online buffer exchange column: Reiko Kyonani1; Weijing Liu1; Rosa Viner1; Min Du2; Thermo Fisher Scientific, San Jose, CA; Thermo Fisher Scientific, Boston, MA

WP 301 High Resolution mass spectrometry-based profiling of putative DNA adducts derived from trans,trans,2,4-decadienyl (tt-DDE): Yu-Ming Hsu1; Chao-Yi Chen1;2; Tzu-Yu Pan1; Acharee Kawaiyaoong1; Min-Zong Huang1; Chi-Fang Wu1,3; Research Center for Precision Environmental Medicine, Kaohsiung Medical University, Kaohsiung city, Taiwan; 2International Master Program of Translational Medicine, National United University, Miaoli city, Taiwan
| WP 302 | Comprehensive analysis of instrument parameters to achieve high-level ion focusing in linear time-of-flight mass spectrometry; Yi-Hong Cai; Yi-Sheng Wang; 1Genomics Research Center, Academia Sinica, Taipei, Taiwan |
| WP 303 | Unlocking the potential of large-cohort proteomics studies with a novel high-resolution accurate mass platform; Yue Xuan; Anna Pushkova; Martin Zeller; Colin Tobias Wirth; Jens Grote; Andreas Kuehn; Tabiwang N. Arrey; Eugen Damoc; Sally Webb; Thomas Moehring; 1Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; 2Thermo Fisher Scientific, San Jose, CA |
| WP 304 | Untargeted PFAS identification and targeted PFAS library screening workflows for groundwater analysis using a QTof mass spectrometer; Ethan R Hain; Kathleen Luo; Om Shrestha; Christopher Gilles; Evelyn Wang; Xiaomeng Xia; Robert English; Tiffany Liden; 1Shimadzu Scientific Instruments, Columbia, MD |
| WP 305 | A new approach for the comprehensive chemical description of complex pharmaceutical products via comprehensive gas chromatography and high-resolution mass spectrometry; Ole Tiemann; Lukas Schwalb1;2, Christopher Paul Rüger; Martha Liliana Chacón-patiño; Thomas Gröger; Ralf Zimmermann1,2; 1Joint Mass Spectrometry Centre, Chair of Analytical Chemistry, University of Rostock, Rostock, Germany; 2Joint Mass Spectrometry Centre (JMSC), Cooperation Group Comprehensive Mass Spectrometric Analytics, "Comprehensive Molecular Analytics" (CMA), Helmholtz Zentrum München GmbH, German Research Center for Environmental Health, Neuherberg, Germany; 3National High Magnetic Field Laboratory, Tallahassee, FL |
| WP 306 | Qualitative and quantitative analysis of Organic Solvents in lithium battery electrolysis by LC-QTOF; Haiyang Wang1; Zhihui Lin; Jianzhong LP; Peibin Hu; 1Agilent Technologies, Inc, Guangdong, China; 2Agilent Technologies, Inc, Beijing, China; 3Agilent Technologies, Inc, Chengdu, China |
| WP 307 | Determination of Oxytocin in the mouse brain by HR-UHPLC-MS: Method Development and Validation; Hanin Diab1; Jonathan Thompson; Klementina Fon Tacer; Tara Bayat1; 1Texas Tech University, Amarillo, TX; 2School of Veterinary Medicine, Amarillo, Texas, United States; 3Amarillo, Texas |
| WP 308 | A novel Ion Processor Device for High-Throughput Analysis in a High-Resolution Mass Analyzer; Christian Hock; Hamish Stewart; Eduard Denisov; Amelia Peterson; Nicolaie Eugen Damoc; Martin Zeller; Tabiwang N. Arrey; Anna Pushkova; Alexander Wagner; Wilko Balschmiter; Dmitry Grinfeld; Alexander A Makarov; 1Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany |
| WP 309 | Evaluation of Mass Correction Strategies for Accurate Mass Measurements of Pulsed Ionization Sources by Infrared Matrix-Assisted Laser Desorption Electrospray Ionization; Alexandria L. Sohn1; David C Muddiman; 1North Carolina State University, Raleigh, NC |
| WP 310 | Identification for Anions in Electrolyte of Lithium Battery Using Ion Chromatography - Quadrupole-Time of Flight Mass Spectrometry; Zhihui Lin1; Haiyang Wang; Jianzhong LP; Peibin Hu; 1Agilent Technologies, Inc, Guangzhou, China; 2Agilent Technologies, Inc, Beijing, China; 3Agilent Technologies, Inc, Chengdu, China |
| WP 311 | A Universal High-resolution Liquid Chromatography-Tandem Mass Spectrometry for the Analysis of Nitrosodimethylamine in Pharmaceutical Products; Donghee Lee1; Se Hee Hong; Sang Beom Han; 1Department of Pharmaceutical Analysis, College of Pharmacy, Chung-Ang University, 84 Heukseok-ro, Dongjak-gu, Seoul, South Korea |
| WP 312 | Data Independent Analysis Evolution: Exploring the Use of High Resolving Power Multi-Reflecting Time-of-Flight Mass Spectrometry Selectivity for Metabolite Identification; Michael McCullagh; Stephen Griffin; Emma Marsden-Edwards; David Eatough; Dale Cooper-Shepherd; Martin Palmer; 1Waters Corporation, Wilmslow, United Kingdom; 2Waters corp, milford, MA |
| WP 313 | The Impact of ppb Mass Accuracy Upon Biotransformation Product Identification Using Negative Ion Non-targeted Urinary Screening Multi-Reflecting Time-of-Flight LCMS; Michael McCullagh1; Iggy Kass; Emma Marsden-Edwards; David Eatough; Dale Cooper-Shepherd; Martin Palmer; 1Waters Corporation, Wilmslow, United Kingdom; 2Waters, Milford, MA |
| WP 314 | Thermal Analysis High-Resolution Mass Spectrometry in Material Sciences: Application towards Fiber-Reinforced Plastics/Concrete and their Thermal Stress and Recycling/Production Behavior; Christopher Paul Rüger1,2; Lukas Friedenri; Anika Neumann; Arne Koc; Martha Liliana Chacón-patiño1;2, Paolo Bombieri; Thorsten Streibel1,2; Murray Gray1,2; Ralf Zimmermann1,2; 1Mass Spectrometry Centre, Chair of Analytical Chemistry, University of Rostock, Rostock, Germany; 2International Joint Laboratory - i2CMC: Complex Matrices Molecular Characterization, TRTG, Harleuf, France; 3National High Magnetic Field Laboratory, Tallahassee, FL; 4Alberta Innovates, Calgary, AB; 5Joint Mass Spectrometry Centre, Cooperation Group Comprehensive Mass Spectrometric Analytics, Helmholtz Zentrum München, German Research Center for Environmental Health, Neuherberg, Germany; 6University of Alberta, Edmonton, AB |
| WP 315 | Unveiling the performance of a novel high-resolution accurate mass platform for proteomics applications; Tabiwang N. Arrey; Amirmansoor Hakimi; Eduard Denisov; Nicolaie Eugen Damoc; 1Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; 2Thermo Fisher Scientific, San Jose, California |
| WP 316 | Metabolomics and Lipidomics Profiling Applied to Bioprocessing using a Standardized, Quantitative Protocol with High-Resolution Mass Spectrometry; Hoorn Y Park; Stephen DeArth; Hai Pham-Tuan; Agnes Scharrer; Vyncent Nguyen; Didar Aisk; Chengjian Tu; Ronny Dosanjh1,2; John Point; George Bu1; Elizabeth S Dodson; 1Thermo Fisher Scientific, Hunt Valley, MD; 2Biocrates Life Sciences AG, Innsbruck, Austria; 3Thermo Fisher Scientific, Grand Island, NY |
| WP 317 | Evaluation of a novel Tribrid Orbitrap Ascend system for in-depth high-throughput proteomics and phosphoproteomics; Yuchen He1; Koenraad Overmyer1,2; Dayn R Brademan; Patricia Bergmeyer; Jingbing Huang1;2; Romain Huegret1; Michael W. Senko;2; Vlad Zabrouskov;2; Michael S. Westphall;2; Evgenia Shistikova;2; Graeme C McAlister;2; Joshua J. Coon1,2; 1University of Wisconsin-Madison, Madison, WI; 2Morgridge Institute for Research, Madison, WI; 3Thermo Fisher Scientific, San Jose, CA |
| WP 318 | Enhanced ionization efficiency of astrobiologically relevant biomarkers via secondary plate selection for Laser Desorption Ionization Mass Spectrometry (LDMS); Ashley M Hanna; Ziqin Ni3; Adrian Southard2; Ricardo Arevalo Jr.3; 1University of Maryland, College Park, MD; 2University of Maryland College Park, College Park, MD; 3University of Maryland, College Park, College Park, MD |
| WP 319 | Optimizing 7 Tesla FT-ICR MS equipped with frequency multiple detection and absorption mode processing for high throughput organic matter analysis; Kevin J Zemaitis1; Eric Choi1; Rosalie Chu1; Yuri E. Corilo; Sai Munikoti; Jordan Rabus; Jan Strube2; William Kew; 1Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, Washington 99354; 2Pacific Northwest National Laboratory, Richland, WA |
WP 320 Urinary Forensic Toxicology Data Independent Analysis Screening: Using High Resolving Power Multi-Reflecting Time-of-Flight Mass Spectrometry; Michael McCullagh1; Johannes PC Vissers1; Martin Palmer2; Jane Cooper1; Michelle Wood1; Emma Maraden-Edwards1; Nayan Mistry1; 1Waters Corporation, Wilmslow, United Kingdom

WP 321 New Tribrid MS ion optics and electronics improve sensitivity, duty cycle, and extend the MS range; Graeme McAlister1; Xiao Wang2; Mike Goodwin1; Christopher Mullin1; Jesse D. Canterbury3; Raman Mathur4; Romain Huguet4; David Berger4; Jingjing Huang5; Michael W. Senko5; Vlad Zabrotskii6; Thermo Fisher Scientific, San Jose, California

WP 322 Linking imaging mass spectrometry analysis of sepsis-induced metabolic rewiring and dichloroacetate treatment to septic cardiomyopathy; Yu Lin1; Manal L. Zablawi1; Lane M. Smith1; Peter W. Stacpoole1; Charles E. McCall1; Boone M. Prentice1; 1Department of Chemistry, University of Florida, Gainesville, FL; 2Department of Internal Medicine/Molecular Medicine and Department of Microbiology and Immunology, Wake Forest School of Medicine, Winston-Salem, NC; 3Department of Anesthesiology, University of Michigan Medical School, Ann Arbor, MI; 4Department of Medicine, Division of Endocrinology, Diabetes & Metabolism, and Department of Biochemistry and Molecular Biology, University of Michigan College of Medicine, Gainesville, FL

WP 323 High resolution isomer resolved lipid imaging of the breast cancer tumor microenvironment; Brett S.R. Claes1; Annet A.M. Duivenvoorden1; Caitlin M. Tressler2; Ethan Yang2; Kanchan Sonkar2; Shane R. Ellis1,3; Kristine Giulden2; Ron M a. Heeren3; 1Maastricht University, Maastricht, Netherlands; 2Joens Hopkins University School of Medicine, Baltimore, MD; 3University of Wollongong, Wollongong, Australia

WP 324 Quantification of cholesterol metabolites in the brain by on-tissue derivatization mass spectrometry imaging in a mouse model of Huntington’s disease; Alice Passoni1; Angela Marika Siciliano1; Monica Favagrossa1; Alessia Lanno1; Laura Colombo1; Mario Saliona1; Renzo Bagnati1; Enrico Davoli1; 1Istituto di Ricerche Farmacologiche Mario Negri IRCCS, Milano, Italy

WP 325 Mass spectrometry imaging and LC/MS/MS profiling of changes in host lipid metabolism of Mycobacterium tuberculosis infected MGL-1 deficient mice.; Reina Paeg1; Sadhana Chauhan1; Kubra F. Naqvi1; Janice Endsley1; Brendan Prideaux1; 1University of Texas Medical Branch, Galveston, TX; 2University of Texas Southwestern Medical Center, Dallas, TX

WP 326 Discovery of Metabolite Biomarkers in Post-traumatic stress disorder (PTSD) Using Mass Spectrometry Imaging (MSI); Huiling Guo1; Shuli Tang1; Jiaxin Feng1; Luchen Wuyang1; Xin Yan1; 1Texas A&M University, College Station, TX

WP 327 Spatial metabolomics identifies adenosine as a new biomarker for pathology in patients with non-macroalbinuric diabetic kidney disease; Guanshi Zhang1; Leila Hejazi2,3; Petter Bjornstad1; Hak Joo Lee1; Nerlyn Garcia Ponce De Leon1; Christopher R. Anderton1; Theodore Alexandrov2; Manjiri A. Venkatachalam1; Kumar Sharma1; 1UT Health San Antonio, San Antonio, TX; 2University of Colorado Anschutz Medical Campus, Aurora, CO; 3Pacific Northwest National Laboratory, Richland, WA

WP 328 Spatial Mapping of Lids and Elements by Mass Microscopy and Integration with LA-ICP-MS in the Diabetic Mouse Pancreata; Koji Okuda1; Ei-ichi Matsuo1; Jeffrey Dahle1; Toshiya Matsubara1; Jannine I. Gamyato2; Shihuei Chen3; Christine M. Kusminski3; Philipp E. Scherer3; Ruth Gordillo3; 1Shimadzu Corporation, Kyoto, Japan; 2Shimadzu Scientific Instrument, Columbia, Maryland; 3University of Texas Southwestern Medical Center, Dallas, TX

WP 330 Spatially resolved characterization of regulated molecules in host–parasite interactions using HP-AP-SMALDI MSI; Katia R Wiedermann1; Stefanie Gerbig1; Parviz Ghezelli2; Nils H Anschtz1; Alejandra Peter Ventura1; Martin Roderfeld2; Ekke Roeb2; Thomas Quack2; Christoph G Greveling3; Liliana M R Silva4; Carlos R Hermosilla5; Anja Taubert5; Kerstin Strupat5; Bernhard Spengler6; 1Institute of Inorganic and Analytical Chemistry, Justus Liebig University Giessen, 35392 Giessen, Germany; 2Gastroenterology, Justus Liebig University Giessen, 35392 Giessen, Germany; 3Institute of Parasitology, Justus Liebig University Giessen, 35392 Giessen, Germany; 4Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany

WP 331 Revealing molecular alterations in gliomeruli with various lesions using CODEX Multiplex Immunofluorescence and MALDI MS: Ellie L Pingly1,2; Melissa A Farrow1,2; Nathan Heath Patterson1,2; Martin Dufresne1,2; Jamie L Allen1,2; Angela RS Kruse1,2,3; Agnes B Fogo1,4,5,6; Mark P Decaestecker2,4; Jeffrey M Spraggins1,2,3,7; 1Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; 2Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; 3Department of Biochemistry and Molecular Biology, Vanderbilt University, Nashville, TN; 4Department of Nephrology, Department of Medicine, Vanderbilt University Medical Center, Nashville, TN; 5Department of Pathology, Microbiology, and Immunology, Vanderbilt University Medical Center, Nashville, TN; 6Department of Pediatrics, Vanderbilt University Medical Center, Nashville, TN; 7Department of Pathology, University of Texas Southwestern Medical Center, Dallas, TX

WP 332 MALDI HIPLEX-IHC on Tissue Microarrays in Neuropathology Research; Yassemin Ucal1; D.R. Naomi Vos1; S. Alexander Iakab1; Henri Bogumill1; Rouzbeh Benan1; Garvey B Yagm1; Signe Frost Friedrickson1; Corinna Henkel1; Mark Lim1; Andreas Von Deimling2,4; Carsten Hopf1,5; 1Center for Mass Spectrometry and Optical Spectroscopy (CeMOS), Mannheim University of Applied Sciences, Mannheim, Germany; 2Department of Neuropathology, Institute of Pathology, Heidelberg University Hospital, Heidelberg, Germany; 3AmberGen, Inc., Billerica, MA; 4Bruker Daltonik GmbH, Bremen, Germany; 5Klinische Kooperationseinheit Neuropathologie, Deutsches Kribsforschungszentrum (DKFZ), Heidelberg, Germany; 6Medical Faculty, Heidelberg University, Heidelberg, Germany

WP 333 Imaging Mass Spectrometry Spectral Analysis of Gastric Proteome Changes after Helicobacter Pylori Infection in Gerbils; Michelle L. Ruyzer1; Jennifer Shuman1; Audra M. Judd1; Hayes McDonald1; Kevin L. Schey1; Timothy L. Cover1,2; Richard M Caprioli1; 1Vanderbilt University, Nashville, TN; 2Veterans Affairs Tennessee Valley Health Care System, Nashville, TN

WP 334 Multidimensional Mass Spectrometry Imaging of Key Biomarkers To Study Ocular Disease: Joshua J O Millar1; Susan Campbell1; Catherine Duckett1; Sarah Doyle1; Laura Cole1; 1Sheffield Hallam University, Sheffield, United Kingdom; 2Trinity College Dublin, Dublin, Ireland

WP 335 Imaging of Fatty Acids in Brains Influenced by Cannabis and the Control of Unwanted Lipid Fragmentation; Samantha L. Cousineau1; Mohammed H. Sarikahya1; Kristina Juricic1; Steven R. Laviolette1; Ken K.-C. Yeung1; 1University of Western Ontario, London, ON

WP 336 Integrating label-free MALDI, MALDI HIPLEX-IHC and SepQuant mass spectrometry imaging to drive drug discovery and development; Bingming Chen1; Jarod Fincher1; Mark P Decaestecker1; 1Institute of Inorganic and Analytical Chemistry, Justus Liebig University Giessen, 35392 Giessen, Germany

WP 337 Enhancement of Lipid Signals in Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry with
WP 338 Label-Free High-Resolution Molecular Imaging of Stratum Corneum by Cluster Secondary Ion Mass Spectrometry (Cluster SIMS) - Naveo Sano; Kate McHardy; Paul Blenkinsopp; Ionoptika Ltd, Eastleigh, United Kingdom

WP 339 Multi-step workflow for visualisation of drug/metabolites and metabolism with DESI-ToF and DESI-Q-ToF mass spectrometers - Emmanuelle Claude; Nyasha Mungoma; Alex Birsan; Ian D Wilson; Joanne B Falanytne; Water & Jones, Inc, Wil. Blvd, United Kingdom; 3Waters Limited, Quebec, N/A; 4Division of Systems Medicine, Department of Metabolism Department of Metabolism, Digestion and Reproduction, Imperial College, Burlington Danes Building, Du Cane Road, London, United Kingdom

WP 340 Mass Spectrometry Profiling of N-Glycans in the Diabetic Pancreas - David A. Tabang; Hua Zhang; Daniel M. Tremmel; Sara Dutton Sackett; Jon Orochi; Lingjun Li; 1Department of Chemistry, University of Wisconsin-Madison, Madison, WI; 2School of Pharmacy, University of Wisconsin-Madison, Madison, WI; 3Department of Surgery, University of Wisconsin-Madison, Madison, WI; 4Department of Surgery, Boston Children’s Hospital, Boston, MA

WP 341 Improving spatial distribution sensitivity and selectivity in MSI, using a novel DESI-Q-ToF and HR-Multi Reflecting ToF systems - Emmanuelle Claude; Farid Jahouh; Martin E. Palmer; Inneke Wynant; Filip Cuyckens; Marjolein Van Heerden; Jan Claereboudt; Bob J Vreken; 1Water & Jones, Inc, Wil. Blvd, United Kingdom; 2Preclinical Sciences & Translational Safety, Jansen Life Sciences, Beerse, Belgium; 3Waters Corporation, Antwerpen, Belgium; 4Maastritch University, Maastricht, Netherlands; 5Waters Corporation, Milford, MA

WP 342 Targeted Quantitative Analysis of the Effect of Fomepizole on Acetaminophen Nephrotoxicity with a DESI Tandem Quadrupole MS Imaging Platform, Jephte Akkapho; Anthony Midley; Bindesh Shrestha; Hartmut Jaeschke; Anup Ramachandran; 1University of Kansas Medical Center, Kansas City, KS; 2Waters Corporation, Milford, MA

WP 343 Mapping Physiologically Relevant Concentrations of Morphine in the Brain by IR-MALDESI MSI - Yury Desyaterik; Audrey Minot; Almira M. Rademeyer; Mary Peace McCrae; Angela D. M. Kashuba; Elias P. Rosen; 1UNC, Chapel Hill, NC; 2Virginia Commonwealth University, Richmond, VA

WP 344 MALDI MSI visualizes the efficacy of cell therapy for treatment of mucopolysaccharidosis in murine brain - Axel Treu; Panagiotis Douvaras; Tim Brandenburger; Beatrice Schnipper; Diego F. Buenaventura; Ashley Lepack; Christoph Patsch; Uwe Thuss; 1Bayer AG, Wuppertal, Germany; 2BlueRock Therapeutics, New York City, NY

WP 345 Enhanced Detection of Brain Charged N-glycans by Infrared Matrix-Assisted Laser Desorption Electrospray Ionization Mass Spectrometric Imaging (IR-MALDESI-MSI) - Juhu Samar; Tanya V. Palomino; Judy Chen; David C Muddiman; Tatiana Segura; 1Duke University, Durham, NC; 2North Carolina State University, Raleigh, NC

WP 346 Glycosphingolipids are important for immune response in Schistosoma mansoni infected hamster liver - tissue studies with high resolution AP-SMALDI MSI - David Luh; Sven Heiles; 1Martin Roderfeld; Christoph G. Greveling; Elke Roeb; Kerstin Strupat; Bernhard Spegler; 1Institute of Inorganic and Analytical Chemistry, Justus Liebig University Giessen, 35392 Giessen, Germany; 2Leibniz Institute for Analytical Sciences - ISAS - e.V., 44139 Dortmund, Germany; 3Lipidomics, Faculty of Chemistry, University of Duisburg-Essen, 45141 Essen, Germany; 4Gastroenterology, Justus Liebig University Giessen, 35392 Giessen, Germany; 5Institute for Parasitology, Justus Liebig University Giessen, 35392 Giessen, Germany; 6Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany

WP 347 Desorption electrospray ionization – mass spectrometry imaging using cyclic ion mobility improves for the separation of lipids isoforms - Ludovic Muller; Nivedita Hegdekar; Chimnoy Sarkar; Marta M. Lipinska; 1Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; 2Department of Chemistry, University of Wisconsin-Madison, Madison, WI; 3Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; 4Vanderbilt University, Department of Biochemistry, Nashville, TN; 5Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; 6Department of Chemistry, Vanderbilt University, Nashville, TN

WP 348 MALDI IMS Reproducibility for the Study of Large Sample Cohorts - Katerina V Djambaysova; Lukasz G Migas; Martin Dufresne; Jamie L. Allen; 1Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; 2Vanderbilt University Medical Center, Nashville, TN; 3Department of Chemistry, University of Wisconsin-Madison, Madison, WI; 4Department of Surgery, University of Wisconsin-Madison, Madison, WI; 5Department of Surgery, Boston Children’s Hospital, Boston, MA

WP 349 Mapping Alzheimer’s disease with integrated MALDI IMS and highly multiplexed immunofluorescence microscopy - Claire F. Scott; Cody R Marshall; Wilber Romero Fernandez; Melissa A Farrow; Angela Kruse; Allison B Esselman; 1Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; 2Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; 3Vanderbilt University, Department of Biochemistry, Nashville, TN; 4Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; 5Biomolecular Multimodal Imaging Center, Vanderbilt University, Nashville, TN; 6Chemical Physical Biology Program, Vanderbilt University School of Medicine, Nashville, TN; 7Department of Pathology, Vanderbilt University, Nashville, TN; 8Department of Biochemistry, Vanderbilt University, Nashville, TN; 9Department of Chemistry, Vanderbilt University, Nashville, TN; 10Cerebral Amyloid Angiopathy Clinic, Vanderbilt University Medical Center, Nashville, TN

WP 350 Metabolite biomarkers associated to specific anatomotopical changes for non-invasive, high-sensitivity and high-resolution in vivo imaging by MALDI-MSI functionalized with focalized femtosecond pulsed infrared laser - Sumin Na; Young-Jin Lee; 1Iowa State University, Ames, IA; 2University of Texas, Austin, TX

WP 351 Mass spectrometry imaging of lipidome in a mouse model of blast-induced traumatic brain injury (TBI) - Michal Falet; 1Manjhi Pratap; 2Manxi Yang; 3Palek Manchanda; 4Julia Laskin; 5Gaurav Chopra; 6Purdue University, West Lafayette, IN; 7Purdue University, WEST LAFAYETTE, IN

WP 352 Exploring in vivo deuteron labeling in surface tissues of Arabidopsis thaliana using MALDI-MS imaging - Troy R. Scoogins; Amanda Pebenito; Jonathan T. Specker; 1Duke University, Durham, NC; 2North Carolina State University, Raleigh, NC
WP 354 Rapid and high spatial mapping of drugs by atmospheric pressure matrix-assisted laser desorption ionization mass spectrometry imaging: REPORT.

WP 355 Mass Spectrometry Imaging of Neuropeptide Neuropeptides in DOX-Administered BRC2 Knockout Mice

WP 356 Trace Level Quantification of Nitrosamine Impurities in Tuberculosis Medicines by LC-MS/MS; Qiya Li; Qun Xu; Nadine Lo; Alain Leeks; Mark Han; Marcela Nelliu; Jack Simpso; Jennifer Belsky; Michael Chapman; Richard Chapman; Neil Landers; Waters corp, milford, MA; Waters Corporation, Milford, MA

WP 357 Native Datalake; enabling a Data Pipeline for Data Analysis with small to medium Native datasets; Ryan P Marchand; Richard Chapman; Neil Landers; Waters corp, milford, MA; Waters Corporation, Milford, MA

WP 358 Rapid and high spatial mapping of drugs by atmospheric pressure matrix-assisted laser desorption ionization mass spectrometry imaging: REPORT.

WP 359 Identification of Unknown Compounds Observed in the Leachables Study of a Protein Drug by Liquid Chromatography High-Resolution Mass Spectrometry: Jie Du; Tracy Zhou; Sven Hackbusch; Kelly Broster; Genentech Inc., South San Francisco, CA; Thermo Fisher Scientific, San Jose, CA; Thermo Fisher Scientific, Hemel, United Kingdom

WP 360 Sequence confirmation and impurity characterization of therapeutic oligonucleotides – A quality by design approach: Giovanni Calderisi; Patrik Platter; Agron Selami; Bachem AG, Bubendorf, Switzerland

WP 361 Enhanced screening for Active Pharmaceutical Ingredients (APIs) through the integration of a single quadrupole mass spectrometer; Kathleen K Luu; Ethan R Hain; Om K Shrestha; Evelyn H Wang; Xiaomeng Xia; Robert English; Tiffany Liden; Christopher Gilles; Shimadzu Scientific Instruments, Columbia, MD

WP 362 Quantitative Analysis of Azido Impurities in Five Sartan Drug Substances using a Triple Quadrupole Mass Spectrometer: Kate (xiaomeng) Xia; Loqan Miller; Evelyn H. Wang; Taira Ogura; Yoshiyuki Okamura; Shimadzu Scientific Instruments, Columbia, MD

WP 363 Novel Time-Of-Flight Residual Gas Analyzer (TOF-RGA) for in situ real-time Process Monitoring: Lukas Hölter; Sébastien Gasc; SpaceTech Technology AG, Gümlegen, Switzerland

WP 364 Method for non-destructively screening wine cork stoppers for 2,4,6-trichloroanisole below the perception threshold at a sampling speed of 2 seconds; Luca Cappellini; Luigi Cioti; Manuel Hutteri; Michael Groessel; TOFWERK, Thuin, Switzerland

WP 365 An Improved Method for Quantifying Glyphosate Impurity in Glyphosate API using LC/MS/MS via Standard Addition; Chun-Ye Sun; Shao-Zhen Wang

WP 366 Chemical composition profiles of residues from in situ burning of fresh and weathered conventional and unconventional oils; Ashish Sarker; Trent University, Peterborough, ON

WP 367 Identification and quantification of 25 crystallization solvents in support of pharmaceutical solid-form screening studies using a single SIFT-MS method; Frank Tarczynski; Joanna Bis; Elliott Franco; Leslie Silva; Vaughan Langford; Alcamo Corporation, Morrisville, NC; Syft Technologies, Los Angeles, CA; Syft Technologies, Christchurch Central City, New Zealand

WP 368 Operating, maintaining, and troubleshooting the sensitivity and robustness of timeTOF platforms for proteomics studies: Benoit Fatou; Conor Mullens; Elizabeth Gordon; Diego Assis; Alvaro Sebastian Vaca; Michael Krawitzky; Matt Willetts; Bruker Scientific LLC, Billerica, MA; Bruker Scientific LLC, San Jose, CA

WP 369 Equipment and facility decontamination of de-lactams and other allergenic pharmaceutical products using Chloride dioxide with LC/MS/MS monitoring; Robert D. Voykner; Paul Lorcheme; LCMs Limited, Durham, NC; Cidor/isys Solutions Inc., Branchburg, NJ

WP 370 Improving Precision and Accuracy of a LC/MS-MS Quantitation Method by Implementing Automation of Sample Extraction Procedures; Junlong Shao; Pharmaron ABS, Germantown, MD

WP 371 Understanding K. phaffii (Pichia pastoris) Host Cell Protein Clearance through Flow-Through Affinity in Biomunagering using Proteomics Approaches; Taufika Islam Williams; Leonard B Collins; Suhbana Srirapa; Stefano Menegatti; NCSU, Raleigh, NC

WP 372 PTM localization score MaxTopos for data-independent acquisition data through Affinity in the phosphoproteomics provides accurate site localization; Pelagia Kyriakidou; Shamil Urazbakhtin; Tanja Bange; Maria Robles; Juergen Cox; Computational Systems Biochemistry Research Group, Max-Planck Institute of Biochemistry, Martinsried, Germany; Institute of Medical Psychology and Biomedical Center, Faculty of Medicine, Ludwig-Maximilians-University, Munich, Germany

WP 373 XMass: XBoost-based peptide spectral library prediction integrated into MaxQuant for DIA and DIA data analysis; Shamil Urazbakhtin; Favo Salinas-Soto; Pelagia Kyriakidou; Juan Luis Restrepo-Lopez; Juergen Cox; Computational Systems Biochemistry Research Group, Max-Planck Institute of Biochemistry, Martinsried, Germany

WP 374 Mass spec ver. 4 – An open-source MS data viewer with enhanced basic functions and easy implementation of external software: Satoshi Tanaka; Masaki Murase; Masaki Kato; Hiroyuki Yamamoto; Tsuyoshi Tabata; Maiko Kusano; Shin Kawano; Susumu Goto; Yasushi Ishihama; Akyasu C. Yoshizawa; Shamil Urazbakhtin; Tanja Bange; Maria Robles; Juergen Cox; Computational Systems Biochemistry Research Group, Max-Planck Institute of Biochemistry, Martinsried, Germany; Institute of Medical Psychology and Biomedical Center, Faculty of Medicine, Ludwig-Maximilians-University, Munich, Germany; School of Medicine, Showa Univ., Shinagawa, Japan; Tayaama Univ., Tayaama, Japan; DBCLS, DS, ROIS, Kashawa, Japan

WP 375 Fully automated and spectrum-centric processing of parallel reaction monitoring (PRM) data: Daniel P. Zolg; Tobias Schmidt; Siegried Gessult; Florian Seefried; Samia Ben Fredj; Mathias Wilhelm; Martin Heinrich Frejno; MSAID GmbH, Garching b.München, Germany; Computational Mass Spectrometry, Technical University of Munich, Freising, Germany

WP 376 Tissue deconvolution using cell-type specific protein profiles: The whole is more than the sum of its parts; Justus Zeinert; Bernhard Y Renard; Christoph N Schlaaffner; Data Analytics and Computational Statistics Group, Hasso Plattner Institute, University of Potsdam, Potsdam, Germany

WP 377 Aligning DIA Proteomics Data in Space: A Large-Scale Citizen Science Projects; Toon Callens; Tine Claes; Sander Willems; Maarten Dhaeneens; Lennart Martens; VIB-Ugent Center for Medical Biotechnology, Gent, Belgium

WP 378 Operating, maintaining, and troubleshooting the sensitivity and robustness of timeTOF platforms for proteomics studies: Benoit Fatou; Conor Mullens; Elizabeth Gordon; Diego Assis; Alvaro Sebastian Vaca; Michael Krawitzky; Matt Willetts; Bruker Scientific LLC, Billerica, MA; Bruker Scientific LLC, San Jose, CA

WP 379 Equipment and facility decontamination of de-lactams and other allergenic pharmaceutical products using Chloride dioxide with LC/MS/MS monitoring; Robert D. Voykner; Paul Lorcheme; LCMs Limited, Durham, NC; Cidor/isys Solutions Inc., Branchburg, NJ

WP 380 Improving Precision and Accuracy of a LC/MS-MS Quantitation Method by Implementing Automation of Sample Extraction Procedures; Junlong Shao; Pharmaron ABS, Germantown, MD
WP 378 midiaID: A spectra-centric pipeline for the analysis of the midiaPASEF data; Mateusz Krzyztof Lacki1; Ute Distler2; Michał Piotr Startek1,2; David Teschner3; Sven Brehmer2; Jens Deckert2; Thilo Schöld1; Jonathan R Krieger1; Florian Krohs2; Oliver Raether2; Andreas Hildebrandt2; Stefan Tenzer2
1 University Medical Center, Johannes Gutenberg University, Mainz, Germany; 2Faculty of Mathematics, Informatics, and Mechanics, University of Warsaw, Warsaw, Poland; 3Institute for Informatics, Johannes-Gutenberg University, Mainz, Germany; 4Bruker Daltonics GmbH & Co.KG, Bremen, Germany; 5University Medical Center of Mainz, Mainz, Germany; 6Bruker Ltd., Milton, ON

WP 380 MicId: a MS-based Workflow for Fast and Accurate Microbe Identification, Antibiotic Resistance Protein Identification, and Biological Activity Estimation; Christian Alves1; Aleksy E Ogurtsov2; Roger Karlsson1; Daniel Jaen-Luchoro1; Beatriz Piñero-Iglesias3; Francisco Salví-Serra4; Björn Andersson2; Edward R B Moore2; Yi-Kuo Yu1; 1CBB NCBI NLM NIH, Bethesda, MD; 2University of Gothenburg, Gothenburg, Sweden

WP 381 A Protein Functional Map Learned from Pan-cancer Multi-Omics Data Enlightens Somatic Mutations, Understudied Genes, and Cancer Hallmarks; Zhiao Shi1; Jonathan Lei1; Bing Zhang1; 1Baylor College of Medicine, Houston, TX

WP 382 Finding Cancer Hallmarks Through Changes in mRNA/protein Relationships; Jose Humberto Giraldez Chávez1; Samuel H Payne1; 1Brigham Young University, Provo, UT

WP 383 Untangling the Connection between Caloric Restriction and Prolonged Survival in Non-human Primates through a Multi-omics Approach; Salma Ibrahim1; Abuehlela Hassan2; Katherine A. Oyeneweri3; Timmy W. Rhoads4,5; Rosalyn M. Anderson4,5,6; Joshua J. Coon4,5,7; 1University of Wisconsin-Madison, Madison, WI; 2Department of Biomedical Chemistry, University of Wisconsin - Madison, Madison, WI; 3Morgue Institute for Research, Madison, WI; 4Department of Nutritional Sciences, University of Wisconsin-Madison, Madison, WI; 5Department of Medicine, University of Wisconsin-Madison, Madison, WI; 6Geriatric Research, Education, and Clinical Center, William S. Middleton Memorial Veterans Hospital, Madison, WI; 7Department of Chemistry, University of Wisconsin-Madison, Madison, WI

WP 384 Multimodal analysis of COVID-19 samples to identify molecular signatures; Baptiste Bauvin1,2; Claudia Carpentier1,2; Thibaud Godon2,4; Maxime Derasee2; Jacques Corbel1,5; 1Corbell Laboratory, CRCHU de Quebec - Université Laval, Quebec, QC; 2GRAIL, Université Laval, Quebec, Quebec

WP 385 Novel tandem nano and capillary flow LCMS-based approach for facile 24/7 proteome profiling with near 100% MS; Runsheng Zheng1; Martin Rendl2; Christopher Swaney1; Adolfo Garcia-Sastre1; Clare Jolly2; Lorena Zuliani-Alvarez2; Greg Towers3; Nevan J Krogan3; 1UCSF, San Francisco, CA; 2Texas Biomedical Research Institute, San Antonio, Texas; 3Icahn School of Medicine at Mount Sinai, New York, NY; 4University College London, London, United Kingdom; 5University College London, London, United Kingdom; 6Novartis Institutes for Biomedical Research, Inc., Cambridge, MA

WP 386 Systems proteomics reveals SARS-CoV-2 variants evolve convergent molecular strategies to remodel host signaling and protein complexes; Mehdi Boughrara1; Athina-Kathrin Reusch1,2; Benjamin Pelacco3; Lucy G Thorne2; Manisha Ummadevi2; Chengjin Ye2; Luis Martinez-Sobrido4; Lisa Miorini4; Kris White5; Danielle L Madonet; Aedel Garcia-Sastre5; William Bellamy6; Ilona Rejman6; Matthew Willetts1; 1University of Wisconsin - Madison, Madison, WI; 2Baylor College of Medicine, Houston, Texas; 3UCSF, San Francisco, CA; 4University College London, London, United Kingdom; 5University College London, London, United Kingdom; 6Novartis Institutes for Biomedical Research, Inc., Cambridge, MA

WP 387 A complete, modular, and flexible proteogenomic pipeline for peptide neoantigen discovery and verification, Tyler Jubenville1; James E Johnson1; Sue Rathe2; Flavia Popescu3; Kyle Richards3; Suzanne Coleman4; Reid Wagner1; Fengchao Yu5; Alexey I. Nesvizhskii1; Subina Mehta1; Pratik D Jagtap1; David Largaespada1,2; Timothy J. Griffin5; 1University of Minnesota, Minneapolis, MN; 2University of Michigan, Ann Arbor, MI
WP 398 High-Resolution Separation of Biosolmers Using Ion Cloud Profiling Method: Xiaoyu Zhou1; Zhufan Wang2; Jingin Fan3; Zheng Ouyang3; Tsinhua University, Beijing, China

WP 399 The new type of electron impact mass spectrometer of ultra high resolution on the bases of multielectrode harmonized Kingdom trap: Eugene Kevych1; Oleg Kharybin2; Gleb Vladimirov3; Sergey Gorbatov4; Anton Liozov5; Petr Borisovets1; Alexander Semenov1; Skolkovo institute of science and technology, Moscow Region, Russian Federation

WP 400 Depth Profiling Study on Organic Monolayer by using Ar-GCIB and LDI-ToFMS: Ji Young Baek1; Chang Min Choi2; Korea Basic Science Institute, Cheoungju, South Korea; 2Korea Basic Science Institute, Cheoungju, South Korea

WP 401 Probing the First Stages of Photoinitiated Polymerisation with an On-Line Photochemical Reactor Coupled Mass Spectrometer: Oisin J Shiels1; Maria Mentli-Platten2; Brett Burns2; Paul Keller2; Philip J Barker2; Adam J Treadwell1; Adam Treadwell, University of Wollongong, Wollongong, Australia; 2University of Wollongong, School of Chemistry, Wollongong, Wollongong, Australia

WP 402 A novel high capacity ion trap to enhance duty cycle of time of flight mass spectrometer: Masayuki Sugiyama1; Shun Kumano1; Yuichiro Hashimoto2; Akihiro Nojima3; 1Research & Development Group, Hitachi Ltd., Kokubunji, Japan; 2Hitachi-HighTech Corporation, Hitachinaka-shi, Japan

WP 403 Characterization of a Novel PTR-TOFMS Instrument for Next Level Analysis of the Gas and Particle Phase: Alfons Jordan1; Christian Lindinger1; Markus Müller1; Tobias Reinecke1; Markus Leiminger1; Klaus Winkler1; Lukas Märk1; Todd Rogers1; Philipp Sulzer2; 1IONICON Analytik GmbH, Innsbruck, Austria; 2Trace VOC, Kennewick, WA

WP 404 An innovative prototype of mass spectrometry system based on a nano-opto-electromechanical (NOEMS) resonator sensor: Wioletta Trzpił1; Adrien Reynaud1; Louis Dartiguemaille2; Vaiton Cumakú1; Guillaume Jourd11; Sébastien Hentz1; Christophe Masselolin2; Marc Sansa2; 1CEA-LETI, Université Grenoble Alpes, F-38000, Grenoble, France; 2Oberon Sciences, 300 avenue des papeteries, Villard-Bonnot, France; 3Villard-Bonnot, France; 4CEA, IRIG, Grenoble, France; 5CEA, LITEN, Grenoble, France

WP 405 Development and hybridization of orthogonal acceleration ToFMS and QIT-ToF-SIMS: Jaevoing Eo1; Chang Min Choi1; 1Korea Basic Science Institute, Daejeon, South Korea; 2Korea Basic Science Institute, Cheoungju, South Korea

WP 406 A Study of the Improved Limitations of Bicubic Interpolation for both Field Analysis and Trajectory Calculations in SIMION: Robert Jackson1; Mark Osgood1; 1Ashwood Labs, LLC, Wilton, NH

WP 407 Characterization of a detection system with high sensitivity and dynamic range for a novel HRAM mass spectrometer: Johannes Petzoldt1; Toby Stanley1; Wilko Balachun1; Philipp Cochems1; Bernd Hagedorn1; Christian Hock1; Barbara Lavi1; Daniel Mourad1; Maximilian Ohmann1; Robert Ostermann1; Semyon Shofman1; Alexander Kadyshevitch1; 1El-Mul Technologies, Rehovot, Israel

WP 408 Versatile, long-lifetime, wide dynamic range detector for TOF applications: Jonathan Gare1; Amit Weingarten1; Semyon Shofman1; Alexander Kadyshevitch1; 1El-Mul Technologies, Rehovot, Israel

WP 409 Detection and accurate mass measurement of difficult to handle negatively charged compounds using Chemical Ionization MS (CIMS): Alan T. Taylor1; Colin L. Mackay1; 1University of Edinburgh, Edinburgh, United Kingdom

WP 410 TENG for the Masses: A Low-cost Triboelectric Ion Source for Lipid Double Bond Localization and Other Nanoelectrospray Applications: Carter A Sel1; Facundo Fernandez1; 1Georgia Institute of Technology, Atlanta, GA

WP 411 On-Paper Electrokinetic Separation and Stacking Coupled to Paper Spray MS for Sub-ppt Screening of Per-polyfluoroalkyl substances (PFAS) In Tap Water: Magnus P Ryberg1; Nicholas Manicke1; 1Indiana University Purdue University Indianapolis, Indianapolis, IN

WP 412 Development and Evaluation of a Novel Accumulation Ion Source for Chemically Instable Compounds: Joshua Rieger1; Sanna Benter1; Markus Langner1; Niklas Pengemann1; Philipp Rogtinger1; Hendrik Kees1; Thorsten Benter1; 1University of Wuppertal, Wuppertal, Germany

WP 413 Localization of labile tyrosine sulfation using an alternative electron-based MS/MS approach in positive and negative ion modes: Mark Lies1; Haichuan Liu1; Takashi Baba1; Zee Zhang1; Elliott Jones1; 1Sciox, Brea, CA; 2SCIEX, Redwood City, CA; 3University of California, Los Angeles, CA; 4Emory, GA

WP 414 LIFDI technique coupled to Orbitrap Explor MS: Mathias Linden1; Tobias P. Wörner1; Kerstin Strupat1; 1Linden CMS, Weyhe, Germany; 2Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany

WP 415 Catalyst-free high yield post column online microdroplet derivatization for LC/MS detection of depurinating DNA adducts: Hugam J.S. Kaleem1; Shu-Hui Chen1; 1National Cheng Kung University, Tainan, Taiwan

WP 416 Automated microfluidic open interface for direct coupling of solid-phase microextraction to mass spectrometry to facilitate rapid and high-throughput analysis: Wei Zhou1; Enir Nazdrajic1; Janusz Pawliszyn1; 1University of Waterloo, Waterloo, Ontario

WP 417 Automating Minimally-Invasive Liquid Microinjection Sampling to Profile Large, Intact Objects: Yiming Wang1; Shimadzu Research Laboratory (Shanghai) Co., Ltd., Shanghai, China

WP 418 Characterization and comparison of theta-capillary and single-channel capillary tip generation for use in nano-electrospray ionization: Jacob P. Hatvany1; Craig A. Aspinwall2; 1Baylor University, Waco, TX; 2University of Arizona, Tuscon, Arizona

WP 419 Development of a compact TLC sampler for MS and its applications: Yiming Wang1; Shimadzu Research Laboratory (Shanghai) Co., Ltd., Shanghai, China

WP 420 AMMONIA project: “Detection of Ammonium Compounds in Marine Systems using Membrane Inlet Laser-Photolysis Mass Spectrometry (PIMS)”: Christian Gehm1; Caroline Schwarz2; Sven Ehler1; Denis Starostin-Penner1; Johannes Passig3; Dominik Kastner4; Christian Menhard5; Eric Achterberg1; Andreas Walte1; Ralf Zimmermann1; 1Leibniz Institute for Baltic Sea Research, Rostock, Germany; 2Joint Mass Spectrometry Centre, Chair of Analytical Chemistry, University of Rostock, Rostock, Germany; 3Photonion GmbH, Schwerin, Germany; 4InnoLas Laser GmbH, Kralling, Germany; 5GEOMAR Helmholtz Centre for Ocean Research Kiel, Kiel, Germany

WP 421 Effect of PEG-modification to capillary surfaces for analysis of carbohydrates and carbohydrate-containing molecules using nano-electrospray ionization-mass spectrometry: Emma-Le P. Olsen1; Jacob B. Hatvany1; Chih-Chieh Hsieh1; Craig A. Aspinwall2; G. Le Olsen3; Elsya S. Gallagher1; 1Baylor University, Waco, TX; 2University of Arizona, Tuscon, Arizona
WP 422 Electrochemically etched tapered-tip stainless-steel electrospray-ionization emitters; Jordan T. Aerts; Per E. Andren; Erik T. Jansson; Uppsala University, Uppsala, Sweden

WP 423 In-Situ Liquid Biopsy Combined with Native Surface Mass Spectrometry and Top-Down-Bottom-Up Proteomics: Raul Villacobo; Sarah C Bено; Neda Feizi Gilandeh; Touradj Solouki; Baylor University, Waco, TX

WP 424 Direct Sampling and Ionization of E-Cigarette Aerosol; Nicole C Auel; Mark E Bier; Carnegie Mellon University, Pittsburgh, PA

WP 425 Controlled synthesis of oligopeptides from simple amino acids in aqueous microdroplets by triboelectric nanogenerator non-electrospray mass spectrometry; Ziad Mahmoud; Daniel V. Vallejo; Facundo M Fernandez; School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA

WP 426 A NOVEL METHOD FOR THE SAMPLING OF NATIVE IONS FROM A DISTANT LOCATION; Hendrik Kersten

WP 427 In-tip microextraction enables fast profiling of phospholipid isomers in plasma by mass spectrometry; Qiqian Zhang; Penglong Lian; Zheng Quyang; Wenpeng Zhang; State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instrument, Tsinghua University, Beijing, China

WP 428 Deep Ultraviolet Laser Ablation and Capture for Off-line Mass Spectrometry; Kadeem O Hayes; Blessing Egbejioju; Neda Feizi Gilandeh; Kelcey B. Hines; Touradj Solouki; Kermit K. Murray; Louisiana State University, Baton Rouge, LA; Baylor University, Waco, TX

WP 429 High-Throughput 'Dip-n-Sip' OPI-MS/MS sampling; Nate Hoxie; Savannah Wood; Vijay Veenvisetty; Anthony Garrison; Pranav Bende; John Janiszewski; Jonathan Shrimp; Colin Kelly; Meghav Verma; Charles Bonney; Sam Michael; Matthew Hull; Peter Korkavi; Chang Liu; Thomas R. Covey; NIHN/CATS, Rockville, MD; SCIX, Concord, ON

WP 430 Developing a low-cost general-purpose corporate multiport inlet for immediately accessible atmospheric pressure and vacuum ionization methods; Charles N McEwen; Mila Pophristic; Research and Development, MSTM, LLC, Philadelphia, Pennsylvania; Saint Joseph's University, Philadelphia, PA, United States, Philadelphia, Pennsylvania

WP 431 Construction and applications of a “plate-source” on API mass spectrometers: a robust, fast, and sensitive ionization method operating from AP; Sarah Trimpin; Trine Halvorsen; James Wagner-Miller; Ken Mackie; Milan Pophristic; Charles McEwen; Ellen Inutani; Wayne State University, Detroit, MI; Department of Pharmacy, University of Oslo, Oslo, Norway; Psychological and Brain Sciences Campus, IU Bloomington, Bloomington, IN; Department of Chemistry, Mindanao State University-Iligan Institute of Technology, Iligan City, Philippines

WP 432 Detection of plasma ions by coupling a high resolution TOF-MS at minimum distance to EUV-light focus point; Niklas Pengemann; Adelind Eilash; Ismael Giisch; Hendrik Kersten; Sascha Brosse; Carlo Holty; Peter Gust; Thorsten Benter; University of Wuppertal, Wuppertal, Germany; RWTH Aachen University, Aachen, Germany

WP 433 Structural characterization and identity confirmation of anthocyanins in plant extracts by direct injection ion mobility-mass spectrometry; River Pachulicz; Long Yu; Blagojce Jovcevski; Vincent Bulone; Tiera L Fukala; Finders University, Adelaide, Australia; ABANova University Centre, Stockholm, Sweden

WP 434 Separation and Quantification of Fentanyl Isomers with Liquid Chromatography-Ion Mobility-Mass Spectrometry (LC-IM-MS); Ralph Aderoh; Christopher D. Chouinard; Clemson University, Clemson, SC

WP 435 Differentiation of Regioisomers of Sulfonylazic Acid by Traveling-wave Ion Mobility Mass Spectrometry (TW-IM-MS); Athula Attigalle; Jinxin Zhang; Meenu Kumar; Spencer Pinto; Stevens Institute of Technology, Hoboken, NJ

WP 436 Ion mobility tandem mass spectrometry of chondroitin sulfate disaccharide domains in biglycan; Mirela Sarbu; Raluca Ica; Edie Sharan; David E. Olemmer; Alina D. Zamir; National Inst for R&D in Electrochemistry and Condensed Matter, Timisoara, Romania; Institute University Bloomington, Bloomington, IN; Department of Technical and Natural Sciences, Aurel Vlaicu University of Arad, Arad, Romania

WP 437 Separation and sequencing of isomeric proteoforms of intact proteins with multiple post-translational modifications by top-down IMS-MS/MS; Francis Berthias; Maša Babović; Nurgül Bilgin; Jasmin Mecinovic; Ole Norregaard Jensen; Department of Biochemistry and Molecular Biology, VILLUM Center for Bioanalytical Sciences, University of Southern Denmark, Odense, Denmark; Department of Physics, Chemistry and Pharmacy, University of Southern Denmark, Odense, Denmark

WP 438 Development of Automated Online, High-Throughput Native Ion Mobility Mass Spectrometry Methodologies for Biotherapeutic Screening; Brock R Juliano; Henry W Li; Anna G Anders; Zhuoer Xie; Brandon T Ruotolo; University of Michigan, Ann Arbor, MI; Angen, Inc., Thousand Oaks, CA

WP 439 Analysis of Copper Ether-Alkali Metal Complexes Derived from Monomeric and Polydisperse Polymer Samples; Hawkins Shepard; Jody C. May; David M Hercules; John A. McLean; Vanderbilt University, Nashville, TN

WP 440 Detection and Characterization of Bacteria in Surface Water using LC-IM-MS/MS; Kimberly Y Kartowikromo; Orocola E Olajide; Ahmed M Hamid; Auburn University, Auburn, AL

WP 441 Characterization of Diabetes Biomarkers using High Resolution Ion Mobility – Mass Spectrometry; Michael W Christopher; Daniel Debord; Boone M. Prentice; Richard A. Yost; Timothy J. Garrett; University of Florida, Chemistry Department, Analytical Chemistry Division, Gainesville, FL; MOBILion Systems, Inc., Chadds Ford, PA

WP 442 Improving confidence in identification of per- and polyfluoroalkyl substances (PFAS) in abandoned eggs using ion mobility and time-of-flight mass spectrometry; Zacheriah A Gernold; Joshua S. Wallace; Alicia Perez-Fuentetaja; Diana Aga; University at Buffalo, Buffalo, NY; RENEW Institute, Buffalo, New York; Buffalo State, The State University of New York, Buffalo, New York

WP 443 CCS-saveware-wise scope target screening utilizing LC-TIMS-HRMS and a new heatedESI source—the answer to environmental and human biomonitoring challenges; Konstantina S. Diamanti; Reza Aalizadeh; Dimitrios E. Damalas; Georgios O. Gkotsis; Bob Galvin; Artem Filipenko; Carsten Baessmann; Nikolaos S. Thomaidis; National and Kapodistrian University of Athens, Athens, Greece; Bruker UK Ltd., Coventry, United Kingdom; Bruker Daltonics, Billerica, MA; Bruker Daltonics GmbH & Co. KG, Bremen, Germany

WP 444 A facile method to generate DDA spectral libraries for DIA analysis provides comparable proteome coverage to a library-free approach; Jessica Wohlfahrt; Emilee Musto; Jennifer Guerard; Lindley B. Shaw; Sidney Stevens Jr.; University of South Florida, Tampa, FL
WP 445  Peptide collision cross section of 22 post-translational modifications; Andreas Will; Denys Olinykov; Florian Meier-Rosar; Jena University Hospital, Jena, Germany

WP 446  Comprehensive 4D workflow for targeted and untargeted screening of PFAS in organisms from different trophic levels utilizing LC-VIP HESI(T)-TIMS-QToF MS; Georgios O. Gkotsis; Dimitrios E. Damalas; Maria-Christina Nika; Bob Galvin; Carsten Baessmann; Nikolas S. Thomaidis; National and Kapodistrian University of Athens, Athens, Greece; Bruker UK Ltd., Coventry, United Kingdom; Bruker Daltonics GmbH & Co. KG, Bremen, Germany

WP 447  Analyzing Polysorbates with a High Resolution Ion Mobility Platform Based on SLIM Technology; Dustin Klein; Komal Kedia; Adam Sutton; Jon Degnore; Daniel Debord; Xuanwen Shawn Li; Hillary A. Schuessler; Merck & Co., West Point, PA; MOBILion Systems, Inc, Chadds Ford, PA

WP 448  Unlocking new levels of structural information for proteins relevant to cultural heritage using native and top-down mass spectrometry; Daniel D Vallejo; Vaclav Krupicka; Aleksandra Popowich; Julle Arslanoglu; Caroline Tokarski; Facundo M Fernandez; Georgia Institute of Technology, Atlanta, GA; Institute of Chemistry and Biology of Membrane and NanoObjects (CBMN), CNRS UMR 5248, Bordeaux Proteome, University of Bordeaux, Bordeaux, France; The Metropolitan Museum of Art, New York City, NY

WP 449  Characterization of polyubiquitinated proteins using ion mobility-mass spectrometry (IM-MS) supplemented with the collisional activation of ions; Elizaveta Shrestopova; Eric Striter; University of Massachusetts Amherst, Amherst, MA

WP 450  Native Hi-Res-MS Eliminates Chemical Noise and Enables Quantitative Structure Analysis of ALS-associated SOD1 Proteoforms; Md Amin Hossain; Brandon C. Miller; Roman Manetsch; Jared R. Auclair; Jeffrey N. Agar; Northeastern University, Boston, MA; Harvard Medical School, Boston, MA

WP 451  High Performance Ion Mobility Spectrometry for Plasma Cleaning Validation: Directspray for Real-Time Analysis vs. Autosampler for High-Throughput Sample Analysis; Julia Kaszczik; Rory McCormin; Ching Wu; ExcelLims Corporation, Acton, MA

WP 452  Prediction of ion mobilities using molecular dynamics based ion-neutral collisions in an open simulation framework (iDSimF); Michelle Raikovic; Maja Hammelrath; Walter Wissdorf; Thorsten Benter; University of Wuppertal, Wuppertal, Germany

WP 453  Ion Clustering and Transformation Reactions during Transit in the HIKE-IMS: Comparing Measurement and Model; Alexander Haack; Christoph Schaefer; Scott Hopkins; Stefan Zimmermann; Leibniz University Hannover, Hannover, Germany; University of Waterloo, Waterloo, ON

WP 454  Simulation of Ion Trajectories in Travelling Wave IMS with an Open Simulation Framework (iDSimF); Maja Hammelrath; Michelle Raikovic; Walter Wissdorf; Thorsten Benter; University of Wuppertal, Wuppertal, Germany

WP 455  Cutting Corners with SLIM: New Rounded Turn Design Improves IM Resolution and Mobility Range of HRIM System; Lui Lin Deng; Adam Engel; Miriam Fico; Daniel Debord; MOBILion Systems, Chadds Ford, PA

WP 456  Deep Ultraviolet Laser Ablation Electrospay Ionization for Native Mass Spectrometry; Kelcey B. Hines; Neda Gilianideh; Raul Villacob; Touradj Solouki; Kermit K. Murray; University of State Louisiana, Baton Rouge, LA; Baylor University, Waco, TX

WP 457  Enabling High Accuracy Collision Cross Section Measurements using Cyclic Ion Mobility-Mass Spectrometry; Devin M. Makey; Ryan Schroeder; Keith Richardson; David Langridge; Jakub Ujma; Kevin Giles; Brandon T. Ruotolo; University of Michigan, Ann Arbor, MI; Waters Corporation, Wilmslow, United Kingdom

WP 458  Using Rigid Molecules to Probe Roles of Charge State, Charge Distribution, and Mass Distribution on Ion Mobility; David V. Dearden; Savannah R. Porter; Jamir Shrestha; Tina Heravi; Brigham Young University, Provo, UT; Intel Corporation, Portland, OR; ARUP Laboratories, Salt Lake City, UT

WP 459  Ramping up the Performance in SLIM: Traveling Waveform Gradients Enhance Mobility, Resolution, Range, and Throughput; Leonard Romer; Ryan Clingman; Sidney Buttrill; Gordon A. Anderson; Miriam Fico; Daniel Debord; MOBILion Systems, Inc., Chadds Ford, PA; Consultant, Palo Alto, CA; GAA Custom Electronics, LLC, Benton City, WA

WP 460  Time-resolved tandem-trapped ion mobility spectrometry/mass spectrometry reveals cooperativity in the unfolding of native-like proteins; Tyler C. Cropley, Fanny C. Liu, Mengei Chai; Christian Bleiholder; Florida State University, Tallahassee, FL

WP 461  Measuring the Conformational Ensemble of Caspase-9 using Ion Mobility-Mass Spectrometry and Collision-Induced Unfolding; Trisha W. Brady; Stacey Nash; Kristalle G. Cruz; Ishan V. Soni; Jeanne A. Hardy; Richard W. Vachet; University of Massachusetts Amherst, Amherst, MA

WP 462  Multi-faceted MS-Enabled Discovery, Characterization, and Localization of a Novel D-Amino Acid-Containing Neuropeptide in the American Lobster Nervous System; Gaoyuan Lu; Wenxin Wu; Vu Ngoc Huong Tran; Hua Zhang; Min Ma; Zhijun Zhu; Shuling Xu; Lingjun Li; University of Wisconsin-Madison, Madison, WI

WP 463  Labeling strategies for inducing mass distribution shifts in high-resolution cyclic ion mobility separations coupled to mass spectrometry; David L. Williamson; Gabe Nagy; University of Utah, Salt Lake City, UT

WP 464  Regulations of Many Solution Structures of Chymotrypsin Inhibitor 2 though ESI-IMS-MS Measurements; Hua Pan; Shannon A. Raab; Lucas W. Henderson; Samantha R. Schrecker; Arthur Laganowsky; David H. Russell; David E. Clemmer; Indiana University Bloomington, Bloomington, IN; Texas A&M University, College Station, TX

WP 465  Characterization of Conformational Isomers of Proteins using Ion Mobility and Collision Induced Unfolding; Michael L. Moore; Stacey Nash; Richard W Vachet; University of Massachusetts Amherst, Amherst, MA

WP 466  Determining the Independence of Stability of chlorophenolphen acetyltransferase (CAT) and the effects of ligand binding; Alexis N. Edwards; Anthony J. Blue; Michael S. Cordes; Jessica M. Conforti; Michael A. Traksellas; Elyssia S. Gallagher; Baylor University, Waco, TX

WP 467  Composite Multidimensional Ion Mobility-Mass Spectrometry for Improved Differentiation of Stereocahemical Modifications; Xia Xu; Li Han; Zhen Zheng; Rui Zhao; Lingjun Li; Xiueuang Shao; Gongyu Li; Nankai University, Tianjin, China; Tianjin Medical University, Tianjin, China; University of Wisconsin-Madison, Madison, WI

WP 468  Ion Mobility and Collision Induced Unfolding Reveal Lipid Nanoparticle-Induced Changes in RNA Structure and Stability; Anna G. Anders; Brandon T. Ruotolo; University of Michigan, Ann Arbor, MI

WP 469  IMS-IMS on a Cyclic Ion Mobility Instrument Coupled to Variable Temperature Electrospray Ionization Elucidates Structural Landscapes of Tetrameric Proteins; Edie M. Sharon; Lucas W. Henderson; Sarah M. O’Keefe; David E. Clemmer; Indiana University Bloomington, Bloomington, IN

WP 470  Trapped ion mobility mass spectrometry in nucleic acid drug-discovery: revealing conformation-specific
preferential binding to regulatory structures of the SARS-CoV-2 genome; Ghazaleh Yassagheli; Thomas Kenderdine; Jyotsna Kumar; Daniela Fabris; University of Connecticut, Storrs, CT

WP 471 Structural Characterization of Isomeric Indium-Doped Octanuclear Iron-Oxo Clusters with Cucube Core using Ion Mobility Mass Spectrometry; Solita Marie Wilson; Holly Bohlin; Susana Herrera; Raphael Raptis; Julia Laskin; Purdue University, West Lafayette, IN; Florida International University, Miami, FL

WP 472 Correlating Conformation to Function of Disease-linked Labile Protein Surface Modifications Using Glycoform-resolved Quantitative Unfolding Mass Spectrometry; Yifei Jia; Yamei Wang; Gongyu Li; Nankai University, Tianjin, China

WP 473 Predicting Collisional Cross Section at Ultra-High Precision Using Comprehensive Physics and Translational-Rotational Energy Partitioning; Christopher Hamilal; Sandiya V.B. Garimella; Jaejun Chun; Yehia M. Ibrahim; David E. Clemmer; NIST, Gaithersburg, MD; Boeing, Huntsville, AL; NBI, Copenhagen, Denmark

WP 474 Introducing a Novel Protocol for the Identification of Optimal Elution Conditions for Lipid Analysis using 2D-ESI-MS/MS; Shenglong Yin; Zhen Xu; Xiaoyu Zhu; Sciex Corporation, Concord, ON, Canada; Guangzhou University of Science and Technology, Guangzhou, China; Macau University, Macau, China; Shanghai Rising Medical Science Co., Ltd., Shanghai, China

WP 475 Characterizing Perfluorohexanesulfonic acid Isomers with Multi-Pass Cyclic Ion Mobility Mass Spectrometry Combined with Collision Cross Section and Retention Time Modeling; Jonathan Antle; Sarah Dowd; Diana Aga; University at Buffalo, Buffalo, NY; Waters Corporation, Milford, MA

WP 476 Elucidation of denatured protein structures through Ion Mobility Spectrometry Mass Spectrometry by comparison to Gas Phase Ion Structures of homopolymers; Leyan Hua; Ganndhi D Viraj; Carlos Larriba-Andaluz; IUPUI, Indianapolis, IN; Purdue University, WEST LAFAYETTE, IN

WP 477 How good are the models proposed to rationalize the transformation and transformation of gas-phase tautomeric ions; Athula B. Attigale; Stevens Institute of Technology, Hoboken, NJ

WP 478 Protein and Protein-DNA Thermal Conformational Changes studied by IR Laser-Assisted nESI-TIMS-ToF MS; Samuel A Miller; Kevin Jeanne Dit Fouque; Fernei Leng; Francisco Alberto Fernandez Lima; Florida International University, Miami, FL

WP 479 Distinguishing Photo crosslinked and non-Photo crosslinked Human Telomers by Ion Mobility Mass Spectrometry; Hein-Chieh Yang; Savannah Scruggs; Mengdi Cha; John Stephen Taylor; Michael L. Gross; Washington University in St. Louis, saint louis, MO

WP 480 Thermal Stabilities of Disulphide-Reduced Lysozyme Conformations by Cyclic Mobility Spectrometry; Sarah O'Keefe; Lucas Henderson; Edie M. Sharon; David E. Ciemmer; Indiana University, Bloomington, IN; Indiana University Bloomington, Bloomington, Indiana; Indiana University, bloomington, IN

WP 481 Conformation identification of disaccharides by complexed with cyclodextrins and metal ions using ion mobility spectrometry and its application in foods; Yinghua Yan; Chuan-Fan Ding; Ningbo University, Ningbo, China; Ningbo University, Ningbo, China

WP 482 Trapped ion mobility separation (tims) of glucose -6 phosphate and fructose 6 phosphate; Surendar Tadi; Xuejun Peng; Beixi Wang; Erica Forsberg; Matthew Lewis; Bruker Daltonics, Billerica, MA; Bruker Scientific, San Jose, CA; Bruker Daltonics, Billerica, MA; Bruker Daltonics GmbH & Co KG, Bremen, Germany

WP 483 Characterization of adeno-associated virus (AAV) capsid protein using microflow LC-MS/MS; Lingsheng Chen; Tie Gao; Ji Luo; Lihai Guo; Xiang Li; Hongxu Chen; SCIENCE, Beijing, China; SCIENCE, Shanghai, China; Division of Recombinant Biological Projects, National Institutes for Food and Drug Control, Beijing, China

WP 484 Low level quantitation of seven N-nitrosamines in Monoclonal antibody (mAb) formulations by using LC-MS/MS; Nitish Ramchandra Suryawanshi; Ashutosh Shelar; Deepthi Maheshwarri; Samruddha Chavan; Nitin Shukla; Nilesh Patil; Purushottam Sutar; Dr. Jitendra Kelkar; Dr. Pratap Rasam; Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India; Spino Biotech Pvt Ltd., Mumbai, India

WP 485 High-Throughput Quantification of Creatine Levels in Dried Blood Spot; Keesley Jo Alexander; Fiona Hubbard; Frances Morris; Kavinda Desilva; Mariko Nakano, Phd; Charles Sailey, Md; Zane Hauck, Phd; Molecular Testing Labs, Vancouver, WA; Molecular testing labs, Vancouver, WA

WP 486 Investigation of Ionization Mechanisms and Fragmentation Pathways of an Energetic Material Via Liquid Chromatography-High Resolution Mass Spectrometry (LC-MS); Kevin Pederson; Elizabeth Grose; Andrew Horan; Ashly Huber; Joseph Worthington; Alisia Broderick; John Brady; Signature Science, LLC; Egg Harbor Township, NJ; Transportation Security Laboratory, Atlantic City, NJ

WP 487 Ultrafast LC-MS Analyses using Short 10 mm Columns; Matthew James; Tony Edge; David Dunthorne; Mark Fever; Katie Lawlor; Lewis Couchman; Keng Tiong Ng; Leon Barrown; Geoff Faden; Avantor, Theale, United Kingdom; Department of Analytical, Environmental and Forensic Sciences, King's College London, London, United Kingdom; Analytical Services International, St. George's - University of London, London, United Kingdom; Environmental Research Group, School of Public Health, Imperial College London, London, United Kingdom; MAC-MOD Analytical Inc., Chadds Ford, PA

WP 488 Analysis and simultaneous quantitation of isoform-specific phosphoinositide 3-kinase (PI3K) inhibitors in mice plasma by LC-MS/MS and its application to pharmacokinetics; Michelle L Spruill; Ritu Bohal; Howard Martin; Weiyi Peng; Xinli Liu; Department of Pharmacological and Pharmaceutical Sciences, University of Houston, Houston, TX; Department of Biology and Biochemistry, University of Houston, Houston, TX; Sagis Diagnostic, Houston, TX

WP 489 Microflow 4D-Proteomics for robust, high-throughput sample analysis; Florian Busch; Andreas Schmidt; Johanna Tüshaus; Eike Mucha; Thomas Kosinski; Stephanie Kaspar-Schoenefeld; Christoph Krisp; Christoph Gebhardt; Julie Munoz; Jean-Francois Greisch; Axel Maibaum; Markus Lubeck; Bernhard Küster; Gary Krapap; Bruker Daltonics GmbH & Co. KG, Bremen, Germany; Chair of Proteomics and Bioanalytics, TUM, Freising, Germany; Bruker Switzerland AG, Faelanden, Switzerland; Bruker S.R.O., Brno, Czech Republic

WP 490 Highly sensitive quantitation of N-nitroso-propranolol in Propranolol hydrochloride formulation and its placebo by using LC-MS/MS; Nitin Shukla; Nitish Ramchandra Suryawanshi; Purushottam Sutar; Samruddha Chavan; Nilesh Patil; Dr. Jitendra Kelkar; Dr. Pratap Rasam; Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India

WP 491 Optimization of search engines and data processing strategies using benchmark peptides enables highly sensitive and robust data analysis in the NHC Indian Liver Disease cohort study; Sailee Rasam; Xiaoyu Zhu; Timothy Sikorski; Thomas Angel; John T Mehler; Jun Qu; Department of
Biochemistry, State University of New York, Buffalo, NY; 2Department of Pharmaceutical Sciences, State University of New York, Buffalo, NY; 3GlxoSmithKline, Collegeville, PA

WP 492 LC-MS determination of bleomycin in biological and pharmacologic specimens: Helena Plešnık1, 2; Maša Božnjak1, 2; Maja Čemažar4, 5; Gregor Serša4, 5; Tina Kosjek4, 5; 1International Postgraduate School Jožef Stefan, Ljubljana, Slovenia; 2Jožef Stefan Institute, Ljubljana, Slovenia; 3Faculty of Pharmacy, University of Ljubljana, Ljubljana, Slovenia; 4Faculty of Health Sciences, University of Ljubljana, Ljubljana, Slovenia; 5Department of Experimental Oncology, Institute of Oncology Ljubljana, Ljubljana, Slovenia; 6Faculty of Health Sciences, University of Ljubljana, Ljubljana, Slovenia

WP 493 Taking the characterization of bispecific antibodies with RPLC-MS to the next level by improving speed and selectivity: Amarande Murisier1; Valentina D’Atri1; Vincent Larraitel2; Sebastian Pirner2; Miroslav Nikolov2; Davy Guilarme1; School of Pharmaceutical Sciences, Institute of Pharmaceutical Sciences of Western Switzerland, University of Geneva, Geneva, Switzerland; 2Roche Pharma Research and Early Development, Large Molecule Research, Penzberg, Germany

WP 494 It’s All About the Solubility: Prodrug and Parent Bioanalysis Using LC-MS/MS: Lin Bu1; Woo Hyun Yoon1; Danielle Toney2; Purvi Jejurikar3; Abbvie, South San Francisco, CA

WP 495 Analysis of Alkylphenol Ethoxylates (APEOs) and Alkylphenols (APs) in Textiles by UHPLC-MS/MS: Jamie Foss1; Francisco A. Ferron2; Roberto Bozic2; 1PerkinElmer, Shelton, CT; 2PerkinElmer, Milan, Italy

WP 496 Global metabolic profiling of E. coli strains for producing soluble recombinant protein: Mehnah Shivastava1; Shashidhar Ganjave2; Deepth Sahayabuddhie2; Vivek Mishra3; Prajval Nakrani3; Pramod P. Wangikar2; 1Indian Institute of Technology, Bombay, Bombay, India; 2Indian Institute of Technology Townsend, Bombay, Mumbai, India; 3Indian Institute of Technology Bombay, Mumbai, India; 4Clarity Bio Systems India Pvt Ltd, Pune, India

WP 497 Development of an analytical method by LC–HRMS for the analysis of saxitoxin and related Paralytic Shellfish Poisoning Toxins: Salomé Chaume1; Clotilde Favino1; Charlotte Maiga2; Christian Albare2; Emmanuel Joubert2; Anne Bossée2; 1DGA, Vert-le-Petit, France

WP 498 Untargeted differential metabolomics of S. mutans biofilm on dental composites: Chien-chia Chen1; Karabi Mondal1; Evan P. O’Brien1; Karl J. Rockne1; James L. Drummond2; Luke Hanley2; University of Illinois at Chicago, Chicago, IL

WP 499 Characterization of a Diverse Sample Collection by UPLC-MS: Wilfredo Pinto1; Foster Tenkorang1; 1Merck, Rahway, NJ

WP 500 New Approach for Quantitation and Measurement of Carbon Isotopes of Drugs with LC Coupled to FID and IRMS: Herbert Tobias1; Andrew Jones1; Tommy Saunders2; J. Thomas Brenna3; 1University of Texas at Austin, Austin, TX; 2Activated Research Company, Eden Prairie, MN

WP 501 Quantification of Psilocybin and Psilocin Content Variety in Psilocybe cubensis Strains with LC-MS; Roman Goff1; Morgan Smith1; Jonathan Ferguson2; Kevin A. Schug1; Sue Sisley3; Paige Wicker4; 1University of Texas at Arlington, Arlington, TX; 2Shimadzu Scientific Instrument, Columbia, MD; 3Scottsdale Research Institute, Scottsdale, AZ

WP 502 Development of an integrated and purpose-designed quality control workflow and dashboard for evaluation of LCMS proteomic platforms: Lee K Palmer1; Aaron O Bailey1; William Russell1; 1University of Texas Medical Branch at Galveston, Galveston, TX

WP 503 Development and validation of a liquid chromatography-tandem mass spectrometry method for determination of phthalate and DINCH metabolites in human urine: Žan Rekar1, 2; Agneta Aninka Runkel1;

WP 504 Direct Quantitation of Five Immunosuppressant Drugs in Volumetric-Controlled Dried Whole Blood Spots by a Fully Automated DSM-LC-MS System: Richard Gibson1; Jingshu Guo1; Stephanie N. Samra2; 1Thermo Scientific, San Jose, CA; 2Thermo Scientific, San Jose, California

WP 505 Untargeted Mass Spectrometry for Analysis of Chemical Trends in Municipal Wastewater Before, During, and After the 2022 World Athletics Championships: Sam Bassett1; Luke Marney2; Jeffrey Morre3; Thando Mawasha3; Michael Harry4; Casey Kanalos4; Corey De La Cruz4; Daphne Guo4; Cheng Shi4; Lya Carini5; Kyle Barber6; Gerrad Jones6; Christine Kelly7; Tyler Radneick8; Claudia Maier2, 5; 1Department of Biochemistry and Biophysics, Oregon State University, Corvallis, OR; 2Department of Chemistry, Oregon State University, Corvallis, OR; 3Department of Biochemical Engineering, Oregon State University, Corvallis, OR; 4Department of Biological and Ecological Engineering, Oregon State University, Corvallis, OR; 5Athletics Integrity Unit, World Athletics, Monaco, Monaco; 6Linus Pauling Institute, Oregon State University, Corvallis, OR

WP 506 Maximizing Sensitivity by Multifactorial Optimization of Method Parameters for Clinical Mass Spectrometry: Evan W. McConnell1; Christopher M. Shuford2; Russell P. Grant3; Labcorp, Burlington, NC

WP 507 Simultaneous detection and quantification of anticancer drug labatinib, capetitabine, and 5-fluorouracil in blood and tissue by isotope dilution LC-MS/MS method: Sana Shafi1; Sujit Biswas2; Michelle L Marshall3; 1University of Houston, Houston, TX; 2Trinity University, San Antonio, TX

WP 508 Chiral LC-MS/MS Methods for the Direct Separation and Analysis of Enantiomers to Understand Conversion in vitro and in vivo: Yongjun Yao1; Bo Liu1; Wenchen Luo1; Cassandra Shu1; Daniella Tonev1; Purvi Jejurikar1; Abbvie, South San Francisco, CA

WP 509 Testosterone, Progesterone and Cortisol analysis by LC-MS/MS for Dried Blood Spot and Serum Samples in a 96-well preparation: X. Johnson; Molecular testing labs, Vancouver, WA

WP 510 The impact of posttranslational and chemical modifications on peptides retention in reversed-phase HPLC: a compendium of chromatographic data for proteomics: Quinn Neale1; Alexandre Prefontained1; Darien Yeung1; Victor Spencer1; Nideljko Budisaa1; Helene Perreault1; Rene Zahedi1; Darrin V. Koohkin2; 1University of Manitoba, Winnipeg, MB; 2University of Manitoba, Winnipeg, MB

WP 511 Structural characterization of SARS-CoV-2 dimeric ORF9b reveals potential fold switching trigger mechanism: Xiuye Jin1; Xue Sun2; Yan Chai3; Yu Bai3; Ying Li4; Tianjiao Hao5; Jianxun Qi6; Hao Song7; Catherine Cl Wong8, 9; George Fu Gao8; University of Science and Technology of China, Hefei, China; 9Peking University, Beijing, China; 2Institute of Microbiology, Chinese Academy of Sciences, Beijing, China; 3Peking University, Beijing, China; 4Tsinghua-Peking University Joint Center for Life Sciences, Beijing, China; 5Peking Union Medical College Hospital, Beijing, China

WP 512 Direct analysis of in vitro oxidation of neural phospholipids via LC-MS/MS and GC-MS/MS: Secilia Garza1; Genevieve James1; Hikyu Park1; Paul Baker2; 1University of Texas, Austin, TX; 2SCIEI, Redwood city, CA

WP 513 Deep Profiling of Plasmalogens by Coupling the Paterno–Büchi Reactions with Tandem Mass Spectrometry: Yehun Wang1; Yu Xia1; 1Tsinghua University, Beijing, China

WP 514 Assessment of multiple separation dimensions for confident annotation of novel microbial conjugated bile
acids (MCBAs) using ion mobility spectrometry-mass spectrometry; James Dodds; Allison K Stewart; Emily C Gentry; Matthew H Foley; Lee R Hagey; Pieter C Dorresteijn; Casey M Theriot; Erin S Baker; University of North Carolina at Chapel Hill, Chapel Hill, NC; 1Thermo Fisher Scientific, West Palm Beach, FL; 2Virginia Tech, Blacksburg, VA; 3North Carolina State University, Raleigh, NC; 4University of California San Diego, San Diego, CA

WP 515 A method for comprehensive investigation of lipid ligands using LC-FRC/HRMS/MS: Noriyuki Tomiyasu; Yoshihiro Izumi; Masatomo Takahashi; Naoya Nishimura; Kenji Toyonaga; Sho Yamashita; Takeshi Bamba; 1Kyushu University, Fukuoka, Japan; 2Medical Institute of Bioregulation, Fukuoka, Japan; 3Research Institute for Microbial Diseases, Suita, Japan

WP 516 A charge-switching reagent for structure elucidation of branched-chain fatty acids via radical-directed dissociation; Ruijun Jian; Yu Xia; 1Tsinghua University, Beijing, China

WP 517 Enhanced ionization of Low-Abundant Lipid Species using Experimentally Generated Libraries: Nicholas S Ly; Jeremy K Chan; Cunjie Zhang; Andrew T Quaile; Kelly Lovozovitch; Stephanie Z Xie; J. Rafael Montenegro-Burke; 1Donnelly Centre for Cellular and Biomolecular Research, Toronto, ON; 2Princess Margaret Cancer Centre, University Health Network, Toronto, ON

WP 518 Improving the performance of automated lipid identification for untargeted lipidomics; William Xu; Adriana Zardini Buzzato; Elvis Lo; Shuang Zhao; Liang Li; 1The Metabolomics Innovation Centre (TMIC), Edmonton, AB; 2University of Alberta, Edmonton, AB

WP 519 Comprehensive characterization of the lipid nanoparticle (LNP) ALC-0315 and its impurities using electron-activated dissociation (EAD): Zhichang Yang; Sahana Malliah; Paul Baker; Robert Proksa; Jon Le Huray; 1SCIex, Brea, CA; 2SCIEX, Redwood City, CA; 3SCIex, Framingham, MA; 4Acutas Therapeutics Inc., Vancouver, BC

WP 520 Identifying Double-Bond-Positions of Phospholipids in Mouse Liver by Using Simultaneous Positive/Negative Ion Switching Analysis of LCMS-9050 and OAD-MS/MS: Yohei Arai; Xu Zhao; Tatsuhiko Takahashi; 1SHIMADZU Corporation, Kyoto, Japan

WP 521 The Caenorhabditis elegans lipidome – established using UHPLC- QTOF-MS and UHPLC-IMS-QTOF-MS: Michael Tan; Lisa Salzer; Alko Barsh; Sven W. Meyer; Stefanie Wernisch; Matthew R. Lewis; Michael Witting; 1Metabolomics and Proteomics Core, Helmholtz Munich, Neubergerberg, Germany; 2Bruker Daltonics GmbH & Co. KG, Bremen, Germany; 3Chair of Analytical Foodchemistry, TUM School of Life Sciences, Technical University of Munich, Freising-Weihenstephan, Germany

WP 522 Understanding lipid metabolism in Type 1 Diabetes development of an IMS-MS with oxygen-induced dissociation and deep learning-based tool LipidOz: Dylan H. Ross; Soumyadeep Sarkar; Aivett Bilbao; Joon-Yong Lee; Daniel J Oron; Josie G. Eder; Meagan C. Burnet; Richard D. Smith; Jennifer E. Kyle; Ernesto S. Nakayasu; Xueyuan Zheng; 1Pacific Northwest National Laboratory, Richland, WA

WP 523 Profiling double bond location of unsaturated lipids in human plasma with Total Correlation Mass Spectrometry (TOC-MS); Jack Rice; Svitlana Liashenko; Nathan Cassidy; Peter B. O’Connor; 1Verdel Instruments Ltd, Camberley, United Kingdom; 2University of Warwick, Coventry, United Kingdom

WP 524 The complexity of methyl-branched unsaturated fatty acids in the skin lipidome of newborns: Lukáš Cudiman; Jan Philipp Menzel; Monica Liu; Prabhu Rangabashyam; Venkatwesara R Narreddula; Stephen J Blanksby; Josef Cvačka; 1Institute of Organic Chemistry and Biochemistry of the CAS, Prague, Czech Republic; 2Department of Analytical Chemistry, Faculty of Science, Charles University, Prague, Czech Republic; 3School of Chemistry and Physics, Queensland University of Technology, Brisbane, Australia; 4University of Wollongong, Wollongong, Australia

WP 525 Gas-Phase Ion/Ion Strategy for the Differentiation of Isomeric Bis(monoacylglycerol)phosphate and Phosphatidylglycerol Species by Shotgun Lipidomics: De’shovon M. Shenault; Caitlin E. Randolph; Sarah T. Nsiiah; Scott A. McCleucky; 1Purdue University, Lafayette, IN

WP 526 Tracking the metabolism of unsaturated fatty acids in Staphylococcus aureus using online Paterno-Büchi reactions; Emily L Prull; Lixin Xu; 1University of Washington, Seattle, WA

WP 527 High-Energy Collision-Induced Dissociation and Ion-source Decay MALDI of Metal-adducted Fatty acids; Chioma J Akor; The University of Alabama, Tuscaloosa, AL

WP 528 Lipid Nanoparticle Impurity Identification Using Single Quadrupole Mass Detection for Regulated Environments: Duanduan Han; Robert E. Birdsell; Ying Qiang Yu; 1Waters Corporation, Milford, MA

WP 529 The atlan of brain glycosphingolipids revealed by selective enrichment and structural lipidotyping: Zidan Wang; Donghui Zheng; Wenpeng Zheng; Yu Xia; 1Tsinghua university, Beijing, China; 2Tsinghua University, Beijing, China

WP 530 Identification and Characterization of Impurities in Lipid Nanoparticle Components Using TOF-MS with In-silico Fragmentation Data Processing; Kellen Delaney; Duanduan Han; Robert E. Birdsell; Ying Qiang Yu; 1Waters Corporation, Milford, MA

WP 531 Determining Double Bond Positions of Lipids using Supercritical Fluid Chromatography Photoionization Mass Spectrometry and Collision-Induced Dissociation of Radical Cations; Patrick Mueller; Gérard Hopfgartner; 1University of Geneva, Geneva, Switzerland

WP 532 Resolve gut bacterial lipid isomerism by coupling mCPBA epoxidation with RPLC-MS/MS; Kai-Li Chen; Ting-Hao Kuo; 1Department of Chemistry, National Taiwan University, Taipei, Taiwan

WP 533 Localization of Methyl branching and Unsaturated Sites on Fatty Acids and Ganglioside with Radical-Initiated Dissociation via Charge-Switch Chemistry and LC/MS; Shane M Finn; Wilthun Gilles; Rayan Murtada; Jinshan Gao; 1Montclair State University, Montclair, NJ

WP 534 Improved Separation of Lipid Extracts Using High Resolution Ion Mobility Incorporating Structures for Lossless Ion Manipulation in LC-HRIM-HRMS; Allison R. Reardon; Katrina L. Leaplatrol; Jody C. May; John A. McLean; 1Vanderbilt University, Nashville, TN

WP 535 Structural diversity of Leptospiro lipid A: what can it reveal about pathogenesis?: Helena Petrossova; Abanoub Mikhail; Matthew Shuman; Sophie Culos; 1Alexandre Giraud-Gatineau; Alloysius M. Gomez; 2Robert K Emst; 3Caroline E. Cameron; 4Elisio A. Wunder Jr.; 5Mathieu Picardeau; 6David R Goodlett; 7University of Victoria, Victoria, BC; 8University of Victoria Genome British Columbia Proteomics Center, Victoria, BC; 9University of Maryland, Baltimore, MD; 10Institut Pasteur, Paris, France; 11University of Washington, Seattle, WA; 12Yale School of Public Health, New Haven, CT

WP 536 Ozone-enabled fatty acid discovery reveals unexpected diversity in the human lipidome: Jan Philipp Menzel; Reuben S. E. Young; Aurelie H. Benfield; Julia S. Scott; Puttandon Wongsonboon; Lukáš Cudiman; 1Josef Cvačka; 1Lisa M. Butler; 2Sonia T. Henriques; Berwyck Pead; 3Stephen J Blanksby; 4School of Chemistry and Physics, Queensland University of Technology, Brisbane, Australia; 5University of Wollongong, Wollongong, Australia;
WP 537 A comparative study on the identification of plasma lipids using collision-induced dissociation and electron-activated dissociation; Kiran Maan1; Dipankar Malakar1; Cagakan Ozbaic2; 1SCIENCE, Bangalore, India; 2SCIX, Alderley Park, United Kingdom

WP 538 Detection and Characterization of Intact Oxidized Phospholipids Following Oxidative Insult of Immortalized Microglial Cells; Yulemni Morel1; Nivedita Hegdekar2; Chinmay Sarkar1; Marta Lipinski1; Jace W Jones1; 1University of Maryland, Baltimore School of Pharmacy, Baltimore, MD; 2University of Maryland, Baltimore School of Medicine, Baltimore, Maryland

WP 539 Pathogenic Leptospira lipA structural changes induced by growth conditions; Sophie Culos1; Helena Petrosova1,2; Abanoub Mikhail1; Alexandra Giraud-Galineau2; Elisio A. Wunder Jr.1; Matheiu Picardeau1; David R Goodlett1,2; 1UVic Genome BC Proteomics Centre, Victoria, BC; 2Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC; 3Biology of Spirochetes Unit, Institut Pasteur, Paris, France; 4Department of Epidemiology of Microbial Diseases, Yale School of Public Health, New Haven, CT

WP 540 Enhance lipid isomer analysis by online photochemical derivatization with capillary electrophoresis-mass-spectrometry; Junhan Wu1; Yikun Liu1; Wenpeng Zhang1; Zheng Ouyang1; 1Tsinghua University, Beijing, China

WP 541 Structure-centric annotation of phospholipids by Electron Activated Dissociation; Vincent Wu1; Mario Povoa Correia2; Adrian Ruiz1; Nicola Zamboni1; 1ETH Zurich, Zurich, Switzerland; 2BCG Health Sciences Centre, Oshawa, ON, Canada

WP 542 Activated Electron Photodetachment and Ultraviolet Photodissociation for Top-Down Characterization of Intact Bacterial Lipopolysaccharides; James E Keener1; Jennifer S Brodbelt1; 1University of Texas at Austin, Austin, TX

WP 543 Lipidomic Profiling of Patients and Long-Term Survivors with Pancreatic Ductal Adenocarcinoma Using Reverse-Phase UHPLC/MS; Zuzana Valtková1; Ondřej Peterka1; Jakub Idkowiak1; Robert Jírásko1; Beatrice Mohelníková Duchonková1; Martin Loveček1; Bohuslav Melichar1; Michal Holáček1; 1University of Pardubice, Pardubice, Czech Republic; 2University Hospital Olomouc, Olomouc, Czech Republic

WP 544 High-coverage targeted lipidomics analysis by LC-MS/MS in mouse brain prepared by laser-capture microdissection; Chunchun Zhong; SCIEX, Shanghai, China

WP 545 Identification and quantification of unsaturated fatty acids using electron-activated dissociation (EAD) fragmentation; Zhour Man1; Dandan Si1; Zhimin Long2; sciex, beijing, China; 1SCIEX, Beijing, China

WP 546 Comparison of Plasma Triacylglycerols and Cholesterol Esters Measured via Supercritical Fluid Chromatography and Normal Phase LC-MS/MS; Eunice A Grigorutu1; Michael S Gardner1; Susan Kuklenyk1; John R Barr1; 1Centers for Disease Control and Prevention, Chamblee, GA

WP 547 Azidination-Based13C-Isotope Labeled Tag for Lipid Absolute Relative Quantitation at the Isomer Level; Honyuan Yang1; Shuli Tang1; Syuan-Ting Kuo1; Xin Yan1; 1Texas A&M Chemistry, College Station, TX

WP 548 An LC-MS/MS Method for Measurement of Sphingolipids in the Plasma of Pediatric Patients with Disorders of Sphingolipid Metabolism; Joanna Y. Lee1; Julie D. Saba1; Hui Zhao1; Yanan Yang1; 1Department of Pediatrics, Division of Hematology/Oncology, University of California-San Francisco, Oakland, CA; 2Agilent Technologies, Santa Clara, CA

WP 549 A C30 RP-LC-MS/MS method for the determination of cholesterol esters from fed and fasted human plasma and cells; Trevor B Romsdahl1; Jennifer J Linares1; William K Russell1; 1Mass Spectrometry Facility - University of Texas Medical Branch, Galveston, TX

WP 550 Method for analyzing lipids and vitamins in media using HPLC-MS and GC-MS; Hee-Jin Yoo1; Duck-Hyun Kim1; Moonhee Park2; Kun Cho1; 1Korea Basic Science Institute, Ochang, South Korea; 2Korea Basic Science Institute, Ochang, South Korea

WP 551 Development and Analytical Validation of a Sphingolipid Targeted Panel; Crystal L. Pace1; Bradley C. Cochran1; Richard J. Robinson1; Metabolon, Morrisville, NC

WP 552 Robust UPLC-MRM-MS workflow that allows combined quantification of oxylipins and PUFAs in a single analysis; Monia Khorani1; Liping Yang1; Jaewoo Choi2; Lynne H. Shint0; Claudia S. Maier1,2; 1Department of Chemistry, Oregon State University, Corvallis, OR; 2Linus Pauling Institute, Oregon State University, Corvallis, OR; 3Department of Neurology, Oregon Health & Science University, Portland, Oregon

WP 553 Alterations of Brain Bioactive Lipids after Microglia Elimination in Alzheimer’s Disease: A Functional Lipidomics Study; Ziyong Xu1; Juan Pablo Palavisi1,2; Sepideh Kiani Shabestari1,2; Matthew Blurton-Jones1,2,3; Kevin F. Brieniek1; Xiaolin Han1; John Goodkin4; 1Barshop Institute for Longevity and Aging Studies, University of Texas Health Science Center at San Antonio, San Antonio, Texas; 2Department of Medicine, UT Health San Antonio, San Antonio, Texas; 3Department of Neurobiology & Behavior, UC Irvine, Irvine, California; 4Sue and Bill Gross Stem Cell Research Center, UC Irvine, Irvine, California; 5Institute for Memory Impairments and Neurological Disorders, UC Irvine, Irvine, California; 6Department of Pathology, Glenn Biggs Institute for Alzheimer’s and Neurodegenerative Diseases, UT Health San Antonio, San Antonio, Texas

WP 554 Dual Cyclization tandem mass for quantification of phosphatidylcholines using 6-plex isobaric tagging; Mahmoud Elhusseiny Mostafa1; Julius Agongo1; Reagan McGuffee1; Scott Grady1; Christopher Amatt1; David Ford1; 1Pharmaceutical Analysis, University of Maryland, College Park, MD

WP 555 PCU2-MS/MS for Quantitation of a Panel of Polyunsaturated Fatty Acids and their Eicosanoid Oxylipin Metabolites; Guille Metzler1; Carmen Fernandez-Metzler1; Richard C. King1; 1PharmaCadenza Analytical Services, Hatfield, PA

WP 556 Lipid Mass Tags via Azidination for Probing Unsatuated Lipid Isomers and Accurate Relative Quantification; Tingyuan Yang1; Shuli Tang1; Syuan-Ting Kuo1; Daisu Freitas1; Madison Edwards1; Hongying Wang1; Yuxiang Sun1; Xin Yan1; 1Texas A&M University, College Station, TX

WP 557 Targeted 4D PASEF-based quantitation strategy for clinical lipidomics; Dhanwri Bajekal1; Raissan Lerner1; Laura Bindla1; 1University of Texas Medical Center of Mainz, Mainz, Germany; 2University Medical Center of Mainz, Mainz, Germany

WP 558 Phytosterols profiling in human serum using a liquid chromatography tandem mass spectrometry; Kerstl Karu; UCL Chemistry Mass Spectrometry Facility, London, United Kingdom

WP 559 A targeted LC-MS method for identification and quantification of 10 different classes of phospholipids; Rohit B. Kamble1; Qibin Zhang1,2; 1Center for Translational
Biomedical Research, University of North Carolina at Greensboro, North Carolina Research Campus, Kannapolis, NC; 2Department of Chemistry & Biochemistry, University of North Carolina at Greensboro, Greensboro, NC.

WP 560 A derivatization strategy using isotope-labeled 3-NPH for absolute quantitation of free fatty acids from human plasma by LC-MS/MS; Jennifer J Linares; Trevor Romsdahl; William Russell; UTMB Health Mass Spectrometry Facility, Galveston, TX.

WP 561 An automated LC-PB-MS workflow for large-scale analysis of lipid C-S isomers; Nan Zhang; Wenhu Pang; Jiexun Bu; Wenpeng Zhang; Zheng Gouyang; PürSpec Technology (Beijing) Ltd., Beijing, China; Tsinghua University, Beijing, China.

WP 562 Direct Comparison of Targeted Ganglioside Analysis Using Multiple Reaction Monitoring (MRM) and Parallel Reaction Monitoring (PRM) LC-MS/MS; Arvin Saffarian Dekhosh; Akemi Sanni; Judith Nwaiwu; Andrew I. Bennett; Cristiano D. Gutierrez; Reyes; Yehia Mechefri; Texas Tech University, Lubbock, Texas.

WP 563 Paternó-Büchi (PB) reaction-based isobaric mass tags for accurate relative quantitation of fatty acids at the isomer level; Xi Chen; Gopal Reddy Ramidi; Suyan-Ting Kuo; Dallas Freitas; Luchen Wuyang; Aidan Slagter; Peiyi Cai; Ashok Polu; Xin Yan; Texas A&M University, College Station, TX.

WP 564 Targeted Lipidomic Analysis of Pediatric Leukemia Cells Using LC-MS/MS Triple Quadrapole; Lilhua Jiang; Ruqiang Jia; Tiffany Triinh; Hui Zhao; Yanan Yang; Mark Sartain; Maya Kasowski; Michael Snyder; Department of Genetics, Stanford University, Stanford, CA; Agilent Technologies, Wilmington, DE; Agilent Technologies, Santa Clara, CA; School of Medicine, Pathology, Stanford University, Stanford, CA.

WP 565 Rethinking lipidomic sample normalization: Using the sulfo-phospho-vanillin assay for lipid pre-quantitation in untargeted LC-MS/MS lipidomic applications; Laura Bailey; Kari B Basso; University of Florida, Gainesville, Florida; University of Florida, Gainesville, FL.

WP 566 Comparison of online and offline HILIC and C20 Reverse Phase Liquid Chromatography coupled to Accurate MS for Quantitative Lipidomic Analysis: Thu Huong (Nicole) Pham; Raymond Thomas; Lakshman W Galagedara; Memorial University of Newfoundland, Corner Brook, NL; Department of Biology, Faculty of Science, Western University, London, ON; School of Science and the Environment, Grenfell Campus, Memorial University of Newfoundland, Corner Brook, NL.

WP 567 A lipidomics atlas of the diabetic liver in mice; Meixia Pan; Juan Pablo Palavicini; Xinlin Han; Barshop Institute for Longevity and Aging Studies, University of Texas Health Science Center at San Antonio, San Antonio, Texas.

WP 568 The effects of systemic lupus erythematosus (SLE) on unsaturated lipids uptakes and their oxidative metabolism in the western population; Elham Pourmand; Kin Sing Lee; James Pestka; Jennifer Fenton; Emily Somers; Faith Strickland; Tracy Fuller; Angel Edwards; Suzu Thompson; Michigan State University, EAST LANSING; University of Michigan-Ann Arbor, Ann Arbor, MI.

WP 569 Metabolomics Evaluation of the Impact of Violet-Blue Light (405 nm) on Platelet Concentrate; Jinchun Sun; Neetu Dahiya; Tom Schmitt; Caitlin Stewart; John Anderson; Scott MacGregor; Michelle MacLean; Richard Beger; Chintamani D. Atreya; NCTR / USFDA, Jefferson, AR; Office of Blood Research and Review, Center for Biologics Evaluation and Research, United States Food and Drug Administration, Silver Spring, MD; The Robertson Trust Laboratory for Electronic Sterilization Technology, Department of Electronic and Electrical Engineering, University of Strathclyde, Glasgow, United Kingdom.

WP 570 A high-resolution LC-MS based metabolomics method for spent media analysis in biopharmaceutical cell culture process; Xiali Gao; George Goneya; Keegan Orzechowski; Alena La; Nafees Norris; Juan Aon; Matthew Maust; GSK, Collegeville, Pennsylvania.

WP 571 Combined GC-TOF-MS and LC-TOF-MS/MS Untargeted Metabolomics Yields Insight into Pathophysiology of Parkinson’s Disease; Lina Dahabiyeh; Jeremiah D Wells; Refat Nimer; Oliver Fiehn; University of California, Davis, Davis, CA; The University of Jordan, Amman, Jordan; Jordan University of Science and Technology, Irbid, Jordan.

WP 572 Untargeted metabolic and proteomic analysis of proximal and distal locations in colon and fecal samples by LC-MS/MS; Oriana Zambiti; Leanne Ohlund; Nejia Lassoudi; Rododile Soret; Nicolas Pliron; Lekha Sleno; University of Quebec in Montreal (UQAM), Chemistry department, Montreal, QC; University of Quebec in Montreal (UQAM), Biology Department, Montreal, QC; CERMO-FC, CNRS, Université de Recherche sur les Maladies Orphelines-Fondation Courtois, Montreal, QC.

WP 573 Combining real time and post-acquisition quality control (QC) for metabolomics workflows; Aiko Barsch; Patrick Groos; Nikolaus Kessler; Matthias Szegnys; Sven W. Meyer; Ilmari Krebs; Heiko Neuweeger; Matthew R Lewis; Bruker Daltonics GmbH & Co. KG, Bremen, Germany; Bruker Daltonics GmbH & Co.KG, Bremen, Germany.

WP 574 Development of an Offline Two-dimensional LC-MS Method for Chemical Isotope Labeling (CIL)-Based Metabolome Profiling; Sicheng Quan; Shuang Zhao; Liang Li; University of Alberta, Edmonton, AB; The Metabolomics Innovation Centre (TMIC) - University of Alberta, Edmonton, AB.

WP 575 Using Multiple Serum Sample Cohorts with Chemical Isotope Labeling LC-MS to Discover Biomarkers of Rheumatoid Arthritis with Different Seropositivity Status; Xiaohong Wang; Wei Han; Walter P. Maksymovych; Liang Li; The Metabolomics Innovation Centre (TMIC), Edmonton, AB; Canadian Research and Education (CaRe) Arthritis, Edmonton, AB; Department of Laboratory Medicine, University of Alberta, Edmonton, AB.

WP 576 Optimization of mass spectrometric parameters in data dependent acquisition for untargeted metabolomics; Hailemarjum Abraha Assress; Mario G Ferruzzi; Kenny Lan; University of Arkansas for Medical Sciences, Little Rock, AR; Arkansas Children’s Nutrition Center, Little Rock, AR.

WP 577 A biological model of the ageing metabolome reveals potential clinically relevant biomarkers; Domenica Berardi; Emily Armitage; Simon Ashton; Alan Barnes; Neil Lofthus; Gillian Farrell; Abdullah Al Sultan; Ashley McCulloch; David Watson; Matthew Baker; Zahra Rattray; Nicholas JW Rattray; Strathclyde Institute of Pharmacy and Biomedical Sciences, University of Strathclyde, Glasgow, United Kingdom; Chimera Corporation, Manchester, United Kingdom; School of Medicine, Faculty of Clinical and Biomedical Sciences University of Central Lancashire, Preston, United Kingdom.

WP 578 Untargeted spatial metabolomic analysis on Ankylosing Spondylitis preclinical model using MALDI-FTICR-Mass Spectrometry Imaging – Novel analysis approach for biomarker discovery; Adele-Asia Ponzioli; Silvia Speca; Amandine Gerstenberg; Aurore Tomezyk; Mathieu Gaudin; Rebecca Deprez-Pouliain; David Launay; Benoit Deprez; Corinne Ramos; ImaBiotech, Loos, France; CAPSTONE-ETN MSCA network, Lille, France; Institute for Translational Research in Inflammation (INFINITE), U1286, Univ. Lille, Inserm, CHU Lille, Lille, France; Electronic Sterilization Technologies, University of Strathclyde, Glasgow, United Kingdom; Institut Pasteur de Lille, Lille, France.
WP 579  Quantifying spatial and temporal changes of Populus root exometabolites during nutrient-deprived growth conditions; Manasa R. Appidi1; Sameer Mudhanari1,2; Kevin Cope2; Dana L Carper2; Richard J Giannone2; Udaya C Kalluri1; Robert L Hettick1; Paul Abraham1,3; Graduate School of Genome Science and Technology, University of Tennessee, Knoxville, TN, USA; Knoxvile, Tennessee; 2Biosciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, USA; Oak Ridge, Tennessee

WP 580  Non-targeted LC-MS analysis of indoor dust in cockroach-infested households; Daniel Krakko1; Whitney L Stutta1; Madhavi Kakumani2; Coby Schal3; Molecular Education, Technology and Research Innovation Center (METRIC), North Carolina State University, Raleigh, NC; 2Department of Entomology and Plant Pathology, North Carolina State University, Raleigh, NC

WP 581  Untargeted Metabolomic Profile of Kaposi’s Sarcoma-Associated Herpesvirus (KSHV) Infection by Reversed phase Liquid Chromatography-High-Resolution Mass Spectrometry (LC-HRMS); Abdulkarem M Alfaghi1; Bernadett Papp2; Timothy J. Garrett3; University of Florida, Gainesville, Florida; 2University of Florida College of Dentistry, Gainesville, FL; 3University of Florida, Gainesville, FL

WP 582  Application of Chemical Isotope Labelling LC-MS Metabolomics to Bovine Pregnancy Investigation; Daniel Patten1; Shuang Zhao1; Marcos Colazo1; Graham Plastow2; Elda Dervish2; Liang Li1,3; 1The Metabolomics Innovation Centre (TMIC), Edmonton, AB; 2Department of Agriculture, Food and Nutritional Science, University of Alberta, Edmonton, AB; 3Department of Agriculture, Food and Nutritional Science, University of Alberta, Edmonton, AB

WP 584  Analysis of Anaplerotic Metabolic Incorporation of Dodecanedioic Acid In Cellular Model of Skin Fibroblasts; Igor Radzikh1; Yan Sanders1; 1Cleveland State University, Cleveland, OH

WP 585  Untargeted Urinary Metabolic Profiling of Patients With Medium-Chain Acyl-Coenzyme A Dehydrogenase Deficiency; Patrick T Stump1; Frangol Tampalboon2; Denise Z Salazar1; Scott M Goldman1; Nigel J Clarke2; 1Quest Diagnostics, San Juan Capistrano, CA; 2Department of Pathology and Laboratory Medicine, University of California, San Diego, La Jolla, CA

WP 586  Using linkage patterns to validate Internal Standard to natural-abundance Isotopic Envelope paired systems; Chris Beecher1; Felice De Jong1; 1IROA Technologies, Chapel Hill, NC

WP 587  Untargeted metabolomics of Bombus impatiensshort-term responses to cold exposure via GC-MS; Hunter Taylor1; Keaveny Ellen1; Michael Dillon1; Franco Basile2; 1University of Wyoming, Laramie, WY

WP 588  Serum Metabolomics and Lipidomics Studies to Identify Biomarkers for Hepatocellular Carcinoma; Md Mamunur Rashid1; Rency S Varghese1; Habtom Ressom1; 1Georgetown University, Washington, DC

WP 589  Sexual Dimorphism of Rewarding System in Mouse Brain Revealed by Parallel Metabolomics and Lipidomics; Huaxu Yu1; Tao Huan1; 1University of British Columbia, Vancouver, BC

WP 590  Tracing the origin of Chinese Lotus root varieties using high-resolution mass spectrometry; Jiao Liu1; Luqing Zhao1; Jinmei Chen1; Zong Yang2; Bingjie Liu1; Lihai Guo2; 1Hubei Academy of Agricultural Sciences, Wuhan, China; 2SCiEX, Shanghai, China; 3SCiEX, Beijing, China

WP 591  Spatial metabolomics of polymicrobial wound infections and associated adhesive bandages; Monica Ness1; Avery Holmes2; Laura-Isselot McCall2,3; Carolyn Ibberson4; 1University of Oklahoma, Norman, OK; 2University of Oklahoma, Department of Microbiology and Plant Biology, Norman, OK; 3University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK

WP 592  Leveraging TENG-MS Untargeted Lipidomics to Study Mesenchymal Stromal Cell Senescence at Low Sample Volumes; Joseph L. Cortsveld1; Daniel D. Vallee2; Molly E. Ogle1; Johnna S. Temenoff1; Facundo Fernandez1; 1Georgia Institute of Technology, Atlanta, GA

WP 593  Segment Scan Mass Spectral Acquisition for Increasing Metabolite Detectability in Chemical Isotope Labeling LC-MS Metabolome Analysis; Chu-Fan Wang1; Liang Li2; 1Department of Chemistry, University of Alberta, Edmonton, AB

WP 594  Developing Workflows to Effectively Probe the Cheese Rind Microbiome Metabolome; Celine A Ertekine1; Laura Sanchez2; Gordon Lui3; 1University of California, Santa Cruz, Santa Cruz, CA

WP 595  Study of changes in amyloid protein conformations upon metal binding using top-down protein analysis with TIMS-FTICR-MS; Francesca O. Bellingeri1; Meng Li2; Yuko P. Y. Lam1; Christopher A. Wotton3; Mark P. Barrow1; Joanna F. Collingwood1; Peter B. O’Connor4; 1University of Warick, Coventry, UK; 2Bruker Dalton’s GmbH & Co KG, Bremen, Germany

WP 596  CSF proteomic identification of disease-associated protein networks that distinguish between parkinsonian disorders; Sophia Weiner1; Mathias Sauer2; Julius Constantinescu1; Radu Constantinescu1; Caj Binnew2; Henrik Zetterberg1,2,3; Johan Gobom1; 1Institute of Neuroscience and Physiology, Department of Psychiatry and Neurochemistry, University of Gothenburg, Mölndal, Sweden; 2Clinical Neurochemistry Lab, Institute of Neuroscience and Physiology, Sahlgrenska University Hospital, Mölndal, Sweden; 3Institute of Neuroscience and Physiology, Department of Neurology, the Sahlgrenska Academy at the University of Gothenburg, Gothenburg, Sweden; 4Department of Neurodegenerative Disease, UCL Institute of Neurology, London, United Kingdom; 5UK Dementia Research Institute, London, United Kingdom; 6Hong Kong Center for Neurodegenerative Diseases, Hong Kong, China; 7Wisconsin Alzheimer’s Disease Research Center, University of Wisconsin School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI

WP 597  Protein and Peptide Signatures Separate Healthy Aging, Mild Cognitive Impairment and Alzheimer’s Disease in a Paired CSF and Plasma Study; Marco Toenneti1,2; Yuehan Feng1; Roland Bruderer1; Dominique Kamber1; Jacqueline Darrow2; Alexandra Lewis2; Abhay Moghekar2; Lukas Reiter1; Biognosys AG, Schlieren, Switzerland; 2Johns Hopkins University School of Medicine, Baltimore, MD

WP 598  Challenges in hypothesis building through multi-omics analysis of Alzheimer’s disease plasma; Yoshiya Oda1; Suzumi M To1; Junya Takei2; 1Fox Chase Cancer Center, Philadelphia, PA; 2Cleveland Clinic, Cleveland, OH

WP 599  Global and targeted proteomics analysis of mitophagy associated withparkinson’s disease; Ricardo Ando1; M Alfaez1; Udaya Moghekar1; 1Axcelead Drug Discovery Partners Inc., Fujisawa, Japan

WP 600  Laser capture microdissection (LCM) enriched transcriptome and proteome differences between...
substantia nigra and ventral tegmental area human midbrain dopamine neurons: Rahul A Bharadwaj; Lieber Institute for Brain Development, Baltimore, MD

WP 601 Using Native Mass Spectrometry to Deduce the Sizes of Amyloidogenic Protein Oligomers Linked to Neurodegenerative Diseases: Eileen Jacqueline Olivares1; Carter Lantz2; Rachel R Ogorzalek Loo1; Joseph A. Loo1; 1University of California, Los Angeles, Los Angeles, CA

WP 602 Deep phosphoproteomic investigation of reactive primary astrocytes with implications in neuroinflammation through serial metal-affinity-capture (SMAC) single-shot DIA mass spectrometry (DIA-MS): Mahmud Hossain1; Francesca Rapino1; Dimitri Ottingen1; Nellwyn Hagan1; Bailin Zhang1; Dhiman Ghosh1; 1Sanofi, Cambridge, MA

WP 603 Detection of epoxides and vicinal diols of docosahexaenoic acid in rat retinas by LC/MS/MS: Genevieve E James1; Cecilia Garza2; Hikyu Park3; 1Paul Baker2; Mikhail Shcherinov3; J. Thomas Brenna3; 1University of Texas at Austin, Austin, TX; 2Dell Medical School, Department of Pediatrics, Austin, TX; 3Sciex, Framingham, MA; Biovia, Los Altos, California

WP 604 Understanding Lipid Accumulation in and Around Amyloid Plaques Using Nano-DESI Mass Spectrometry Imaging: Manxi Yang1; Emerson Hemly1; Palak Machanda1; Kaushik Sharma1; Connor Beveridge1; Mushiqiao Iqfath1; Matthew Muhoberac1; Gaurav Chopra1; Julia Laskin1; 1Purdue University, West Lafayette, IN

WP 605 Characterization of brain O-glycosylation of mice with depressive-like behavior: Youngsuk Seo1; Byoung Lee1; 1Center for Cognition and Sociality, Institute for Basic Science, Daejeon, South Korea

WP 606 Brain region-specific Lipidomics Profiling of Lipid Droplets in Alzheimer’s Disease and Aging: Caitlin E Randolph1; Palak Manchanda1; Connor Beveridge1; Kanchan Bisht1; Berwyn Poad2; Stephen J Blanksby2; Gaurav Chopra1; 1Purdue University, WEST LAFAYETTE, IN; 2Queensland University of Technology, Brisbane, Australia

WP 607 Qualification of an Immunoaffinity Capture-Liquid Chromatography-Tandem Mass Spectrometry (IAC-LCMS) Assay to Quantify Huntingtin Protein in Human Peripheral Blood Mononuclearocytes (PBMCs): Serge Zemero1; Lana Fabia1; Emma Gromacki1; Richard C. King1; Todd Herbst1; Celia Dominguez2; Edith Monteagudo3; Carmen Fernandez-Metzler4; 1PharmaCadence Analytical Services, LLC, Hatfield, PA; 2Institutional

WP 608 A Comparative Proteomic Analysis of Parkinson’s Disease, Dementia with Lewy Bodies and Multiple Systems Atrophy: Sinead Greally1; Mukesh Kumar1; Christoph N Schlaffner1; Sabrina Berretta2; Hanno Steen3; Judith Steen3; 1Boston Children’s Hospital, Boston, MA; 2Harvard Brain Tissue Resource Center (HBTRC), McLean Hospital, Belmont, MA; 3Boston Childrens Hospital, Boston, MA

WP 609 Dissecting Alzheimer’s Disease (AD) brains with x-ray Phase-contrast microtomography combined with MALDI-Mass Spectrometry Imaging: Masaya Ikegawa1; Soichiro Tokuhira1; Yumiko Toyama1; Takashi Nirasawa1; Masato Hoshino1; Motohiro Nishikawa1; Nobuto Kakuda1; Yoko Sato1; Shigeo Murayama1; Doshisha University, Kyotanabe City, Japan; 2Bruker Japan K.K., Yokohama, Japan; 3Japan Synchrotron Radiation Research Institute (JASRI/SPRING-8), Harima, Japan; 4Kyoto Institute of Nutrition & Pathology, Kyotanabe City, Japan; 5Brain Bank for Aging Research, Tokyo Metropolitan Geriatric Hospital and Institute of Gerontology, Itabashi, Japan

WP 610 The Fragile X Glycoproteome Mass Spectrometric Investigation of Altered Synaptic Plasticity: Ashley Pheatsanthat1; Elliot Patrenets1; Caroline Roycroft1; Hannah N. Miles1; Min Ma1; Pamela R. Westmark2; Cara J. Westmark1; Lingjun Li1; 1University of Wisconsin-Madison, Madison, WI

WP 611 A systematic method to quantify peptides in CSF for the analysis of neurodegenerative diseases: Gennifer Merrich1; Jea Park1; Deanna Pibul1; Julia E Robbins1; Brian C Searle2; Eric Huang1; Christine C. Wu1; Kathleen Poston3; Thomas J. Montine1; Michael J. MacCoss1; 1University of Washington, Seattle, WA; 2Ohio State University, Columbus, OH; 3Stanford University, Stanford, CA

WP 612 Identification of Spontaneous Chemical Modifications in Neurodegenerative Disease Brain Tissue: Brilee L Van Orman1; Ibrar Siddique2; Gal Bittan3; Blaine Roberts3; Ryan R. Julian1; 1University of California, Riverside, Riverside, CA; 2University of California, Los Angeles, Los Angeles, CA; 3Emory University, Atlanta, GA

WP 613 Tissue Specific Interactome of the NPC1 Cholesterol Transporter: Roshan Javanshad1; Thu T. A. Nguyen1; Stephaniehan M Cologna1; 1University of Illinois at Chicago, Chicago, IL

WP 614 Spatiotemporal Proteomics of Human iPSC-derived Neuron Model of Frontotemporal Dementia: Wan Nur Ai7ah Mazi1; Jiawei Ni1; Ashley Frankenfeld1; Ling Hao1; 1Department of Chemistry, George Washington University, Washington, DC

WP 615 Spatial proteomic characterization of amyloid plaques in murine Alzheimer’s disease brains by laser capture microdissection and mass spectrometry: Mengqi Chu1; Huan Sun1; Yun Jiao1; Junmin Peng1; 1Stjude children research hospital, Memphis, TN

WP 616 Comprehensive analysis of protein glycosylation and glycation reveals pathways associated with cognitive decline and protection from cognitive decline: David Morganstern1; Hila Levy1; Nil Ticksykovsky1,2; Aron S. Buchman1; David A. Bennett1; Michal Schneider Beeri1,2; Yishai Levin1; 1Weizmann Institute, Rehovot, Israel; 2Weizmann Institute of Science, Rehovot, Israel; 3The Joseph Sagol Neuroscience Center, Sheba Medical Center, Ramat Gan, Israel; 4The Goodman faculty of life sciences, Bar Ilan University, Ramat Gan, Israel; 5Rush Alzheimer’s Disease Center, Rush University, Chicago, IL; 6Icahn School of Medicine at Mt Sinai, New York, New York, United States, NY

WP 617 Local and global functional protein networks in Huntington’s disease animal models: Todd M. Greco1; Joshua L Justice1; Josiah E Hutton1; Tavis J Reed1,2; Jeffrey P Gentle1; Michelle A Kennedy1; Bokai Song1; Alma M Perez2,3; Ismael Alas2,3; 1CHDI Foundation, Los Altos, CA; 2AB Carroll1; Ileana M Cristea1; 1Princeton University, Princeton, NJ; 2Western Washington University, Department of Psychology, Bellingham, WA; 3Jan and Dan Duncan Neurological Research Institute, Houston, TX; 4Baylor College of Medicine, Department of Molecular and Human Genetics, Houston, TX; 5University of Washington, Department of Neurology, Seattle, WA

WP 618 Amyotrophic Lateral Sclerosis-associated Mutants of SOD1 Module miRNA Biogenesis through aberrant interactions with Exportin 5: Xinyuan Chen1; Xiaomei He1; Yin-Yu Yang1; Yinsheng Wang1; 1University of California, Riverside, Riverside, CA

WP 619 Deep intact proteome quantification of microgram-scale proteome by tandem mass tag labeling and online 2D high-pH/low-pH-RPLC top-down analysis: Yanting Guo1; Trishika Chowdhury1; Walter P. Gale1; Kellye A. Cuff-Sutton1; Dahanu Yu1; Si Wu1; 1University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK

WP 620 Analysis of the Δhnox Caulobacter crescentus proteome and c-di-GMP pools using LC-MS: Cameron C Lee-Lopez1; Md. Shariful Islam1; Erik T Yuki1; 1New Mexico State University, Las Cruces, NM
WEDNESDAY POSTERS

WP 621 Long-term quantitative and qualitative reproducibility of capillary zone electrophoresis-tandem mass spectrometry for top-down proteomics of complex proteome samples: Amirhossein Sadeghi, Qiayi Wang; Wenrong Chen; Xiaowen Kevin Liu; Liangliang Sun; Michigan State University. EAST LANSING; 2Indiana University Purdue University Indianapolis, Indianapolis, IN; 3Tulane Center for Biomedical Informatics and Genomics, Tulane University, New Orleans, LA

WP 622 A multi-layered proteomic atlas to delineate RAS-dependent cellular networks across RAS mutants and isoforms; Syed Azmat Ali; Karim Aljakouch; Jeroen Krijgsveld; German Cancer Research Center, Heidelberg, Germany; 2Heidelberg University, Heidelberg, Germany

WP 623 Exploring RNA Binding Interactome in Mouse Macrophages; Matthew J. Marino; Deepali Rathore; Aleksandra Nita-Lazar; National Institute of Health, Bethesda, MD; NIH/NIAID, Bethesda, MD

WP 624 Label-Free Quantification of Multi-Mixture Proteins using Data-Independent Acquisition (DIA); Randy J. Arnold; Takeshi Shibata; Ushio Takeda; Haruka Kumabe; Takeshi Masuda; Sumio Ohtsuki; Patrick Pribil; 2SCIEX, Bloomington, IN; 3K. A. AB SCIEX, Tokyo, Japan; 4Kumamoto University, Kumamoto, Japan; 5SCIEX, Concord, ON

WP 625 QCQuan: a new tool for rapid quality assessment of quantitative proteomics experiments; Simon Appelantis; Joris Van Houtven; Jef Hooeyberghs; Dirk Valkenberg; 1Hasselt University - DSI, Hasselt, Belgium

WP 626 Brain Organoids in Space: a neurodevelopment proteomic experiment on the effects of microgravity using CubeLab in the International Space Station; Aline M. A. Martins; Livia Luz; Diego Assis; Daniel B. McGlatchy; Jolene K. Diedrich; Alysson Muotri; John Robert Yates III; 1The Scripps Research Institute, La Jolla, CA; 2Sanford Consortium for Regenerative Medicine, UCSD, San Diego, CA; 3Buerk Daltonics, San Jose, CA

WP 627 A complementary ion-based strategy enables multiplexed quantification in ETAU analysis using DeU isoobaric tags; Ting-Jia Gu; Peng-Kai Liu; Danqing Wang; Zichong Li; Wang, Ding; 1School of Pharmacy, University of Wisconsin-Madison, Madison, WI; 2Biophysics Program, University of Wisconsin-Madison, Madison, WI; 3Department of Chemistry, University of Wisconsin-Madison, Madison, WI; 4University of Texas at Austin, Austin, TX

WP 628 Targeted quantification of human and mouse Kv7.2 and Kv7.3 in stably transfected HEK293 cells, mouse and rat brains using MRMs; Rainbow WP Kwan; Stephanie Lee; Gina De Boer; Janette Mezevoya; Richard Dean; Shohei Iwamoto; Luis Sojo; 1Xenon Pharmaceuticals, Burnaby, BC; 2University of Victoria, Victoria, BC

WP 629 Identification of proteins that differentially interact with the phosphorylated and unphosphorylated C-terminal domain of RAP1; Shadi Fredericks; Nolan Bashyal; Mukesh K. Venkat Ramanii; Yan Zhang; Jennifer S. Brodbelt; 1Department of Chemistry, The University of Texas at Austin, Austin, TX; 2Department of Molecular Biosciences, The University of Texas at Austin, Austin, TX

WP 630 Proteomics and honey bee health; Renata Moravcova; Kyung-Mee Moon; Greg R. Stacey; Jason C. Rogalski; Xiaojing Yuan; Stephen F. Pernai; Marta M. Guarna; 1University of Science and Technology, Rolla, MO; 2German Cancer Research Center, Heidelberg, Germany; 3Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany

WP 631 Tandem Mass Tag (TMT) Quantification Using Data Directed Analysis and SELECT SERIESTM MRT Mass Spectrometer; Christopher J. Hughes; Martin E. Palmer; James, 1Lansing, 2Water Corporation, Wilmslow, United Kingdom

WP 632 Accurate and precise label-free quantification with comprehensive proteome coverage using a novel HRAM platform; Zilu Ye; Anna Pashkovka; Ulises H. Guzmán; Florian Harking; Tabibang W. Arrey; Hamish Stewart; Ana Martinez Del Val; Yue Xuan; Eugen Damoc; Jesper V. Olsen; 1Novo Nordisk Foundation Center for Protein Research, Copenhagen, Denmark; 2Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany

WP 633 Evaluation of a novel high-resolution accurate mass platform for its application on TMT-based multiplexing of single cells; Pedro Aragon; Valdemar Penas; Tabibang N. Arrey; Shadi Fredericks; Benjamin Furtwangler; Bo Porse; Hamish Stewart; 1National Institute of Health, Bethesda, MD; NIMH/NIAID, Bethesda, MD

WP 634 Surface characterization in development of CAR-T therapies; Pajoon Fardavoo; Paul Stauffer; Tonya Wendorff; Xueyang Guo; Theodore B. Verhey; Sorana Morissy; 1Department of Biochemistry and Molecular Biology, University of Calgary, Calgary, AB; 2Amie Charbonneau Cancer Institute, Cumming School of Medicine, University of Calgary, Calgary, AB

WP 635 Real-Time Search improves sensitivity of TMTPro complementary ion quantification; Alex Johnson; Jingjing Huang; William D. Barshop; Jesse D. Canterbury; Vlad Zabrouskov; Graeme McAlister; Martin Wühr; 1Princeton University, Princeton, NJ; 2Thermo Fisher Scientific, San Jose, California

WP 636 Quaternary amine tags for improved complement-quantitation in proteomics samples; Nick Brodie; David C. Schriemer; 1University of Calgary, Calgary, AB

WP 637 Quantitative Protein Profiling in Brain Subregions of Mice Exposed to Open-Field Low-intensity Blast Reveals Position-Dependent Blast Effects; Marcus Jackson; Shanyan Chen; Martin Langenderfer; Chao Li; Heather R. Siedhof; Ashley Balderrama; Runtting Li; Catherine E. Johnson; C. Michael Greenleaf; Ibola Cemak; Ralph G Delpalma; Jiankun Cui; Zengping Gu; 1University of Missouri, Columbia, MO; 2University of Science and Technology, Rolda, RO; 3Moor University, Columbus, GA; 4Department of Veterans Affairs, Washington DC, DC; 5University of Missouri, Columbia, MO

WP 638 Functionalized Nanoparticles Enable Quantitative and Precise Large-Scale Unbiased, Deep Plasma Proteomics; Ting Huang; Jian Wang; Alexey Stukalov; Margaret Donovan; Shari Ferrick; David F. Druck; Seth Just; Gabriel Castro; Eithier Elgieran; Ryan Benz; Yingxiang Huang; Khaterat Motamedchaboki; Omid C. Farokhzad; Serafim Batzoglou; Simon Kreimer; Asim Siddiqui; Jennifer E. Van Eyk; Daniel Hornburg; 1Seer, Inc., Redwood City, CA; 2Cedars-Sinai Medical Center, Los Angeles, CA

WP 639 Developing Cell Quenching Method to Facilitate Single Cell Mass Spectrometry Experiments: Deepi Bhushal; Shay Shalikanpally Sunasena Wiye Munigé, Zongkai Peng; Zhibo Yang; 1University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK

WP 640 Single-Cell Proteomic Analysis of Drosophila Oocytes: Merin M. Riien; Rachel R. Ogorzalek Loo; Joseph A. Alexander; 1University of Texas at Austin, Austin, TX; 2University of Texas at Austin, Austin, TX

WP 641 Evaluation of sample preparation methods for single cell MALDI-MS; Stanislav S. Rubakhin; Jonathan V.
WP 642 Data-Dependent Acquisition with Precursor Coisolation Improves Proteome Coverage and Measurement Throughput for Label-Free Single-Cell Proteomics: Thv Tuong1, 2; Madisyn Johnston1; Kei Webber1; Hannah Boekweg1; Caleb Lindgren1; Yiran Liang1; Alissia Nydegger2; Xiaofeng Xie2; Samuel H Payne1; Ryan Kelly1; Brigham Young University, Provo, UT

WP 643 Development of a single-cell proteomic workflow to study the proteomic profiles of PC-12 differentiation: Arpa Ebralidi1; Stanislau Stanishkevicius1; Liping Yang1; Luke C. Marney1; Kavi Ashash Vaidya1; Claudia Maier1; Oregon State University, Corvallis, OR

WP 644 Improving accuracy of protein quantitation in single-cell proteomics: Connor A Peterson1; Hannah Boekweg2; Samuel H Payne1; Brigham Young University, Provo, UT

WP 645 Increasing throughput of single-cell analysis through Hyperplexing and PairQuant Acquisition with inSeqAPI: Tommy K. Cheung1; Hanna G Budayeva2; Yin Zhu2; Christopher M Rose3; Genentech, Inc., South San Francisco, CA; Genentech Inc., South San Francisco, CA

WP 646 Label free single cell proteomics using thermal inkjet dispensing with single cell sensing system: Stanislau Stanishkevicius1; Hyo Sang Jang1; Liping Yang1; Jeffrey Moore1; Claudia Maier1; Oregon State University, Corvallis, OR; HP Inc., Corvallis, Oregon

WP 647 High throughput single cell proteomics using ultrafast gradients and Wide-Window Acquisition to reach unprecedented proteome coverage and quantitative accuracy: Manuel Matzinger1; Rupert L. Mayer2; Karl Menzel3; Protein Chemistry Group, IMP, Vienna, Austria

WP 648 High-throughput nano LC-MS for sample-limited proteomics: Alec C Valenta1; Christopher Pynn2; Dominic Hoch3; Manuel Matzinger1; Rupert L. Mayer2; Alexander Makarov3; Karl Mechtler3; Runsheng Zheng4; Thermo Fisher Scientific, Somerset, NJ; Thermo Fisher Scientific, Germering, Germany; Thermo Fisher Scientific, Reinach, Switzerland; Institute of Molecular Pathology, Vienna, Austria; Thermo Fisher Scientific, Bremen, Germany

WP 649 A single-cell metabolomics approach for the study of the medicinal plant Catharanthus roseus: Anh Hai Vu1; Carlos Eduardo Rodriguez-Lopez2; Delia Ayed Serna Guerrero3; Sarah Ellen O’Connor4; Lorenzo Capelli4; 1Department of Natural Product Biosynthesis, Max Planck Institute for Chemical Ecology, Jena, Germany; 2Escuela de Ingenieria y Ciencias, Tecnologico de Monterrey, Monterrey, Mexico

WP 650 Spectral library based Single-cell proteomics resolves cellular heterogeneity: Lakmini Senavirathna1; Cheng Ma2; Ru Chen3; Sheng Pan1; 1The University of Texas Health Science Center at Houston, Houston, Texas; 2Baylor College of Medicine, Houston, Texas

WP 651 Increasing Depth of Single-Cell Analysis by Feature Matching in diaPASEF Data: Karl K Krull1; Syed Azmal Ali1; Jereon Krijgsvedel2; 1German Cancer Research Center (DKFZ), Heidelberg, Germany; 2Medical Faculty of Heidelberg University, Heidelberg, Germany

WP 652 Enhancing single-cell proteome coverage with a novel high-resolution accuracy mass platform: Valdemar Petrosius1; Tabiwan N. Arrey1; Hamish Stewart2; Nicolaie Eugen Dâmoc3; Vlad Zabrouskov4; Erwin M. Schoof1; 1Technical University of Denmark, Copenhagen, Denmark; 2Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; 3Thermo Fisher Scientific, San Jose, California

WP 653 Innovative in-capillary sample processing coupled to high-sensitivity CE-MS analysis to decipher the proteome and N-glycome of single mammalian cells: Yunfan Gao1; Anne-Lise Marie1; Alexander R. Ivanov1; 1Northeastern University, Boston, MA

WP 654 Automated Single-Cell Metabolomics to Map Molecular Transducers of MSC Senescence: Joseph L. Corstvet1; Samuel M. Ehrlich2; Daniel D. Vallejo3; Molly E. Ogle4; Bo Yang5; Alexandra E. Dunn5; Mohamed W. Badawy6; Johnna S. Temenoff7; Craig R. Forest8; Facundo Fernandez9; 1Georgia Institute of Technology, Atlanta, GA

WP 655 Pipetting-free single cell analysis with the label-free proteoCHIP and the Evotop adapter for high sensitivity proteomics on the timsTOF SCP: Christoph Krisp1; Dorte Bekker-Jensen2; David Hartmyr3; Anjali Seth4; Moritz Heusel5; Magnus Huusfeldt6; Thorstian Lederthiel1; Jean-Francois Greisch1; Andrea Almeida1; Jarrod Sando2; Guilhem Tournaire3; Nicolai Bache1; Markus Lubeck2; Gary Krupp2; Bruker Daltonics GmbH & C.KG, Bremen, Germany; Eevosep, Odense, Denmark; Cellierion SASU, Lyon, France; IonOptix Pty Ltd, Melbourne, Australia; Bruker S.R.O., Brno, Czech Republic

WP 656 Pushing the boundaries for robust and high-throughput single cell analysis with Whisper Flow technology powered by diaPASEF: Dorte B. Bekker-Jensen1; Christoph Krisp2; David Hartmyr2; Anjali Seth3; Ole B. Hoerning4; Moritz Heusel5; Magnus Huusfeldt6; Andrea Almeida1; Jarrod Sando2; Markus Lubeck2; Gary Krupp2; Nicolai Bache1; Eevosep Biosystems, Odense, Denmark; Bruker Daltonics GmbH & C. KG, Bremen, Germany; Cellierion SASU, Lyon, France; IonOptix Pty Ltd, Melbourne, Australia; Bruker S.R.O., Brno, Czech Republic

WP 657 Algorithmic challenges in single-cell proteomics data analysis: Hannah Boekweg1; Samuel H Payne2; Brigham Young University, Provo, UT

WP 658 Metabolomic coverage of small cell populations: Julius Aongo1; James Edwards1; Saint Louis University, Saint Louis, MO

WP 659 Top-Down Proteomics of Human Single Cells using Spray-Capillary Based Microsampling and Online CE-MS Analysis: Walter Galie1; Zhilao Zhao2; Trishika Chowdhury1; Samin Anjum1; Yanting Guo2; Kellely A Cupp-Sutton2; Si Wu1; University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK

WP 660 Applying parallel proteomics and transcriptomics from same single cells to investigate mitotic regulation: James M Fischer1; Thermo Fisher Scientific, Bremen, Germany; Sarah M Williams1; Kristin M Engbrecht2; Ronald J Moore3; William Christer4; Joshua Cantlon5; Johannes W Bagnoli1; Anjali Seth3; Lijiana Pasha-Tolic3; Yin Zhu3; Pacific Northwest National Lab, Richland, WA; Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, Washington; Nuclear, Chemistry, and Biology Division, Pacific Northwest National Laboratory, Richland, Washington; Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA; Cellierion SASU, Lyon, France

WP 661 How many proteins is enough? The race for utility in single-cell proteomics: Alyssa A Nitz1; Jose Humberto Giraldez Chavez2; Samuel H Payne3; Brigham Young University, Provo, UT

WP 662 New functionalities of ms.epfl.ch for advanced on-line processing of High-Resolution MS and MS/MS data: Daniel Trujillo Ortiz1; Ricardo dei Reis Silvestro2; Natalia Gasilova1; Rémi Martine1; Cyril Portmann1; Luc Patiny1; Vincent Mute1; Laure Menin1; EPFL SB ISIC-GE, Lausanne, Switzerland; HES-FO, Fribourg, Switzerland; Infamalps SA, Monthey, Switzerland

WP 663 All-biomass carbon nanofiber for matrix-assisted laser desorption/ionization mass spectrometry: Haoran Zhang1; Wenxin Wu2; Lijing Li3; University of Wisconsin-Madison, Madison, WI

WP 664 Method Validation for the Determination of 11-nor-9-carboxy-Δ9-THC and 11-nor-9-carboxy-Δ9-THC in Human Urine by Liquid Chromatography Coupled to Mass Spectrometry (LC/MS/MS): Adrian Rausch1; Ana
WP 665 Removal Of Potential Pitfalls- Improve Ruggedness of Bioanalytical Method by Focusing On Assay Details; Xiaodong Zhu; Jingguo Hou; Penny Fan; Andrew Cunningham; 1Worldwide Clinical Trials, Austin, TX, 2UC Davis Graduate Studies, Davis, CA; 3UC Davis, Davis, CA

WP 666 Mass Spectrometry-guided Synthesis of Iodoacetyl Black Hole Quenchers; Pradnya Patil; Karine Bagramyan; Daniel Röth; Markus Kalkum; 1City of hope, Duarte, CA

WP 667 Two-Dimensional Ion Chromatography Tandem Mass Spectrometry (2D IC-MS/MS) Method for The Analysis of Phosphate Metabolites in Soil Matrix; George Gachum; 1Aimee Schryer; Steven Siciliano; 2University of Saskatchewan, Saskatoon, SK

WP 668 Method Development for quantitative determination of creatine phosphate, creatine and ATP in rat brain by LC-MS/MS; Wen Lu; Chia-Yi Kuan; Siming Wang; 1Georgia State University, Atlanta, GA; 2University of Virginia, Charlottesville, VA

WP 669 Development of a Biological Reference Material for Accurate Ephedrine Quantification in Urine Using LC-MS/MS; Inseon Kang; Yoondam Seo; Hyeon-Jeong Lee; Junghyun Son; Hophil Min; 1Korea Institute of Science and Technology, Seoul, South Korea

WP 670 Identification of Xenobiotic Plant Metabolites Using Isotopic Enrichment Combined with Plant Cell Culture Experiments; Jesce Balcer;1 Yelena Adelfinskaya; Chris J Brown; Mike Madary; Jeffrey R Gilbert; Suresh Annandudi; 1Corteva Agriscience, Indianapolis, IN

WP 671 Prioritization Strategies for Non-Target Screening and Applications to Recycled Textile Analysis of Emerging Contaminants; Drew Szablewski; Varvara Apostolopoulou Kalkavou; Aij Mathew; Anneli Krueve; 1Stockholm University, Stockholm, Sweden

WP 672 Assessment of quantification process and measurement uncertainty for LC-IM-TOFMS analysis of contaminants of emerging concern in river water; Teresa Steininger-Mairinger; Sven Kochmann; Tim J. Causon; Stephanie Hann; 1Department of Chemistry, University of Natural Resources and Life Sciences (BOKU), Vienna, Austria; 2ACIB (austrian centre of industrial biotechnology), Vienna, Austria

WP 673 Validation of a Robust Quantitative Oral Fluid LC-MS/MS Method Comprised of 54 Analytes; Philip Hackett; Lawrence J. Andrade; Ana Celia Grenier Ph.d.; Amber Awad; 1Dominion Diagnostics, North Kingstown, RI

WP 674 Improved workflow for urinary uromitochondrially disaccharide analysis using AMAC derivatization followed by automated solid phase cleanup and LC-MS/MS analysis; Debashis Ghosh; Michael L Neugent; Karsten Liegmann; Brian Shofran; Nicole J. De Nicolo; Vladimir Shulaev; 1University of North Texas, Denton, TX; 2UT Dallas, Richardson, TX; 3Tecn, Baldwin Park, CA

WP 675 Analytical method for separation of isobaric isotomers of Delta S, 8, and 10 THC and their metabolites utilizing fast LC/MS/MS; Andre Szczesniewski; Agilent Technologies, Wood Dale, IL

WP 676 An Enhanced Avermectin Method for Characterization of Bovine Pharmacokinetics Utilizing Tandem Mass Spectrometry; Greg Jellick; Kim Lohmeyer; Dee Ellis; Stephan BH Bach; 1University of Texas at San Antonio, San Antonio, TX; 2USDA-ARS, Karlville, Texas; 3Texas A&M, College Station, TX

WP 677 Comprehensive analysis of microplastics and their adsorbed environmental matrix constituents using a combination of thermal desorption and pyrolysis with GCxGC-HRTOFMS; David E Alonso; Nick Jones; Joseph Watts; Emily Taylor; Natacha Le Moan; Jeff Cleland; Jennifer Zimmer; 1Alturas Analytics, Inc., Moscow, ID; 2Ashvattha Therapeutics, Redwood City, CA

WP 678 Bioanalysis of hydroxyl-dendrimer therapeutics using LC-MS/MS with in-source fragmentation; Jason S Watts; Emily Taylor; Natacha Le Moan; Jeff Cleland; Jennifer Zimmer; 1Alturas Analytics, Inc., Moscow, ID; 2Ashvattha Therapeutics, Redwood City, CA

WP 679 Deep structural analysis of glycogen in biological samples and in disease states; Yasmine Bouchibti; Cathy Chen; Carlito S. Lebrilla; 1UC Davis Graduate Studies, Davis, CA; 2UC Davis, Davis, CA

WP 680 Tryptophan metabolite microLC-MS/MS method development and its application to clinical research on metabolism relating to aging and chronic diseases; Carolina N. Perez; John J. Thaden; Gabriella A.M. Ten Have; Nicolaas E.P. Deutz; 1Texas A&M University - Center for Translational Research in Aging and Longevity, College Station, TX

WP 681 Simultaneous quantitation of multiple excipients in biological formulation by using LC-MS/MS; Nilesht Patil; Ashutosh Shelar; Samruddha Chavan; Nilish Ramchandra Suryawanshi; Nilit Shukla; Purushottam Sutar; 1Dr. Pratap Rasam; 2Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India

WP 682 Elucidating Gut Microbial Metabolism with Mass Spectrometry Through 13C Labeled Dietary Fiber; Christopher Suarez; Cheng-Yu Weng; Chad Masarweh; David Mills; Carlito Lebrilla; 1University of California, Davis, Davis, CA

WP 683 AGMD-M determines histone methylation with methyl donors from diverse sources using peak pair pruning; Mark Sowers; Kangling Zhang; 1University of Texas Medical Branch at Galveston, Galveston, TX

WP 684 Peak Pair Pruner: an addon to MS-DIAL for peak pair validation and ratio quantification of isotopic labeling LC-MS(MS) data; Ryan A Smith; 1Qibin Zhang; 2Center for Translational Biomedical Research, University of North Carolina at Greensboro, North Carolina Research Campus, Kannapolis, NC 28081, USA, Kannapolis, NC; 3Department of Chemistry & Biochemistry, University of North Carolina at Greensboro, Greensboro, NC

WP 685 Measuring Antimicrobial Resistance in Methicillin-Resistant Staphylococcus aureus using Deuterium Labeling on a Bruker Bioterpy MALDI-TOF; Josiah J. Remnser; Paul Lueb1; Bryan Belleaire; Young Jin Lee; 1Iowa State University, Ames, IA

WP 686 Mass spectrometric characterization of selectively deuterated native bacterial lipids informs design considerations for lipid deuteration and enhances neutron scattering experiments; Matthew J Keller; 1Qiu Zhang; Brian C Sanders; Hugh M O’Neill; Robert L Hetlich; 1Oak Ridge National Laboratory, Oak Ridge, TN; 2University of Tennessee, Knoxville, TN

WP 687 Hydrogen-Deuterium Exchange of Isotopically Labeled Protein Mixtures; Prabav S Dias; Darby Ball; Oladimeji S Olayiwoye; Javier Flores; Sheena D’arcy; 1University of Texas at Dallas, Richardson, TX

WP 688 Discovery of metabolic signature in hepatic fibrosis and pulmonary fibrosis using 13C-MFA; Mieong Kim; 1Ashvattha Therapeutics, Redwood City, CA

WP 689 A New Set of Isobaric Labeling Reagents for Quantitative 16-Plex Proteomics; Xiaolong Qian; Gidan Li; Jin Zhi; Zhanlong Mei; Jie Liu; Yuxing Zhang; Mao Bi; Xingang Liu; Chao Lv; Hequan Yao; Jianguo Sun; Feng Rao; Shuwei Li; Siqi Liu; 1University of Chinese Academy of Sciences, Shenzhen, China; 2BGI Shenzhen, Shenzhen, China; 3School of Life Sciences, Department of Biology, Southern University of Science and Technology, Shenzhen, China; 4Nanjing Apollomics Biotech Inc, Nanjing, China; 5China Pharmaceutical University, Nanjing, China

WP 690 Quantitative flux analysis of compartmentalized NADH metabolism; Yahu Wang; 1Ethan Stanciliffe; Michaela Schweiger-Haber; Leah P. Striver; Gary J. Patti; 1Columbia University, New York, NY; 2Corteva Agriscience, Indianapolis, IN

WP 691 Profiling the human urinary proteome using a dimethyl-based multiplex-DIA workflow; Ericka Itan; Marvin
Data-driven approach to resolve precursor enrichment in metabolic labeling: Henock M. Deberneh1, Justin Zhu1, Rovshan G. Sadygov1,2

Quantifying Protein Synthesis Using Orbitrap Gas Chromatography High-resolution Mass Spectrometry: Xiaorong Fu1, Stanislaw Deja1, Justin Fletcher1, Jeffrey Browning1, Shawn Burgess1, UT Southwestern Medical Center, Dallas, TX, 2UT Southwestern Medical Center, Dallas, Texas.

Dual tagging for multiplex quantitative metabolomics using LC-HRMS: Brianna Mwimkong Tengan1, James Edwards1, Michael Arrambuster1, Saint Louis University, St. Louis, MO.

Slow TCA cycle flux implies suppressed ATP production in solid tumors: Caroline R Bartman1,2,3, Daniel R Weiland1,2, Yihui Shen1,2, Won Dong Lee1,2, Yujiao Han3, Tara Teslai1,2, Connor S. Jankowski1,2, Laith Samarah1,2, Noel R Park1,2, Victoria Da Silva-Diz1, Maya Aleksandrova1, Yetis Guiletkin1,2, Argi Marishta1,4, Lin Wang1,2, Lifeng Yang1,2, Shawn Davidson1, Martin Wuehr1,4, Matthew G Vandenberghe1,3, Daniel Herranz1, Jyoti Yanxiang Guo1, Yibin Kang1,4, Joshua D Rabinowitz1,2,3, Department of Chemistry, Princeton University, Princeton, NJ, Lewis-Sigler Institute for Integrative Genomics, Princeton University, Princeton, NJ, 2Ludwig Institute for Cancer Research, Princeton University, Princeton, NJ, 3Department of Molecular Biology, Princeton University, Princeton, NJ, 4Cancer Institute of New Jersey, Rutgers University, New Brunswick, NJ.

MitoMap – A three-dimensional landscape of mitochondrial architecture: Kerem Can Akkaya1,2,3, Ying Zhi1, Cong Wang1, Dmytro Puchkov1, Martin Lehmann1, Fan Liu1,2,3, Department of Structural Biology, Leibniz-Forschungsinstitut für Molekulare Pharmakologie (FMP), Berlin, Germany, 2Core Facility Cellular Imaging, Leibniz-Forschungsinstitut für Molekulare Pharmakologie (FMP), Berlin, Germany, 3Charité – Universitätsmedizin Berlin, Berlin, Germany.

An integrated nascent proteomics approach to systematically investigate how translation initiation factors shape the cancer proteome: Toman Bortecen1, Robert Wolfgang Kalis1, Johannes Zuber1, Jeroen Krijgsve1, Torsten Müller1, German Cancer Research Center (DKFZ), Heidelberg, Germany, Institute of Molecular Pathology, Vienna, Austria.

Perseus plugin for circadian multi omics data analysis enables accurate prediction of circadian phase from proteomics data: Carlo De Nart1, Fatih Aygenli1,2, Andrea Schmidt1,2, Andreas Schmidt1,2, Abigail Mackey4,5, Michael Kjaer4,5, Marcus Krüger1,2,1CECAD research center, Cologne, Germany, 2Institute for genetics, Cologne University, Cologne, Germany, 3Center for Molecular Medicine Cologne, Cologne, Germany, 4ISMC, Department of Orthopedic Surgery, Copenhagen University Hospital Bispebjerg and Frederiksberg, Copenhagen, Denmark, 5Department of Clinical Medicine, Faculty of Healthy and Medical Sciences, University of Copenhagen, Copenhagen, Denmark.

The Synaptic Proteome of Autism Spectrum Disorder Across Postnatal Development in Human Primary Visual Cortex: Shelby Ruiz-Mitzner1,2, Kevin Xu1, Jin-Hong Du1, Bert Klei2, Berne Devlin1, Matthew L MacDonald1,3, 1University of Pittsburgh, Pittsburgh, PA, 2Carnegie Mellon University, Pittsburgh, PA, 3University of Pittsburgh Medical Center, Pittsburgh, PA.

MaxQuantAtlas creates large-scale, accurate cellular protein concentration maps from heterogeneous proteomics data: Daniela Ferretti1,2, Yatao Shi1, Pavel Sintcyn1,3, Medeni Taxw1,3, Chris Brown1,3, Scott Rusin1, Eric Kuhn2,3, Susanne Breitkopf2,3, Dirk Walth2,3, Juergen Cox1, Kirti Sharma2, 1Max Planck Institute for Biochemistry, Martinsried, Germany, 2Kymera Therapeutics, Watertown, MA, 3Max Planck Institute for Biochemistry, Planegg, Germany.

Proteomic Measurements reveal how the bacterium Thermoaerophilus thermosphaericus executes the uptake and metabolism of diverse carbohydrates for eventual bioproduct production: Megan K Elliott1,2, Kristina T Stephens3, Richard J Giannone1,2, Evert K Holwerda2, Robert L Hettich1,2, Oak Ridge National Laboratory, Oak Ridge, TN, University of Tennessee, Knoxville, TN, Dartmouth College, Hanover, NH.

Development and validation of a multi-omics platform to evaluate compounds in Lead Discovery based on progressive and differentiable cellular phenotypes: Timothy Harnerly1, Tao Wang1, Chris Kwiatkowski1, Karina Edwards1, Heidi Van Every1, Evan Rosa-Roseberry1, Francesca Zappacosta1, Joseph Kozole1, Roland Annan1, GlaxoSmithKline, Collegeville, PA.

USP7 regulates the mTORC1 Polycomb axis to stimulate genomic H2AK119ub1 deposition uncoupled from H3K27me3: Jeroen AA Demmers1,2, Ayestha Sij1, Yaser Atlasi1, Jan A Van Der Knaap1,2, Joyce Wolf1, Van Der Meer1, Gillian E Chalkley1, Karel Beetzstaroti1, Dick HW Dekkers1, Wouter AS Doll1, Zeilja Ozug1, Wilfred FJ Van Ijken1, Peter CP Verneritz1, Eramus Medical Center Rotterdam, Rotterdam, Netherlands, Queen’s University Belfast, United Kingdom.

Proteomic and Transcriptomic analysis of caste transition and aging in the ponerine ant, Harpagognathos saltator: Maxxum Fiorito1, Karl Glastrad2, Michael Gilbert2, Matan Sorek3, Tierney Ganon3, Shelley Berger1, Department of Biochemistry and Biophysics, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA, Department of Cell and Developmental Biology, University of Pennsylvania, Philadelphia, PA.

Multi-omics Evaluation of Progranulin Deficiency in Human iPSCs, iPSC-derived Neurons, and Mouse Brain: Gwangbin Lee1, Haorong Li1, Cha Yang1, Jiawei Ni1, Wan Nur Atiqah Mazli1,2, 1OmicEra Diagnostics, Hong Kong, 2Singapore Institute of Food and Biotechnology Innovation, Singapore, Singapore.

Integrating Metabolomics and Systems Biology to enhance Limonene yield from engineered bacterial cultures: Jasmeet Kaur Khani1, You Ting Hee1, Chew Wee1, Kumar Selvaragoo3,4, 1Singapore Institute of Food and Biotechnology Innovation, Singapore, Singapore, 2Bioinformatics Institute (BII), Agency for Science, Technology and Research (A*STAR), Biopolis, Singapore.
WP 709 Multi-layered Proteomics Analysis of Insulin Signaling in a Hepatic Cell Line Mimicking Insulin Sensitivity and Resistance: Sarah Hyllkevist Jørgensen; Kristina Bennet Emdal; Anna-Kathrine Pedersen; Rita Slaby; Peter Kresten Nielsen; Jesper Velgaa Olsen; Novo Nordisk A/S; Måløv, Denmark; Novo Nordisk Foundation Center for Protein Research, University of Copenhagen, Copenhagen, Denmark

WP 710 GoDig-enabled Targeted Proteomics Assays Using a Commercialized TMT-labeled Yeast Standard: Kevin Dong; Qing Yu; Steven R. Shukin; Edward L Huttin; Steven P Gygi; Joao A Paulo; Harvard Medical School, Boston, MA

WP 711 LC-HRMS Based Proteo-metabolomics to Reveal Molecular Remodeling Underlying Methionine-induced Cell Fate Change in Vertebrate (Frog) Embryos: Jie Li; Kaitlyn E. Stepler; Leena R. Pade; Camille Lombard-Banek; Peter Nemes; University of Maryland College Park, College Park, MD

WP 712 Method Development for Epitope Mapping of Membrane Rearrangements Embedded in Virus-Like Particles: Esther Wolf; Lauri Pei; Joan Tevra; Mart Ustav Jr.; Derek Wilson; York University, North York, ON; Icosagen, Ossu, Estonia

WP 713 Elucidation of the distinct RNA-protein interactomes of SARS CoV-2 genomic and subgenomic RNAs: Isabella T Whitworth; Rachel Knoener; Maritza Puray-Chavez; Peter Hallmann; MBark Baddouh; Sofia Romero; Mark Scall; Yoshishiro Kawakoa; Sebia Kultuyo; Lloyd M Smith; Nathan M Sherrer; University of Wisconsin-Madison, Madison, WI; Washington University in St. Louis, St Louis, MO

WP 714 LC-UV-MS Analysis of Intact Adeno-Associated Virus (AAV) Vector Capsid Proteins: Amber D Henry; Pei Liu; Kevin Ray; Sigma Aldrich, St. Louis, MO

WP 715 Stability Characterization of Multiple Serotypes of Adeno-Associated Virus Using Charge Detection Mass Spectrometry: Rachel Koerber; Susan Abbatiello; Andy Jarrell; Waters Corporation, Milford, MA

WP 716 Characterization of Adeno-associated viral proteins and related proteoforms using top-down approach on a LC-Orbitrap Tribrid MS platform: Reiko Kiyonami; Kristina Szrentic; Kenneth Thompson; Chao Yan Liu; Min Du; Thermo Fisher Scientific, San Jose, CA; Thermo Fisher Scientific, Chi, Switzerland; Thermo Fisher Scientific, Frederick, Maryland; Thermo Fisher Scientific, Cambridge, MA

WP 717 Reassessment of excess DNA packaging in Zamilon virophage using charge-independent nano-resonator MS: Szu-Hsueh Li; Sandra Jeudy; Adrien Reynaud; Bogdan Vysockiy; Yohann Couté; Julia Novion-Ducassous; Jean-Michel Claverie; Sébastien Hentz; Chantal Abregel; Christophe Masselon; Department of Chemistry, National Cheng Kung University, Tainan, Taiwan; UA13, Inserm/CEA/UGA IRIG, Biosciences et biogénierie pour la santé, Grenoble, France; CNRS - UMR 7256 - IGS, IMB, IOM, Marseille, France; Université Grenoble Alpes, CEA, LETI, Grenoble, France

WP 718 Investigating epitranscriptomic communications between selected neuremodulator and HIV-1 lifecycle in the CNS by MS-based techniques: Limin Deng; Jyotsna Kumar; Mikaila French; Danièle Fabris; UConn Chemistry Dept, Storrs, CT

WP 719 Adeno-Associated Virus Capsid Proteins Peptide Mapping by Analytical & Micro Flow Reversed Phase Chromatography Coupled to High Resolution Mass Spectrometry: Sergio Guazzotti; Roxana Eggleston-Rangel; Mastooreh Chamanian; Lorne Nelson; Phenomenex, Alcobendas, Madrid, Spain; Phenomenex, Torrance, CA

WP 720 Peptide mapping and post-translational modifications of AAV5 produced in HEK293: Geoffrey Rule; Agnieszka Lass-Napiorkowska; Pei Liu; Kevin Ray; Cory Muraco; Millipore Sigma, Bellefonte, PA; MilliporeSigma, St. Louis, MO; MilliporeSigma, Bellefonte, PA

WP 721 Detailed Characterization of Adeno-Associated Virus Capsid Proteins by Combining Peptide Mapping and Protein Fingerprinting by Intact Mass: Kevin Ray; MilliporeSigma, St. Louis, MO

WP 722 Arborviral-induced alterations of the mosquito lipidome: Paul S Somja; Oshani Ratnayake; Irma Sanchez-Vargas; Nunya Chotwian; Barbara Graham; Samantha Pinto; Amber Hopf-Jannasch; Rushika Perera; Center for Metabolism of Infectious Diseases, Center for Vector-borne Infectious Diseases, Colorado State University, Fort Collins, CO; Chakri National Medical Institute, Faculty of Medicine Ramathibodi Hospital, Thailand; Bindley Bioscience Center, Purdue University, West Lafayette, Indiana

WP 723 Assessing the fate of Virus-Like-Particles (VLPs) during neutralization before mass analysis: Vaitson Camukou; Mehrzad Roudini; Louis Dartigueolongue; Baslian Pellegrini; Sebastien Ferron; Andreas Mazzella; Christophe Masselon; University of Grenoble Alpes (UGA), Grenoble, France; CEA, IRIG, Grenoble, France; Leibniz Institute for Solid State and Materials Research, IFW Dresden, Dresden, Germany; CEA, LITEN, Grenoble, France

WP 724 Not too heavy, not too light, it’s just right! Using viral molecular mass to discriminate human respiratory viruses: Vaitson Camukou; Thomas Fortin; Sebastien Ferron; Christophe Masselon; University of Grenoble Alpes (UGA), Grenoble, France; CEA, IRIG, Grenoble, France; CEA, LITEN, Grenoble, France

WP 725 Optimized Liquid Chromatography-Mass Spectrometry Methods for Integral Protein Analysis and Peptide Mapping of Adeno-Associated Virus Capsid Proteins: Iain Tuna Sakalligolu; Anjali Alving; Braker Scientific, LLC, Billerica, MA

WP 726 Development of an LC-MS/MS Based Multi-Attribute Characterization Assay for a Live Virus Vaccine: David Foreman; Alyssa Q Stiving; Xuanwen Li; Hillary A. Schuessler; Merck, West Point, PA

WP 727 Mass Spectrometry-based Determination of Tailed Phage Virion Protein Copy Number: Gialinh Vu; Sophia Unwin; Sammy Park; Dan Moleur; Susan Christopher; Susan T. Weintraub; Rochester Institute of Technology, Rochester, NY; Univ. of Texas HSC, San Antonio, TX; Proteome Software, Portland, OR

WP 728 HIV-1 Virion Proteome Analysis Reveals Conserved and Novel Post-Translation Modifications Modulating Viral Function: Claire E Boos; James W Bruce; Mark Scall; Rachel M Miller; Nathan M Sherrer; Lloyd M Smith; University of Wisconsin-Madison, Madison, WI

WP 729 Individual Ion and Charge Detection on the Orbitrap Analyzer for Robust Analysis of Large Native Complexes: Jared O. Kafader; John P. McGee; Pei Su; Michael A. R. Hollas; Ryan T. Fellers; Kenneth R Durbin; Philip D. Compton; Neil L. Kelleher; Northwestern University, Evanston, IL; Integrated Protein Technologies Inc., Carlsbad, CA

WP 730 In-depth Characterization of Adeno-Associated Viruses using Microchip Capillary Electrophoresis Coupled with Mass Spectrometry: Josh Smith; Sara Carillo; Adi M Kulkarni; Erin Redman; Kate Yu; Jonathan Bones; National Institute of Bioprocessing Research and Training, Dublin, Ireland; MDA-089 Devices Inc., Boston, MA; School of Chemical and Bioprocess Engineering, University College Dublin, Dublin, Ireland
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 7:00 - 8:00 pm

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Data-Independent Acquisition II .............................026-046
Education: Teaching MS and Teaching with MS ..........047-052
Elemental Analysis .............................................053-054
Energy: Petroleum, Biofuels, and Algae ......................055-064
Environmental: General III....................................065-089
Environmental: Pharmaceuticals and Pesticides ..........090-101
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Food Safety & Chemistry: Foodomics, Allergens, Bacteria, Foods, and Supplements II.........................122-147
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Small Molecules: Qualitative and Quantitative Analysis II ..................................................714-735

ThP 001 Exploring the Application of Rapid Evaporative Ionisation Mass Spectrometry (REIMS) to Bovine Health Monitoring and Milk Quality Analysis; Rachael Patricia Murdock1; Sharon Huws2; Simon Cameron3; 1Queen’s University Belfast, Belfast, United Kingdom

ThP 002 Rapid, High-Throughput Measurement of Catecholamine Neurotransmitters and Their Metabolites in Urine by Paper Spray Mass Spectrometry (PS-MS); Taelor M. Zarkovic1,2; Jan Palaty2; Jason L. Robinson3; Christopher G. Gill4.5,6,7; 1Appl. Env. Res. Labs. (AERL), Nanaimo, BC; 2University of Victoria, Victoria, BC; 3Fraser Health, New Westminster, BC; 4Health PEI, Charlottetown, PEI; 5Vancouver Island University, Nanaimo, BC; 6Simon Fraser University, Burnaby, BC; 7University of Washington, Seattle, WA

ThP 003 Can the extracted chemical information from FFPE samples using LA-REIMS imaging support pathological diagnosis?; Gabriél Stefan Horkovics-Kováts1,2; Richard Schäffer1; Csaba Hajdu2; Attila Egh1; Fanni Gaža3; Bálint András Deák2; Benedek Gyongyösi2; Gitta Schlosser4; Julia Balog5; 1Édvós Loránd University, Budapest, Hungary; 2Waters Research Center, Budapest, Hungary; 3Department of Pathology, Forensic and Insurance Medicine Semmelweis University, Budapest, Hungary

ThP 004 Field Forward Collection and Analysis: Utilizing Pressure-Sensitive Adhesive Paper Combined with Portable Spectrometry for Detection of Threats; Dan Caram1; Nicholas Manicke2; Elizabeth Dhummakupt2; 1Exct, Gunpowder, MD; 2IUPUI, Indianapolis, IN; 3U.S. Army DEVCOM Chemical Biological Center, Aberdeen Proving Ground, MD

ThP 005 Identification of Ignitabl e Liquids by Gas Chromatography-Mass Spectrometry and Direct Analysis in Real-Time-Mass Spectrometry via Their Marker Compounds; Shrutti Pareja1; Briza Marie Wicks2; 1Kansas State University, Manhattan, KS; 2University of Kansas, Lawrence, KS

ThP 006 Ambient Ionization-Based Screening Protocols for High Priority N-Nitrosamines in Pharmaceutical, Forensic, and Environmental Samples; Ebenerez H. Bondzie1; Trevor J. McDaniell1; Patrick W. Fiedl2; Donald C. Mulligan3; 1Illinois state university, Normal, IL; 2Naval Air Warfare Center, Weapons Division, China Lake, CA; 3Illinois State University, Normal, IL

ThP 007 Rapid, parallel analysis of derivatized volatile phenols in grapes and wines by sorbent sheets (SPMESH) coupled to DART-MS; Terry L Bates1,2; Gavin L. Sacks1; 1Cornell University, Ithaca, NY; 2Bruker Daltonics, Billerica, MA

ThP 008 Biopolymer-based sorptive phases into hypodermic needles: sample preparation and direct ambient mass spectrometry analysis in a single device; Jaime Millán-Santiago1; Rafael Lucena1; Soledad Cárdenas1; 1University of Córdoba, Córdoba, Spain

ThP 009 Accelerated Aza-Michael Addition and SuFEx Reaction in Microdroplets; Jyotirmoy Ghosh1; Joshua Mendoza2; R. Graham Cooks3; 1Purdue University, West Lafayette, IN; 2Purdue University, WEST LAFAYETTE, IN

ThP 010 Differentiation of Poly(vinylidene fluoride) polymers based on their end groups by DART-FT-ICR MS and modified Kendrick mass defect diagram; Pierre Pacholski1,2; Sébastien Schramm2; Frédéric Progent1; Frédéric Aubriet2; 1CEA, DAM, DIF, F-91297 Arpajon, France; 2Laboratoire de Chimie et Physique-Apprcoche Multi-échelles des Milieux Complexes (LCP-A2MC), Université de Lorraine, METZ, France

ThP 011 Rapid Detection of Amino Acid-based Metabolic Disorders by On-Sample Schiff Base Derivatization and Paper Spray Mass Spectrometry; Marcos Bouza Antones1; Daniel Foest2; Sebastian Brandt3; Juan F. García-Reyes4; Joachim Francke5; 1University of Jaén, Jaén, Spain;
**THURSDAY POSTERS**

**ThP 012**

Comparison of LC-MS and Two Ambient Ionization Techniques for the Quantitative Analysis of Phenybutazone and Oxyphenbutazone in Equine Serum

- David Borts
- Laura Burns
- Dwayne Schrunk
- Tom Kane
- Ryan Mckitlisch
- Shane Stevens

- Iowa State University Veterinary Diagnostic Laboratory, Ames, IA
- Restek Corporation, Bellefonte, PA

**ThP 013**

Towards mass spectrometry guided skin cancer surgery

- Lauritz Falkow Borsen
- Fernanda Endringer Pinto
- Martin Glud
- Stine Regin Wiegele
- James McKenzie
- Uwe Paasch
- Merete Handersdal
- Zoltan Takats
- Christian Janfelt
- Catharina Margrethe Lerche
- Bispbjerg Hospital, Copenhagen, Denmark
- University of Copenhagen, Copenhagen, Denmark
- Imperial College, London, London, United Kingdom
- University of Leipzig, Leipzig, Germany

**ThP 014**

Rapid analysis of C6 aldehydes in foodstuffs by sorbent sheet extraction and direct analysis in real-time mass spectrometry (SPMESH-DART-MS)

- Andre P. Kalenak
- Terry L Bates
- Gavin L. Sacks

- Cornell University Dept. of Food Science, Ithaca, NY

**ThP 015**

Quantitation of Lignin/Cel lulose/Hemicellulose and Lignin Monomeric Unit Ratios in Lignocellulosic Biomass via Laser-Assisted Micro-Pyrolysis Flowing Atmospheric-Pressure Afterglow Mass Spectrometry

- Dong Zhang
- Michael Loemer
- Ejpke Akatugba
- Gerardo Gamez
- Texas Tech University, Lubbock, TX

**ThP 016**

Direct analysis and classification of different olive oils by paper spray mass spectrometry

- Ines R Talarico
- Lucia Bartella
- Priscia Rocivo Bautista
- Antonio Molina Diaz
- Leonardo Di Donna
- Juan F Garcia-Reyes

- University of Calabria, Rende, Italy
- Universidad de Jaen, Jaen, Spain
- University of Jaen, Jaen, Spain

**ThP 017**

A Tool Allowing Rapid Acquisition and Extraction for Processing of DESI Screening Application Data

- Mark Towers
- Lisa Reid
- Richard Chapman
- Joanne B Ballantyne
- Rosyton Goodacre
- Ian D Wilson
- Paul Richardson
- Richard Davey
- Waters Corporation
- Wilmslow, United Kingdom
- Waters Corporation, Milford, MA
- University of Liverpool, Liverpool, United Kingdom
- Waters Corporation, Milford, MA

**ThP 018**

4 to 6 Orders of Magnitude More Matter Into The Ion Inlet Tube For IBF “ESI” MS With A Surprise

- Drew Sauter
- Nanoliter, LLC, Henderson, NV

**ThP 019**

Simultaneous Analysis of Methadone, Naltrexone, Naloxone and Nalmefene in Dog Plasma using LC-MS/MS

- Rachel M. Proctor
- Yi Di

- LabExperts sp. z o. o., Gdańsk, Poland
- Bioanalytic sp. z o. o., Wrocław, Poland

**ThP 020**

Automating analyses of confiscated samples for identification of illicit drugs

- Fuju Guan
- Matthew A. Adreance
- Leif McGillorck

- University of Pennsylvania, West Chester, PA
- University of Pennsylvania, Philadelphia, PA

**ThP 021**

Simultaneous Quantification and Confirmation of Oxycodeone and its Metabolites in Equine Urine by UHPLC-MS/MS

- Jaclyn R. Miasanelli
- Youwen You
- Rachel M. Proctor

- Columbia University, New York, NY
- University of Pennsylvania, New Bolton Center Campus, Kennett Square, PA
- Pennsylvania Equine Toxicology and Research Laboratory, West Chester, PA

**ThP 022**

A novel high-throughput GC-MS/MS method for detecting NSAIDs, Steroids, and Cannabinoids in Equine Plasma

- Leif K McGillorck
- Youwen You
- Fuju Guan
- Mary A. Robinson

- Department of Clinical Studies, School of Veterinary Medicine, University of Pennsylvania, New Bolton Center Campus, Kennett Square, PA
- Pennsylvania Equine Toxicology and Research Laboratory, West Chester, PA

**ThP 023**

HR-MS/MS EAD and CID fragmentation leads to selective, sensitive and reliable quantitation of anabolic steroids in urine

- Adrian Soboh
- Rafal Szewczyk
- Anna Lenartowicz
- Juliia Mironienka
- Katarzyna Krupczylyka-Stopa
- Maciej Stopa
- Andrzej Kwasnica

- LabExperts sp. z o. o., Gdańsk, Poland
- Bioanalytic sp. z o. o., Wrocław, Poland

**ThP 024**

Multiplex analysis of muscle developing five monoclonal antibodies in human plasma using LC-HRMS

- Hyoeon-Jeong Lee
- Yoondam Seo
- Insee Kang
- Junghyun Son
- Eugene C. Yi
- Hophil Min

- Korea institute of science and technology, Seoul, South Korea
- Korea University, Seoul, South Korea

**ThP 025**

Using Water Adduction to Differentiate Cannabinoid Isomers in a Quadrupole Ion Trap Mass Spectrometer

- Dini S. Fernando
- Cameron D. Worthington
- Gary L. Glish

- University of North Carolina at Chapel Hill, Chapel Hill, North Carolina, USA

**ThP 026**

Over 150 000 Peptide Precursors Identified in a Single Injection dIA-PASEF Workflow

- Joshua Charkow
- Brenton Seale
- Brett Larson
- Anne-Claude Gingras

- Department of Molecular Genetics, University of Toronto, Toronto, ON
- Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, ON
- Lunenfeld-Tanenbaum Research Institute at Mount Sinai Hospital, Sinai Health, Toronto, ON

**ThP 027**

Quantifying 1000 protein groups per minute of gradient using data-independent acquisition (DIA) on a hybrid quadrupole time-of-flight system

- Nicolle Narrie
- Thor Batruch
- Patrick Pribit

- SCIEX, Macclesfield, United Kingdom
- SCIEX, Concord, ON

**ThP 028**

Integrating DIA-NN software analysis of data-independent acquisition data into a cloud processing pipeline

- Melanie Juba
- Nicolle Morrice
- Alexandria Antonoplis
- Christie Hunter
- Patrick Pribit
- SCIEX, Redwood City, CA
- SCIEX, Alderley Park, United Kingdom
- SCIEX, Redwood city, CA
- SCIEX, Concord, ON

**ThP 029**

Assessment of an optimized DIA-PASEF method for the detection of low-abundant differential proteins in spike-in experiments

- Jeewon Babu Raji
- Christine Schaeffler
- Christine Carapito
- Laboratoire de Spectrométrie de Masse BioOrganique, Institut Pluridisciplinaire Hubert Curien (UMR 7178), Strasbourg, France

**ThP 030**

MaxLFQ algorithm enables accurate hybrid precursor-fragment-based quantification of plexDIA data in MaxQuant: a joint effort of Max Planck Institute of Biochemistry, Martinsried, Germany

**ThP 031**

Proteomic turnover and thermal stability profiling of chromosome 3 aneuploidy in lung cancer

- Yi Di
- Wenzuo Li
- Joao Jose Castellano Perez
- Qian Bai
- Alison M. Taylor
- Yansheng Liu

- Yale University, New Haven, CT
- Yale Cancer Biology Institute, West Haven, CT
- North Carolina University, New York, NY

**ThP 032**

DIA Phosphoproteomics: Comparative Evaluation of Dynamic Range and Quantitative Accuracy across Multiple MS Platforms

- Tanmayi D V Satpathy
- Hualong Li
- Sebastian Vaca
- Claudia Certeck
- Kholi Pham
- Hasim Keshishian
- D. R. Mani

- Stanford University, Stanford, CA

**ThP 033**

Improved library free dIA-PASEF based quantitative proteomics using Spectronaut

- Jejas Gandhi
- Damiano Robbiani
- Anna Susmel

- Biognosys AG, Schlieren, Switzerland

**ThP 034**

Accelerated mass spectrometry imaging via MS/MS spectrum decimation of inter-pixel compositional variations of metabolites

- Dan Li
- Zhou Yang

- State Key Laboratory of Precision Medicine and Theranostics, China Medical University, Shenyang, China
From data-independent acquisition (DIA) to targeted MS/MS: Automatic realignement for additional confirmation in suspect screening; Christian Klein; James S Pyke; Emma E Rennie; Cafe Simmons; Karen E Yannell; Madhusudan Sharma; Li Sun; Kai Chen; Agilent Technologies, Santa Clara, CA.

Comparison of library-free analysis of mice liver proteomics with data-independent acquisition generated by TripleTOF 5600 and ZenoTOF7600; Chang Liu; Tess Puopolo; Huijiang Li; Ang Cai; Hang Ma; Navindra P Seeram; University of Rhode Island, Kingston, RI.

Generating fit-for-purpose targeted assays from a catalog of pre-screened peptides using data-independent acquisition (DIA) based figures of merit; Ariana E Shannon; Yi Wang; Gang Xin; Amanda B. Hummon; Brian C Searle; PELotonia Institute for Immuno-Oncology, Comprehensive Cancer Center The Ohio State University, Columbus, OH; Department of Bioinformatics, The Ohio State University Medical Center, Columbus, Ohio; Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH; Department of Microbial Infection and Immunity, The Ohio State University Medical Center, Columbus, Ohio.

Efficient generation of highly multiplexed serum biomarker panels using gas phase fractionation and DIA libraries; Abigail Burrows Franco; Cecily R Wood; Ohio State University, Columbus, OH; Biomedical Informatics, The Ohio State University, Columbus, OH.

Streamlining biomarker discovery with DIA-MS in large prostate cancer fluid-based clinical cohort; Annie Ha; Amanda Kho; Zhuyu Qiu; Vladimir Ignatrenko; Julius O Nyawente; O. John Senmies; Danny Vespiari; Stanley K. Liu; University of Kentucky, Lexington, KY; Thermo Fisher Scientific, San Jose, CA.

Exploring the benefits of differential mobility separation (DMS) and SWATH data-independent acquisition (DIA) for complex proteomic sample analysis; Reyes Le Blanc; Eva Duchoslav; Lyle Burton; Stephen Tate; Bradley Schneider; ISCIEX, Concord, ON, Canada; TOFSCIEX, Concord, ON.

Investigation of the human lysosomal proteome by targeted proteomics; Stephanie Kaspar-Schoenefeld; Dhitri Arora; Andreas Schmidt; Dominic Winter; Bruker Daltonik GmbH & Co. KG, Bremen, Germany; Institute for Biochemistry and Molecular Biology, Medical Faculty, Rheinische Friedrich-Wilhelms-University of Bonn, Bonn, Germany.

Proteomic Strategies Uncover A Novel Aging Phenotype in the Post-Menopausal Ovary; Christina D King; Shweta S Dipari; Francesca E Duncan; Birgit Schilling; Buck Institute for Research on Aging, Novato, CA; Northwestern University, Evanston, IL; Institute for Molecular Medicine, Gent, Belgium; UGent Department of Biomedical Sciences, Ghent, Belgium.

Label-free quantification of over 5000 protein groups from single-cell sample amounts with median CV approaching 10% using tims-TOF SCP DIA; Peter M Pichler; Manuel Matzinger; Goran Mitulovic; Karl Mechtler; Research Institute of Molecular Pathology, Vienna, Austria; Bruker Daltonics GmbH & Co.KG, Bremen, Germany.

Design of Mass Spectrometry Experiments for Undergraduate Courses; Jixuen Bu; Junhan Wu; Nan Zhang; Yuyu Li; Wenpeng Zhang; Zheng Ouyang; URSPEC Technology (Beijing) Ltd., Beijing, China; Department of Precision Instrument, Tsinghua University, Beijing, China.

Data-centric tutorials for learning mass spectrometry and proteomics; Ansima R Mongane; Luke A Squires; Alyssa A Nitz; Samuel H Payne; Brigham Young University, Provo, UT.

Development of a self-service LC-QTOF-based metabolomics training workflow in an open access core facility; Paul Mathews, Claudia M. Boot; Paul G Mathews; Claudia M Boot; Colorado State University, Fort Collins, CO.

Benchmark MALDI MSI: Mass Spectrometry Imaging on a Budget; Kendra G. Selby; Emily M Hubecky; Gabriel A. Bressendorff; Ashley R Chirichillo; Summy Shrestha; Lynne Ling; Donald Caspary; Kevin R Tucker; Southern Illinois University Edwardsville, Edwardsville, IL; Southern Illinois University School of Medicine, Springfield, IL.

Social Media for Mass Spectrometry; Kermit K. Murray; Louisiana State University, Baton Rouge, LA.

Unlocking the Power of Mass Spectrometry in Biomanufacturing: A Microlearning Approach; M. Cyndell Gracieux-Singleton; Jason Whiteley; Brian Herrng; Marie Vestergaard; Scott Latus; Biomanufacturing Training and Education Center (BTEC), NCSU, Raleigh, NC; Technical University of Denmark, Kgs. Lyngby, Denmark.

Multi-Elemental Analysis of Chemically Defined Cell Culture Media by ICP-MS; Yulan Bian; Aimei Zou; Patrick Simmons; Agilent Technologies, Singapore; Singapore; Agilent Technologies, Santa Clara, CA.

Mpx/hr LA-ICP-TOFMS mapping and data evaluation; Martin Ruthe; Christoph Heinrich; Mathias Wilhelm; Martin Heinrich Freino; TOFwerk, Gwill (Thun), Switzerland; Elemental Scientific Lasers, Huntington, United Kingdom; Elemental Scientific Inc, Melbourne, Australia.
Effects of Aromaticity on Petroleum Acid Fragmentation; Esther Mbuna; Nathan Gard; Andrew Adam; Benjamin Bythell; Ohio University, Athens, OH

Contribution of APCI-FTICR-MS for the molecular characterization of bio-oil from lignocellulosic biomass; Charlotte Mase**1;2; Marie Hubert-Roux**1;3; Carlos Alonso**1;3; Pierre Giusti**1;2,3; 1University of Rouen, Mont Saint Aignan, France; 2TotalEnergies OneTech R&D, TotalEnergies Research & Technology, Gonfreville, France; 3International Joint Laboratory - i2C2M; Complex Matrices Molecular Characterization, TRTG, Hartlepool, France

Unraveling the Structural Secrets of Unique Compositions in Highly Complex Mixtures by High-Resolution Mass Spectrometry; Jens Dreschmann; Wolfgang Schrader; Max-Planck-Institut für Kohlenforschung, Mülheim An Der Ruhr, Germany

Applications of FT-ICR MS for the elucidation of oligomeric structures from thermochemical conversion of lignocellulosic biomass; Evan Terrell**1;2; Melba Domes Denison**1;2; Raizada Mamique Webster**1;2; Anthony Dufour**1;2; Vincent Carre**1; Frederic Aubriet**1; Manuel Garcia-Perez**1; USDA-ARS, Southern Regional Research Center, New Orleans, LA; 2Washington State University, Pullman, WA; 3Universidad Nacional de Colombia, Bogotá, Colombia; 4Université de Lorraine, Nancy, France; 5Universite de Lorraine, Metz, France

Methodology development for the monitoring of the use of Ionic Liquid in the removal of Naphtalenes acids from Oil: Sol Sauna Nety**1; Simiso Dube**1; Mathew M Nind**1; 1University of South Africa, Johannesburg, South Africa; 2UNISA, Florida Park, Roodepoort, South Africa

Derivatized Carbazoles Dissociation Chemistry; Dylan Carter**1; Jaya Paudel**1; Benjamin Bythell**1; Ohio University, Athens, OH

Absorption mode Fourier Transform – Improved data quality for the FT-ICR MS analysis of extremely complex crude oil mixtures; Alessandro Vetere**1; Wolfgang Schrader**1; Max-Planck-Institut für Kohlenforschung, Mülheim An Der Ruhr, Germany

High throughput sequencing of mutant libraries using MALDI-ToF-MS analysis of microbial colonies for selecting fatty acid desaturase variants; Kisurb Choe**1; Mike Jindra**1; Susan Hubbard**1; Blake Mirman**1; Brian F Pfleger**1; Jonathan V. Sweedler**1; 1University of Illinois at Urbana-Champaign, Urbana, IL; 2University of Wisconsin-Madison, Madison, WI

Analysis of Neutral Organic Nitrogen Compound Present in Crude Oil Using Tandem Mass Spectrometry and Computational Chemistry; Jaya Paudel**1; Lauren Davis**1; Dylan Carter**1; Benjamin Bythell**1; Ohio University, Athens, OH

Characterization of pinewood-derived fast pyrolysis oil and its water-insoluble fraction with MRMS using ESI and APCI; Hafiza Sajida Kousar**1; Janne Janis**1; 1Washington State University, Pullman, WA; 2University of Toledo, Toledo, OH; 3The Andersons, Maumee, OH 43537

Identification of Per and Polyfluorinated Alkyl Substances in Alternative Onsite Wastewater Treatment Systems by HRMS; Rachel Smolinski**1; Meghan Oates**1; Amith Maroli**1; Arjun Venkatesan**1; Carrie A McDonough**1; 1Carnegie Mellon University, Pittsburgh, PA; 2New York State Center for Clean Water Technology, Stony Brook, NY; 3Stony Brook University, Stony Brook, NY

Quantitation of Total PFAS including Trifluoroacetic Acid with Fluorine Nuclear Magnetic Resonance (19F-NMR); Dinor Cadzic*; Rebecca A. Dickman*; Abigail S. Joyce*; Joshua S. Wallace*; P. Lee Ferguson*; Diana S. Aga*; University at Buffalo, Buffalo, NY; 2Duke University, Durham, NC

Fast Screening of Perfluorinated Compounds Using Desalting Paper Spray Ionization Mass Spectrometry (DPSI-MS) Method; Md. Tanim-Al Hassan**1; Praneeth Ivan Fnu**1; Yongling Ai**1; Francis J. Osonuga**1; Omowunmi A. Sadik**1; Mengyan Li**1; Hao Chen**1; New Jersey Institute of Technology, Newark, NJ

Analysis of Ultra-Short Through Medium Chain Length PFAS in Ground and Industrial Water by Multimode Chromatography-Mass Spectrometry; Tarva Napolitano*; Zijie Beryl Xia*; Alexander Schrum*; Ronald Benson*; Resonac America, Inc, New York, New York; 2Claros Technologies, Minneapolis, MN

Identifying specific chemicals in aerosol particulate matter from various sources using mass spectrometry and artificial neural network analysis; Geondo Park**1; Seungwoo Son**1; Yongheyeon Yim**1; Sungghan Kim**1; 1Department of Chemistry, Kyungpook National University, Daegu, South Korea; 2Korea Research Institute of Standards and Science (KRISS), Daejeon, South Korea; 3Mass Spectrometry Converging Research Center and Green-Nano Materials Research Center, Daegu, South Korea

PFAS in Alligators of North Carolina’s Cape Fear River: Assessing Spatial and Temporal Trends from 2018 to 2022; Anna K. Boatman*; Kylie D. Rock*; Scott M. Belcher*; Erin S Baker*; 1University of North Carolina at Chapel Hill, Chapel Hill, North Carolina; 2North Carolina State University, Raleigh, NC

Analysis of Targeted and Non-targeted Dye and Emerging Contaminants in the Kali-Loji River, Indonesia, Using UPLC-FT-ICR-MS; Rajiful Alam**1; Dede Henri Yuli Yanto**1; Sunghwan Kim**3,4; 1Kyungpook National University, Daegu, South Korea; 2Research Center for Applied Microbiology, National Research and Innovation Agency (BRN), Bogor, Indonesia; 3Department of Chemistry, Kyungpook National University, Daegu, South Korea; 4Mass Spectrometry Converging Research Center and Green-Nano Materials Research Center, Daegu, South Korea

Utilizing Ion Mobility to Enhance Targeted and Non-Targeted Analysis of PFAS from Environmental Samples Collected at a Ski Resort; Sarah Dowd**1; Kari Organitini**1; Marian Twiohig**1; Jean Carlan**1; Frank Dorman**1,2; 1Waters Corporation, Milford, MA; 2Department of Chemistry, Dartmouth College, Hanover, NH

Analysis of Per- and Poly-fluroalkylated Substances (PFAS) Specified in EPA Method 1633 Using Triple Quadrupole LC-MS/MS; Om k Shrestha**1; Ethan Hain**1; Kathleen Luo**1; Christopher Gilles**3; Evelyn Wang**3; Xiaomeng Xia**1; Robert English**1; Tiffany Liden**2; 1Shimadzu Scientific Instruments, Columbia, MD

Extremely sensitive real-time detection of PFAS in the gas phase; Joel R. Kimmell**1; Abigail Koss**1; Carla Frege**1; 1TOFWERK AG, Boulder, CO; 2Tofwerk AG, Thun, Switzerland

A Comprehensive Workflow for PFAS Analysis in Wastewater with Extended EPA Draft Method 1633 List; Ruoji Luo**1; Emily Parry**1; Matthew Giardina**1; Linfeng Wu**1; Patrick Batoun**1; Tarun Anumol**1; 1Agilent Technologies, Inc., Santa Clara, CA

The Effect of Water Properties on the Adsorption of Microcystins and Nodularin-R from Aqueous Samples by Treated Corncobs; Hasarawuni S Kirdiana**1; Manjula M Kandage**1; Norman Pelffer**1; Michał Marszewski**1; Dragan Isaiovic**1; 1University of Toledo, Toledo, OH; 2The Andersons, Maumee, OH 43537

Quantification of Microplastics and Nanoplastics in firefighting gear and the environment; Tommy M Nguyen**1; O. David Sparkman**1; Liang Xue**1; Harry Allen**1; Terry Ramus**1; 1University of The Pacific, Stockton, CA; 2U.S. Environmental Protection Agency, Signal Hill, CA; 3Diablo Analytical Inc., Antioch, CA

Method development for the non-targeted analysis of complex environmental contaminants - understanding oxidation processes in soil; Wolgang
ThP 079

New Directions in wastewater-based epidemiology. Identification of small and large biomolecules as biomarkers of public health and industrial activities; Ruben Gil Seligone; Jessica Subirats; Montserrat Carrascal; Pablo Gago Ferrero; Antoni Ginebreda; Damia Barceló; IDAEA-CSIC, Barcelona, Spain; 2Info Instituto d'Investigaciones Biomèdiques August Pi i Sunyer, Barcelona, Spain; 3Catalan Institute for Water Research (ICRA), Girona, Spain

ThP 080

Spatial and Temporal Distributions of Per- and Polyfluorinated Alkyl Substances (PFAS) in Galveston Bay, TX; Yina Liu; Michael Shields; Sangeetha Puthigai; Xiaolei Xu; Shari Yvon-Lewis; 1Texas A&M University, College Station, TX

ThP 081

Optimizing a method to quantify per- and polyfluoroalkyl substances (PFAS) in house dust, silicone wristbands and handwipes; Sharon Zhang; 1Grace Campbell; 2Katllyn May; 1North Carolina State University, Raleigh, NC

ThP 082

Untargeted PFAS Suspect Screening and Quantitation of Community Water Samples from North Carolina’s Cape Fear River Basin; Rebecca A Weed; Jeffrey Enders; 1Grace Campbell; 2Katllyn May; 1North Carolina State University, Raleigh, NC

ThP 083

Identification of Novel Degradation Products of Microcystins using UHPLC/MS and Automated Annotation of Their MSn Spectra; Sharmila J Peraino; Judy A Westrick; 2Dragan Isailovic; 1University of Toledo, Toledo, OH; 2Wayne State University, Detroit, MI

ThP 084

Non-Targeted Analysis of Emerging Per- and Polyfluoroalkyl Substances (PFAS) in Rainwater; Yubin Kim; 1Kynald A. Pike; 1Donald Conley; 1Jameson Sprankle; 2Rebekah Gray; 1Christopher Alaimo; 2Thomas Young; 2Jennifer Faust; 1Paul L Edmiston; 1College of Wooster, Wooster, OH; 2University of Wisconsin-Madison, Madison, WI; 3University of California, Davis, Davis, CA

ThP 085

Untargeted Exposure Analysis of Lake Okeechobee Using SPE-MIC-CHRM; 1David Peden; 2Yina Liu; 1Ellen Tiwary; 2Krista McCoy; 2Timothy J. Garrett; 1University of Florida, Gainesville, FL; 2Florida Atlantic University Harbor Branch Oceanographics, Fort Pierce, FL

ThP 086

Comparing a Dried Blood Spot Microfluidic Chip to Whole Blood Analyses for PFAS Detection and Quantitation in Field Studies; Gregory Kudzin; 1James N Dodds; 1Hanah Sternes; 2Zach Mclean; 2Scott M. Belcher; 2Kevin S Baker; 1University of North Carolina at Chapel Hill, Chapel Hill, NC; 2North Carolina State University, Raleigh, NC

ThP 087

GC-MS method with reduced solvent consumption for PBDE quantification in revalorized polymers; Marc-Antoine Vaudreuil; 1Richard Silverwood; 2Alexandra Furtos-Matei; 1Université de Montréal, Montreal, QC; 2Lavergne Inc., Montreal, QC

ThP 088

Direct filter desorption of environmentally relevant chemicals using multi-scheme chemical ionization (MION) mass spectrometry; Joonas Mikkilä; 1Fariba Partovi; 2Jyrki Mikkilä; 1Tuula Jokinen; 1Neha Deoöl; 1Mikko J Sipilä; 2Aleksei Shcherbinin; 2Matti P Rissanen; 1Hi Josef; 1Karsa Ltd., Helsinki, Finland; 2Aerosol Physics Laboratory, Physics Unit, Faculty of Engineering and Natural Sciences, Tampere University, Tampere, Finland; 3Climate and Atmosphere Research Center (CARE-C), The Cyprus Institute, Nikosia, Cyprus; 4Institute for Atmospheric and Earth System Research (INAR), University of Helsinki, Helsinki, Finland

ThP 089

Trimethylation enhancement using diazomethane (TrEnDi) enables enhanced LCMS detection of glufosinate and 3-(methylphosphino)propionic acid from canola samples; Christian A Rosales; 1Krysten L Shedy; 1Karl V Wassen; 2Jeffrey M Manthorpe; 2Jeffrey C Smith; 1Carleton University, Ottawa, ON

ThP 090

Streaming HRMS data acquisition and interpretation for wastewater impact on water quality; Michael Thurman; 1Imma Ferrer; 1James S Pyke; 1University of Colorado, Boulder, CO; 2Agilent Technologies, Santa Clara, CA

ThP 091

Quantification of the Herbicide 2,4-Dichlorophenoxyacetic acid and of Specific Organophosphorous and Synthetic Pyrethroid Insecticides by LC-MS/MS; Dickson Wambua; CDC, Atlanta, GA

ThP 092

Determination of Multiclass Pharmaceuticals in Environmental Samples by Liquid Chromatography-Tandem Mass Spectroscopy; Xiaouo Wei; 1, 2; Yujie Ben; 1Chunniao Zheng; 3, 4; Zongwei Cai; 1, 3; 5State Key Laboratory of Environmental and Biological Analysis, Hong Kong Baptist University, Hong Kong, China; 6Department of Chemistry, Hong Kong Baptist University, Hong Kong, China; 7State Environmental Protection Key Laboratory of Integrated Surface Water-Groundwater Pollution Control, School of Environmental Science and Engineering, Southern University of Science and Technology, Shenzhen, China; 8EIT Institute for Advanced Study, Ningbo, China

ThP 093

Development of a high-resolution LC-MS/MS workflow combining multiple activation methods for the general screening of pesticides; Romain Gauthier; 1Mircia Guna; 2Gérard Hopfgartner; 3ILSIM, Department of Inorganic and Analytical Chemistry, University of Geneva, Geneva, Switzerland; 4SCIEX, Concord, ON

ThP 094

Residue dissipation and dietary risk assessment of cyantraniliprole, spinetoram, and flicamid in celery (Apium graveolens) under field conditions by LC-MS-MS; Yeong-Jin Kim; 1Sung-Gil Choi; 2Young Sang Kwon; 2Deuk-Young Lee; 2Jong-Su Seo; 2Jong-Hwan Kim; 1Environmental Safety Assessment Center, Gyeongnam Branch Institute, Korea Institute of Toxicology, Jinju, South Korea; 2Residue Chemical Assessment Division, Agro-Food Safety and Crop Protection Department, National Institute of Agricultural Sciences, Wanju, South Korea

ThP 095

Water quality determination: a myriad of analysis simplified; Mariia Pugden; 1Luis Oujuela; 1Shimadzu do Brasil LTDA, Barueri, Brazil

ThP 096

Determination of multiresidue pesticides in Arabian Dates using LC and GC Triple Quadrupole Mass Spectrometry; Tuna Oncu; 1Ohran Papak; 2Shimadzu Middle East and Africa FZE, Istanbul, Istanbul, Turkey

ThP 097

Measuring Antibiotics in Shao Creek using Liquid Chromatography-Tandem Mass Spectrometry during the COVID Pandemic; Cheyenne D Copling; 1Jacob Smith; 2Katherine Malloof; 1Jacob Pierson; 2Kathryn Nansch; 2Leslie Kupferle; 2Adam Sullivan; 2Megan Davis; 2Chloé Pancake; 2Samuel Bickford; 2Robert Dixon; 2Kevin R Tucker; 1Southern Illinois University of Edwardsville, White/Caucasian, IL; 2Southern Illinois University of Edwardsville

ThP 098

Pesticides residue pre-screening using KARA MION INLET CUPLED TO ORBITRAP MASS SPECTROMETER WITH SELECTIVE CHEMICAL IONIZATION; Fariba Partovi; 1Joonas Mikkilä; 2Jussi Kontro; 3Jyrki Mikkilä; 3Nasib Naseri; 2Aleksei Shcherbinin; 2Paxton Juuti; 3Suvi Ojanperä; 2Matti Rissanen; 1Yves Leblanc; 1Aerosol Physics Laboratory, Physics Unit, Faculty of Engineering and Natural Sciences, Tampere University, Tampere, Finland; 2Karsa Ltd., Helsinki, Finland; 3Finnish Customs, Helsinki, Finland; 4Aerosol Physics Laboratory, Physics Unit, Faculty of Engineering and Natural Sciences, Tampere University, Tampere, Finland; 5Department of Chemistry, University of Helsinki, Helsinki, Finland

ThP 099

A Highly sensitive method for the determination of carbamates in water as per ASTM D-7645 by LCMS-8045; Shailiesh Sadashiv Damale; 1Jessin Mathai; 1Kumar
ThP 100  Rapid low-cost testing of urine for unknown pesticide variants: Alexey Melnik; 1, 3 Olusola Onawoga; 2, 3 David Chick; 2 Silverio Iacono; 2, 3 Alexander Aksenov; 2, 3 University of Connecticut, Storrs, CT; 3 Atomix Inc., Farmington, CT; 3 TomTec, Hamden, CT; 4 University of Connecticut, Storrs, CT

ThP 101  Impact of Using 1.5 mm Column ID and Various Stationary Phases on LC/MS Pesticide Screening Analysis: Stephanie Schuster; 1 Peter Pellegrinelli; 2 Conner W. McHale; 2 Benjamin Libert; 2 Taylor Harmon; 2 Advanced Materials Technology, Inc., Pittsburgh, PA.

ThP 102  FluoroMatch 3.0 – Automated PFAS Non-Targeted Analysis and Visualizations Applied to Mammalian Biofluids; Michael Kummer; 1 Nandarani Abril; 2 Emilie Parr; 2 Sheng Liu; 2 Carrie A McDonough; 2 David Duke; 2 David Godin; 3 Elizabeth Z. Lin; 3 Emma E Rennie; 3 Jeremy Koelmel; 3 Kristal JG Pollitt; 3 Innovative Omics, Sarasota, FL; 3 Agilent Technologies, Santa Clara, CA; 3 University of South Florida, Tampa, Florida; 3 University of Louisville, Louisville, KY.

ThP 103  HRMS-based Exposomics for Evaluating Embryonic Exposure Concentration and Cross-Platens Transfer of Xenobiotics: Max L Feuerstein; 1, 2 Tira Buerki-Thummer; 2 Benedikt Wardth; 2 University of Innsbruck, Faculty of Chemistry, Department of Food Chemistry and Toxicology, Währinger Straße 38, 1090, Vienna, Austria; 3Exposome Austria, Research Infrastructure and National EIRENE Hub, Vienna, Austria; 3Empa, Swiss Federal Laboratories for Materials Science and Technology, 9014 St. Gallen, Switzerland.

ThP 104  Generating MassBank-ready files from accurate mass library spectra: a proof-of-concept study: Andrew McEachran; 1 Tristan Chukka; 2 Alex Chao; 2 Gregory Janesch; 3 Elin Ulrici; 2 Jon Soubis; 2 Antony Williams; 3 Agilent Technologies, Santa Clara, CA; 3Chemical Characterization and Exposure Division, Office of Research and Development, U.S. Environmental Protection Agency, Research Triangle Park, NC; 3ORAU Student Services Contractor to Center for Computational Toxicology and Exposure, Office of Research and Development, U.S. Environmental Protection Agency, Research Triangle Park, NC

ThP 105  Urinary DNA adductomics – a non-invasive, untargeted approach for the assessment of exposure-associated health risks: Carolina Müller; 1 Alexandra Keidl; 2 Jazmine Virzi; 2 Laura Deloso; 2 Yuan-Jhe Chang; 3 Mu-Rong Chao; 4 Chiung-Wen Wu; 4 Marcus C. Hsu; 4 Oxidative Stress Group, Department of Molecular Biosciences, University of South Florida, Tampa, Florida 33620; 5Department of Chemistry, University of South Florida, Tampa, Florida 33620; 5Department of Occupational Safety and Health, Chung Shan Medical University, Taichung, Taiwan; 6Department of Occupational Medicine, Chung Shan Medical University Hospital, Taichung, Taiwan; 7Department of Public Health, Chung Shan Medical University, Taichung, Taiwan.

ThP 106  LC-MS workflow for large-scale profiling of mercapturic acids in human urine: Jin Y Chen; 1 Zhengzhi Xie; 1 Maleesha De Silva; 2 Saurin R. Sutaria; 1 Hong Gao; 1 Sanjay Srivastava; 1 Pawel Lorkiewicz; 1 University of Louisville, Louisville, KY.

ThP 107  Roles of HNOx and Carboxylic Acids in Thermal Stability of Nitroplasticizers: Kitmin Chen; 1 Dalí Yang; 1 Zheng-hua Li; 1 Oana C. Marina; 1 Alexander S. Edgar; 1 Los Alamos National Laboratory, Los Alamos, NM

ThP 108  Exposome-Wide Mapping of Circulating Caffeine Metabolites in Large Prospective Cohort Reveals Biochemical Links between Caffeine Exposure and Parkinson’s Disease Risks: Yunia Lai; 1 Yujia Zhao; 2 Douglas J. Walker; 2 Christina M. Lii; 3 Bastiaan R. Bloem; 4 Sirwan K.L. Darweesh; 5 Susan Peters; 2 Roel Vermeulen; 2, 7 Gary W. Miller; 1 Department of Environmental Health Sciences, Mailman School of Public Health, Columbia University, New York City, NY; 2Institute for Risk Assessment Sciences, Utrecht University, Utrecht, Netherlands; 3Department of Environmental Health, Rollins School of Public Health, Emory University, Atlanta, GA; 4Institute of Epidemiology and Social Medicine, University of Münster, Münster, Germany; 5School of Public Health, Imperial College London, London, United Kingdom; 6Radboud University Medical Center; Donders Institute for Brain, Cognition and Behaviour; Department of Neurology; Center of Expertise for Parkinson & Movement Disorders, Nijmegen, Netherlands; 7University Medical Centre Utrecht, Utrecht, Netherlands

ThP 109  Wristband Personal Passive Samplers and Suspect Screening Methods Highlight Gender Disparities in Chemical Exposures: Nicholas Herkert; 1 Jessica L Levasseur; 1 Kate Hoffman; 1 Gordon Getzinger; 2 P. Lee Ferguson; 3 Anna S Young; 4 Joseph G Allen; 5 Elizabeth Z Lin; 5 Krista Godin-Pollard; 5 Heather Ratnapalan; 5 Anna S Young; 1 Nicholas School of the Environment, Duke University, Durham, NC; 2Department of Civil and Environmental Engineering, Duke University, Durham, NC; 2Department of Environmental Health, Harvard T.H. Chan School of Public Health., Boston, MA; 2Department of Environmental Health Sciences, Yale School of Public Health, New Haven, CT

ThP 110  Comprehensive Targeted Proteomics-Driven Biofluids Profiling of Aerosol Aerosol Exposed NOKI cells: New Insights into the Pathways Involved: Mehari Weldemariam; 1 Tao Ma; 2 Sarah L.J. Michel; 1 Richard N. Dalby; 1 Abraham Schneider; 2 Maureen A. Kane; 3 Department of Pharmaceutical Sciences, University of Maryland School of Pharmacy, Baltimore, Maryland; 2Department of Oncology and Diagnostic Sciences, University of Maryland School of Dentistry, Baltimore, Maryland.

ThP 111  MRM-profiling for detecting emerging contaminants in human biomonitoring: Application to Bisphenol A replacements: Jasmin Chovatlya; 1 Ravikumar Jagani; 1 Manish Arora; 2 Syam S. Andra; 3 Institute for Exposomic Research, Department of Environmental Medicine and Public Health, Icahn School of Medicine at Mount Sinai, New York, NY.

ThP 112  Comprehensive Targeted Exposome Assay for Serum Samples: Jiamin Zheng; 1 Lun Zhang; 1 Mathew Johnson; 1 Rupasri Mandal; 1 David S. Wishart; 1 University of Alberta, Edmonton, AB

ThP 113  Mapping the exposure of firefighters through the lens of mass spectrometry: Xiaoping Lin; 1 Xinmei Zhang; 2 Basil Michael; 1 Xiao Long; 1 Mary Fitzgerald; 1 Karl Christine Nadeau; 1 Michael P. Snyder; 1 Department of Genetics, Stanford University, Stanford, CA; 2Sean N. Parker Center for Allergy and Asthma Research at Stanford University, Stanford, CA

ThP 114  Structural elucidation of metabolites from bisphenol A analogs, BPB, BPAP and TBBPA, by high resolution tandem mass spectrometry: Said Ur Rehman; 1 Fan Ousij; 2 Lekha Steno; 1 University of Quebec in Montreal, Montreal, QC; 2EcoTO network on ecotoxicology research, Quebec, QC; 3University of Quebec in Montreal (UQAM), Chemistry department, Montreal, QC

ThP 115  High-resolution mass spectrometry-based evaluation of limonene metabolites as biomarkers of greenness exposure: Zhengzhi Xie; 1 Saurin R. Sutaria; 1 Jin Y. Chen; 1 Hong Gao; 1 Daniel J. Conklin; 1 Rachel J. Keith; 1 Sanjay Srivastava; 1 Aruni Bhatnagar; 1 Pawel Lorkiewicz; 1 University of Louisville, Louisville, KY

ThP 116  Utilizing Calibration Points to Replace Kovat’s Indices to Confirm Tentatively Identified Compounds: Sarah T Pfahlert; 1 Robert Bradford; 1 Jaehwan Lee; 1 Christine Duran; 2 John T Higgins; 2 Mitch Rubenstein; 2 Yue D. DAYTON, Ohio; 3US AIR FORCE, DAYTON, OH

Raju; Rajendra Makhamale; 1 Atul Narkar; 1 Shimadzu Middle East & Africa FZE, Dubai, United Arab Emirates
ThP 117 Liquid chromatographic retention time prediction models to secure and improve the feature annotation process in high-resolution mass spectrometry; Julien Parinet; Yassine Makni; Thierno Dião; Thierry Guérin; ANSES, Maisons-Alfort, France; ANSES Maisons-Alfort, France

ThP 119 Quality Control of Electronic-Cigarette Liquids by Helium-Plasma Ionization (HePi) Mass Spectrometry; Kinchan Kharangara; Logan Buddenbaum; Sijang Xu; Athula B. Attigallie; David Douce; Steve Bajic; Stevens Institute of Technology, Hoboken, NJ; Waters Corporation, Milford, MA

ThP 120 Consumer Product Non-targeted Exposomics for Proactive Human Health; Jenna Hua; Kristin A Favela; William D Watson; Jake A Janssen; Michael J Hanhett; Heath A Spidle; Jared Grossman; Maxwells Markam, Inc., Berkeley, CA; Southwest Research Institute, San Antonio, TX; Agilent Technologies, Santa Clara, CA

ThP 121 Comparison of Targeted and Untargeted DNA Adductomics methods on an LC/qToF platform; Nathan Montgomery; Corey Broeckling; Colorado State University, Fort Collins, CO; University of California, Davis, CA

ThP 122 Determination of Variance of Secondary Metabolites in Lettuces Grown Under Different Light Sources by FIMS and ANOVA-PCA; Jinghao Sun1,2; Mengliang Zhang; Nicola Kuzbodela; Yaguan Luo; James Harney; Pei Chen; USDA-ARS, Beltsville, MD; Middle Tennessee State University, Murfreesboro, TN

ThP 123 Nitrofuran Metabolites and Chlorophenicol in Aquaculture Products using LC-MS/MS; Brian Veach; Food and Drug Administration, Jefferson, AR

ThP 124 Determination of Benzophenone Derivatives in Breads in Taiwan by Solid–liquid Extraction-based UHPLC–MS/MS and Dietary Risk Assessment; Yu-Fang Huang1,2; Xuan-Rui Liu; Chen-Ting Wu; Institute of Environmental and Occupational Health Sciences, National Yang Ming Chiao Tung University, Taipei, Taiwan; Institute of Food Safety, Health and Environmental Engineering, National United University, Miaoli, Taiwan; Institute of Food Safety and Health Risk Assessment, National Yang-Ming Chiao Tung University, Taipei, Taiwan

ThP 125 Routine Quantitation of 17 Underivatized Amino Acids in Nutraceuticals and Animal Feed using HPLC with a Fit-for-Purpose MSD Detector; Gram Thompson; Sue D’Antonio; Donna Payne; Hui Zhao; Mike Adams; Agilent Technologies, Wilmington, DE; Agilent Technologies, Wilmington, Delaware; AnalytEval, SMITHVILLE, TX; CWChem Labs, Smithville, TX

ThP 126 Micro-QuEChERS coupled with UHPLC-MS/MS for Determination of Benzophenones and Parabens from Tea in Taiwan; Ting Liu; Wei-Chun Wang; Institute of Food Safety and Health Risk Assessment, National Yang Ming Chiao Tung University, Taipei, Taiwan; Institute of Environmental and Occupational Health Sciences, National Yang Ming Chiao Tung University, Taipei, Taiwan

ThP 127 The application of a QTOF instrument to enable traceability of the origin of ginger; Liuqing Zhao; Xiaoqiang Zhang; Zong Yang; Bingjie Lu; Lihai Uno; SCIEX, Shanghai, China; SCIEX, Shanghai, China

ThP 128 Development of a Multi Analyte Method for the Screening of Dietary Supplement Products; Christopher R. Beekman; Rahul Pawar; U.S. Food and Drug Administration, College Park, MD

ThP 129 Simultaneous Quantification of South Korea representative Allergenic Foods with Optimized HPLC-MS/MS Approaches; Min-Kyung Jun; Kyungdo Kim; Zee-Yong Park; Sangsuk Oh; School of Life Science, Gwangju Institute of Science and Technology, Cheonmadangwagi123, Buk-gu, Gwangju, South Korea; Department of Food Science and Technology, College of Engineering, Ewha Womans University, Seoul, South Korea

ThP 130 Parallel-reaction monitoring detection of egg proteins for food allergen control: target peptide refinement and optimization; Luyun Zhang; Philip Johnson; Melanie Downs; Food Allergy Research and Resource Program, Department of Food Science and Technology, University of Nebraska-Lincoln, Lincoln, Nebraska, Lincoln, NE

ThP 131 Determination of authenticity of Manuka honey by MALDI-TOF mass spectrometry; Simona Salvo; Tom K. Abban; Mathew O’Dwyer; Richard Carter; Oliver Fiehn; University of California, Davis, CA

ThP 132 Tracing the origins of red cabbage moss using a QTOF instrument for rapid nutrient identification; Qing Liu; Liu-qing Zhao; Zong Yang; Bing ji Lu; Li hai Guo; SCIEX, nanchang, China; SCIEX, Shanghai, China; SCIEX, Shanghai, China; SCIEX, Beijing, China; SCIEX, China, Beijing, China

ThP 133 Quantitation of Polysaccharides in food using LC-MS/MS; Jiani Jiang; Nikita P. Bacalzo, Jr.; Carillo B. Lebrilla; University of California, Davis, Davis, CA

ThP 134 Immunoaffinity Plastic Blade Spray Mass Spectrometry for Rapid Confirmatory Analysis of Food Contaminants; Arandi Gebehall; Reda Hamour; Marco Blokland; Michel Nielen; Wageningen Food Safety Research (WFSR) part of Wageningen University & Research, Wageningen, Netherlands; Laboratory of Organic Chemistry, Wageningen University, Wageningen, Netherlands

ThP 135 Analysis of volatile compound in bovine milk samples using static headspace gas chromatography-mass spectrometry: Deyukwon Kwong; Hyojin Hwang; Jeongkwon Kim; Department of Chemistry, Chungnam National University, Daejeon, South Korea

ThP 136 High-throughput UHPLC-MS/MS Analyses Optimizing the Flavor of Dairy Products; Florian Ute; Andrea Spaccasassi; Tim D. Stark; Johanna Kreisst; Caren Tanger; Ulrich Kulozik; Thomas F. Hofmann; Corinna Dawid; Chair of Food Science and Technology, Technical University of Munich, Freising, Germany; Leibniz-Institute for Food Systems Biology at the Technical University of Munich, Freising, Germany; Chair of Food and Bioprocess Engineering, Technical University of Munich, Freising, Germany

ThP 137 Standardized metabolomics for the analysis of food enables confident and comparable chemical composition data: Jessica Prenni; Jacqueline Chaparro; Corey Broeckling; Nathan Montgomery; Nichole Reisdorph; Richard Reisdorph; Cole Michael; Katrina A Doenges; Arpana Vemula; Oliver Fiehn; Stacy D Sherrod; Katrina L. Leaptrot; Jody C. May; John A. McLean; Chi-Ming Chien; Tracy Shalifazadeh; Steve Watkins; Colorado State University, Fort Collins, CO; University of Colorado Anschutz, Denver, CO; University of California Davis, Davis, CA; Vanderbilt University, Nashville, TN; Verso Bioscienes, San Francisco, CA

ThP 138 Rapid Authentication of Red Wine by MALDI-MS Combined with DART-MS; Xuewei Lin; Hao Wu; Gefei Huang; Qian Wu; Zhongping Yao; The Hong Kong Polytechnic University, Kowloon, Hong Kong, Xiamen University, Xiamen, China

ThP 139 Comprehensive analysis of functional ingredients using LC-MS/MS; Kazuya Katada1,2; Mami Okamoto; Jun Watanabe; Atsuhiko Toyama; Mari Maeda-Yamamoto2,3; Shimadzu Corporation, Kyoto, Japan; Self Care Food Council, Chiyoda-Ku, Japan; National Agriculture and Food Research Organization, Tsukuba, Japan

ThP 140 Retrospective screening of unknown emerging contaminants in tea using LC-HRMS; Gui-Ru Xie; HONG-JHANG Chen; Health and Nutrition, SGS Taiwan
**THURSDAY POSTERS**

*France*; *Waters Corporation, Wilmslow, United Kingdom; Génome métabolique, Genoscope, Institut Français Jacob, CEA, CNRS, Univ Evry, Université Paris-Saclay, Evry, France; Laboratoire de Chimie Moléculaire, CNRS – IP Paris, Ecole polytechnique, Palaiseau, France; IFPM - Sorbonne Université, UMR CNRS 8232, Paris, France; Département de chimie moléculaire, UMR CNRS 5250, Université Grenoble Alpes, Grenoble, France; *Pesticides and Marine Biotoxins unit (PBM), Laboratory for Food Safety, French Agency for Food, Environmental and Occupational Health & Safety (ANSES), Université Paris-Est. Maisons-Alfort, France; *UIMC, Université de Toulouse, Inserm, MetaboHub, Toulouse, France; *IRSD, Université de Toulouse, INSERM, INRA, INP ENV'T, Université de Toulouse 3 Paul Sabatier, Toulouse, France; *Emeritus, Morangis, France*

**ThP 163** Gas-phase fragmentation of symmetric and asymmetric viologen-based host-guest complexes; *Daniel M Hristov*; Hugo Y. Samayoa-Oviedo; *Julia Laskin*; *Purdue University, WEST LAFAYETTE, IN*

**ThP 164** Reactions of [UFXC2H]+(X=F, Cl, Br) with H2O: Competition between the loss of C2H2 and HX; *Samuel J Lenze*; Michael Van Stipdonk; Justin Terhorst; *Duquesne University, Pittsburgh*

**ThP 165** Gas-phase dissociation and thermal decomposition of mono- and di-cation ionic liquids; *Taodig O Abdulraheem*; Amanda Patrick; *Mississippi state university, Starkville, MS*

**ThP 166** Fimsbacin: an ongoing Theoretical Study of bonding to Felli Forming Complexes; *Daryl Giblin*; Michael L. Gross; Timothy Wenczewisk; *Washington University, St Louis, MO; Washington University in St. Louis, St Louis, MO*

**ThP 167** Peptide Chain Extension and Chiral Preference Mediated by Oxazoline Intermediate in Aqueous Microdroplets; *Lingqi Qiu*; R. Graham Cooks; *Purdue University, WEST LAFAYETTE, IN*

**ThP 168** Spontaneous Prebiotic Condensation Reactions in Impinging Streams of Aqueous Microdroplets; *Dylan T. Holden*; Nicolas M. Morato; Myles Q. Edwards; Lingqi Qiu; R. Graham Cooks; *Purdue University Department of Chemistry, West Lafayette, IN*

**ThP 169** A Multidimensional Approach to Probing the Binding Affinities of Poly(Lysine) and Poly(Stryene Sulfonate) Polyelectrolyte Complexes: Calum Bochenek; Addie Keating; Chrys Wesdemiotis; The University of Akron, Akron, OH

**ThP 170** Gas-phase Acidity of D/L-Cysteine-Containing Oligopeptides by Computational and Mass Spectrometry Studies; *Shiyuan Wang*; Yuntao Zhang; Jianhua Ren; *University of the Pacific, Stockton, CA*

**ThP 171** Automated Spectron Annotation and Structure Disambiguation of Released N-linked Glycans; *Gary Wilcox*; Anastasia Chemykh; Rebecah Kawahara; John Skilt; Morton Thyen-Andersen; Marshall Bern; *Protein Metrics, LLC, Cupertino, CA; Macquarie University, Sydney, Australia*

**ThP 172** Absolute and relative quantification of bovine milk oligosaccharides using LC-MS based methods; *Yu Wang*; Yu-Ping Huang; Sierra Durham; Daniela Barile; UC Davis, Davis, CA

**ThP 173** In-depth characterization of non-human sialic acid (Neu5Gc) in human serum using label-free ZIC-HILIC/HRM-MS; *Daum Lee*; Nari Seo; Myung Jin Oh; Hyun Joo An; *Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, South Korea; Asia Glycomics Reference Site, Chungnam National University, Daejeon, South Korea*

**ThP 174** Unusual free oligosaccharides found in human, bovine and caprine milk; *Weichien Weng*; Chi-Kung Ni; *Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei City, Taiwan*

**ThP 175** Ultra-High-Throughput Microchip CE-MS Quantitative Glycomics Enabled by 18-plex Isobaric Multiple Labeling Reagents for Carbonyl-Containing Compound (SUGAR) Tags; *Zicong Wang*; Aditya Kulkarni; Kate Yu; Lingjun Li; University of Wisconsin-Madison, Madison, WI; 9008 Devices, Boston, MA; *School of Pharmacy, University of Wisconsin-Madison, Madison, WI*

**ThP 176** Understanding the Structural Diversity of Immunogenic Glycans in Pig-to-Human Xenotransfusion using PGC-based LC/MS; *Eun Park*; Myungjin Oh; Hyun Joo An; *Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, South Korea; Asian Pacific Glycomics Reference Site, Daejeon, South Korea*

**ThP 177** Absolute pharmacokinetics of heparin in primates by RM: *Ke Xie; Renselaer Polytechnic Institute, Troy, NY*

**ThP 178** Predicting Sialic Acid Content in N-Linked Glycans Using the Isootope Pattern of Chlorine; *Tana Palomino*; David C Muddiman; *North Carolina State University, Raleigh, NC*

**ThP 179** LC-MS/MS Characterization of Glycans in Pig Sertoli Cells to Understand Complement System Behavior; Andrew I. Bennett; Rachel L. Washburn; Jannette M. Dufour; Yehia Mecrel; *Texas Tech University, Lubbock, TX; Texas Tech University Health Sciences Center, Lubbock, Texas*

**ThP 180** N-linked Glycan quantitation, Is relative quantitation altered by label choice?; Hoang Kim Ngan Thai; Ron Orlando; *University of Georgia - Complex Carbohydrate Research Center, Athens, GA*

**ThP 181** N-Glycome Profile of the Spike Protein S1: Systematic and Comparative Analysis of 11 variants of SARS-CoV-2; *Parisa Ahmadi*; Cristian D Gutierrez Reyes; Shereefdeh Orighinde; Akeem Adeyemi Sanni; Andrew I. Bennett; Peilin Jiang; Oluwatosin Daramola; Moijgan Atashi; Vishal Sandiya; Yehia Mecrel; *Texas Tech University, Lubbock*

**ThP 182** De Novo Glycan Sequencing by PGC-nLC-ExD MS/MS and CID/HCD-ExD MS3 on an Omnitrap Orbitrap Hybrid Instrument; Nadia Cherkeskaya; Chaohuang Xie; Margaret Downa; Dimitris Papanastasiou; Athanasios Smyrnakis; Pengyu Hong; Joo An; *Pacific Glycomics Reference Site, Chungnam National University, Daejeon, South Korea; IRSD, Université de Toulouse, INSERM, INRA, INP ENV'T, Université de Toulouse 3 Paul Sabatier, Toulouse, France; IP Paris, Ecole polytechnique, Palaiseau, France; Laboratoire de Chimie Moléculaire, CNRS – IP Paris, Ecole polytechnique, Palaiseau, France; *Pesticides and Marine Biotoxins unit (PBM), Laboratory for Food Safety, French Agency for Food, Environmental and Occupational Health & Safety (ANSES), Université Paris-Est. Maisons-Alfort, France; *UIMC, Université de Toulouse, Inserm, MetaboHub, Toulouse, France; *IRSD, Université de Toulouse, INSERM, INRA, INP ENV'T, Université de Toulouse 3 Paul Sabatier, Toulouse, France; *Emeritus, Morangis, France*

**ThP 183** Field-asymmetry ion mobility spectrometry to improve the separation and identification of released N-glycans; Denis Morfa; Zoltan Szabo; Cornelia L Boeser; *Thermo Fisher Scientific, San Jose, CA*

**ThP 184** Evaluation of chromatographic columns and methods for the analysis of Mannose, Mannose Phosphates Mannose Nucleotides in plasma by LC-MS/MS; Yashmitha Ravindra; WuXi AppTec Research Services Division, Cranbury, NJ

**ThP 185** LC-MS/MS Analysis of Heparan Sulfate and it’s components in cerebrospinal fluid, brain, liver and serum; *Lydia Lu; WuXi AppTec - Research Services Division, Cranbury, NJ*

**ThP 186** Evaluation of chromatographic columns and methods for the analysis sugars and sugar phosphates by LC-MS/MS; Fatemeh Mousavi; WuXi AppTec - Research Services Division, San Diego, CA

**ThP 187** Assessing N-glycan identification and quantitation from NISTmAb using ion mobility-mass spectrometry; Jeffrey Enders; Taufika Islam Williams; Kenneth P Garrard; Steven Broome; Rachel Harris; Shahadat Reza; David C Muddiman; North Carolina State University, Raleigh, NC; MOBiLion Systems, Inc, Chadds Ford, PA

**ThP 188** Improved Hydrophilic Interaction Liquid Chromatography for LC-MS Analysis of Released N-Glycans; Randall Robinson; Nandini Singh; Andrei Bordunov; Steven Mast; Tom Rice; Aled Jones; Oscar
ThP 198
California; Spring House, PA; Weis Veerabahu Shanmugasundaram
Spectrometry (HDX-MS) applications of PEPS Lento, 2, 3, 4
Using a nonlinear two
proteins by TRESI
structural and conformational dynamics of membrane
Birmingham, United Kingdom; Gedchich,
Daniel Serie1; InterVenn Biosciences, South San Francisco, CA; InterVenn Biosciences, Melbourne, Australia
ThP 190
Chemoenzymatic Synthesis of Sialylglycosphingolipids using One-Pot MultiEnzyme (OPME); John Mccarthur1; Pierce Carrouth1; Katie Miller1; Bailey Padgett1; Dana Moore1; L. Andrew Lee1; IMCS, Irno, SC
ThP 191
D-Va: prediction and interpretation of intact N-glycopeptidemembran mass spectra by deep learning; Zhewei Liang1; Matthew P. Campbell2; Richard (Dj)
Shipman1; Monil Gandhi1; Paul Aiyetan2; Norton Kitagawa2; Daniel Serie1; InterVenn Biosciences, South San Francisco, CA; InterVenn Biosciences, Melbourne, Australia
ThP 192
AllostERIC regulation of proteasome function as established by HDX exchange mass spectrometry, cryo-EM, and molecular dynamics simulations; Madison Turner1; Samuel E. Hoff2; Adwath B. Uday3; Algirdas Velyvis3; Natalie Zeytuni4; John Mcarthur1; Pierce Carrouth1; Norton Kitagawa2; Daniel Serie1; InterVenn Biosciences, South San Francisco, CA; InterVenn Biosciences, Melbourne, Australia
ThP 193
Using Mass Spectrometry Techniques to Capture Mechanosensitivity in Cardiac Proteins; Elena S Holden1; Miranda Collier1; Lucia Parolini1; Dirk Aarts1; Katja Gehmlich1; Justin LP Benesch1; maths model fit
University, Facu
of Microbiology, Prague 4, Czech Republic; Petr Man1, 2, 3; Haruka Nishiumi1; Takahiro Maruno1; Jonathan Phillips1; Leigh Oates1; Indian Institute of Science, Bangalore, India; Milan, Czech Republic; Moscow, Russia; Oklahoma City, OK
ThP 194
Using membrane mimics (nanodiscs) to understand the structural and conformational dynamics of membrane proteins by TRESI; Shibata, Taro2; Mok3; Lento1; Derek Wilson1; York University, Toronto, ON
ThP 195
Applications of PEPS-HDX-ESI-MS for measuring protein folding energies and folding/unfolding rates using a nonlinear two-state model fit; Motolani O Mathew1, 2; Rohana Liyanage1, 2; Shivakumar Somnalla1; Thallapuranam Krishnaswamy S Kumar1; Jackson Lay Jr.1; University of Arkansas, FAYETTEVILLE, AR; 2, Arkansas State-wide mass spectrometry facility, FAYETTEVILLE, AR
ThP 196
Establishing HDX-MS and other biophysical approaches to interrogate CC858 mediated GSPT1 degradation; Shruti Navak1; Paul Tava1; Cory Rice1; Michael Eddins1; Thierry Fischmann1; Li Xiao1; Raphaelle Berger1; David G. McLaren1; Haihong Zhou1; Merck & Co., Inc., Kenilworth, New Jersey; 2Merck & Co., Inc., West Point, PA
ThP 197
Sensitivity Improvement of HDX-MS Method and its Applications in Therapeutic Protein Study: Epitope Mapping and Protein Interactions; Xiao Pan1; Genetech, South San Francisco, CA
ThP 198
Differentiating Conformational Changes induced by Degraders & Non-degraders in BCL-6 and ERα using Hydrogen Deuterium Exchange Mass Spectrometry (HDX-MS); Ekaterina G. Devanova1; Richard Y-C Huang1, 2; Robert Langish1; Daia Weiss2; Jinli Zhu3; Andy Christoforou3; Isabella Tran3; Minerva Tran3; Vreerabahu Shannahugasundaram4; Aaron Balog4; David Weiss4; Petia Shikova4; Ingred Wertz4, 5; Bristol-Myers Squibb, Princeton, NJ; 3Janssen Research & Development, Spring House, PA; 4Bristol-Myers Squibb, San Diego, California; 5Lyterian Therapeutics, San Francisco, California; 6Bristol-Myers Squibb, Brisbane, CA
ThP 199
Probing the Effects of Hydrogen-Deuterium Exchange on Protein Stability in Solution and the Gas Phase; Yousef Heidari1; Lars Konermann1; Western University, London, ON
ThP 200
Optimized Hydrogen/Deuterium Exchange Mass Spectrometry Analysis of SARS-Cov-2 Spike Ectodomain Shows Regional Differences in Conformational Dynamics; Christopher A. Haynes1; Theodore R. Keppel1; Christopher A. Haynes1; Adrian R. Woolfitt1; Sarah Osman1; Betlehem Mekonnen1; Adrian R. Woolfitt1; Yu Zhou1; Dongxia Wang1; John R Barr1; Centers for Disease Control and Prevention, Atlanta, GA
ThP 201
Conformational Dynamics Analysis in SARS-CoV-2 Spike Variant Proteins Upon Interaction with Differentially Binding Antibodies Using Hydrogen/Deuterium Exchange Mass Spectrometry; Theodore R. Keppel1; Christopher A. Haynes1; Adrian R. Woolfitt1; Sarah Osman1; Betlehem Mekonnen1; Dongxia Wang1; John R Barr1; CDC, Atlanta, GA
ThP 202
Investigating the Influence of the Lipid Environment in Nanodiscs on the Dynamics and Insertion of Antimicrobial Pore-Forming Peptides; Ron Dennis Siaden Ortega1; Margot Di Cesare2; Jean-Michel Jault2; Cedric Oreille2; Etienne Meunier2; Julien Marcoux2; IBPS Toulouse, Toulouse, France; 3Universite de Lyon, Lyon, France
ThP 203
Epitope mapping of polyclonal antibodies in vaccine-elicted human serum; Mulin Fang1; Oliver Wu1; Joel B. Langford1; Kelley A. Cupp-Sutton1; Kenneth Smith2; Kathleen Norris3; Judith A. James3; Si Wu1; University of Oklahoma, Norman, OK; 2Oklahoma Medical Research Foundation, Oklahoma City, OK
ThP 204
Hydrogen Deuterium Exchange Mass Spectrometry Reveals Protein Conformational Changes Upon N-terminal PEGylation; Trent A. Korch1; Ross Yang1; Hongxia Wang1; Hilary A. Schuessler1; Merck & Co., Inc., Kenilworth, New Jersey
ThP 205
HDX-MS and XL-MS analyses of antigen-IG-FcRilla Interactions; Yukie Yamaguchi1; Natsumi Wakazumi1; Mine Iroha1; Takahiro Matsumoto1; Ko Kawahara1; Haruka Nishiumi1; Rina Yogo2, 3; Saeko Yanaka2, 3; Daisuke Higo2; Tetsuo Torisu2; Koichi Kato2, 3; Susumu Uchiyama1, 2, 3; Osaka University, Suita, Japan; 4Exploratory Research Center on Life and Living Systems (ExCELLS), National Institutes of Natural Sciences, Okazaki, Japan; 5Institute for Molecular Science (IMS), National Institutes of Natural Sciences, Okazaki, Japan; Nagoya City University, Nagoya, Japan; 7Thermo Fisher Scientific, Yokohama, Japan
ThP 206
Structural Mass Spectrometry on the Track of Neurodegenerative Diseases; Petr Man1; Zuzana Kalaninovav1; Son a Galuskova2; Tibor Mosko2; Michael Volny1; Karel Holada1; Petr Novak2; BiocEv - Institute of Microbiology, Prague, CZ; Charles University, Faculty of science, Prague, Czech Republic; 2Charles University, First Medical Faculty, Prague, Czech Republic
ThP 207
Transient structural dynamics during allostERIC activation and inhibition of glycogen phosphorylase from non-equilibrium millisecond HDX-MS; Monika Kist1; Jonathan Phillips1; University of Exeter, Exeter, United Kingdom
ThP 208
The Effects of Kinetic Stabilizers on the Structural Dynamics of Amyloidogenic Immunoglobulin Light Chain Using Hydrogen Deuterium Exchange Mass Spectrometry; Daniele Peterle1; Nicholas L. Yan1; Elena S. Kiimitchuk1; Thomas E. Wales1; Olga Gorsky1; Gareth J. Morgan1; Jeffrey W. Kelly2; John R. Engen2; Department of Chemistry & Chemical Biology, Northeastern University, Boston, MA; 2Department of Chemistry, The Scripps Research Institute, La Jolla, CA; 3Amyloidosis Center,
ThP 211 The Acidic Domain of Asf1 Contributes to Binding Histones H3-H4 and Modulates Histone Acetylation Transferase Rtt109; Kayatoun Morakabi; Noushin Akhavantabi; Darby J Baill; Sheena D'arcy; The University of Texas at Dallas, Richardson, TX; The University of Texas at Dallas, Richardson, Texas; University of Texas Southwestern Medical Center, Dallas, TX; University of Texas Southwestern Medical Center, Dallas, Dallas, Texas, United States, Dallas, TX

ThP 212 Conformational Dynamics of TEM-type Extended Spectrum β-Lactamases as Revealed by Hydrogen-Deuterium Exchange/Mass Spectrometry; Tsz Fung Wong; Pui Kin So; Yu Wai Ho; The Hong Kong Polytechnic University, Kowloon, Hong Kong

ThP 213 Ligand-induced conformational changes on β1-Adrenergic Receptor coupled to miniGs mapped by Hydrogen-Deuterium Exchange Mass Spectrometry; Joanna Toporowska; Parth Kapoor; Jonathan Hopper; Argyris Politis; King's College London, London, United Kingdom; Massachusetts General Hospital, Boston, MA; National Oceanic and Atmospheric Administration, Silver Spring, MD; National Institute on Drug Abuse, National Institutes of Health, Bethesda, MD; University of Wisconsin, Madison, WI; University of Cambridge, Cambridge, United Kingdom; University of Texas at Dallas, Richardson, TX; University of Texas Southwestern Medical Center, Dallas, TX; University of Texas Southwestern Medical Center, Dallas, Dallas, Texas, United States, Dallas, TX

ThP 214 Conformational dynamics of SARS-CoV-2 variant RBDDs and their interactions with ACE2: Insights revealed by HDX-MS; Dong Zhang; Tsz-Fung Wong; Pui-Kin So; Zhongping Yao; The Hong Kong Polytechnic University, Kowloon, Hong Kong

ThP 215 Structural characterization of p97/VP1 AAA+ ATPase via Hydrogen-Deuterium Exchange Mass Spectrometry; Ezgi Basturk; Baran Dingiloglu; Berfin Dogan; Gizem Dinler Doganay; Istanbul Technical University, Istanbul, Turkey

ThP 216 Major Allotrophic Regulation of Pyruvate Kinases by Native and Synthetic Ligands; Evan Bonnond; Agnieszka Bogucka; Marko Hvoßen; Sheena D'arcy; UT Dallas, Richardson, TX; University of Cambridge, Cambridge, United Kingdom

ThP 217 Tuning half-site reactivity: communication of chemically identical but dynamically different active sites over 100Å distance in Mo and β1 AR: Comment; Monika Tokmakova-Lukaszewska; Qi Huang; Luke Berry; Hayden Kallas; John Peters; Lance Seefeldt; Simonne Raugel; Brian Bothner; Montana State University, Bozeman, MT; PNNL, Richland, WA; MSU; BOZEMAN, MT; Bozeman, MT; Utah State University, Logan, UT; University of Oklahoma, Norman, OK

ThP 218 Heparin-induced changes in platelet factor IV conformation implicated in heparin-induced thrombocytopenia explored by H/D exchange; Yi Du; Igor A Kaltashov; University of Massachusetts-Amherst, Amherst, MA

ThP 219 Mechanism of complement cascade activation probed with HDX-MS; Charles Mundorf; Michael Watson; Lauren Carter; Malika R Hale; Adrian Valdez; David J Rawlings; Marion Pepper; Neil KinGu; Miklos Guttman; University of Washington, Seattle, WA

ThP 220 Determination of antibody epitopes against Sars-CoV2 antigens using Hydrogen Deuterium Exchange-Mass Spectrometry; Ankit P Jain; Liu Xu; Filip Frank; Wilbur Lam; Eric Ortlund; Blaine Roberts; Emory School of Medicine, Emory University, Atlanta, GA; Wallace H. Coulter Department of Biomedical Engineering, Georgia Institute of Technology & Emory University, Atlanta, GA; Affiliated Cancer and Blood Disorders Center of Children’s Healthcare of Atlanta, Atlanta, GA; Pediatric Technology Center, Children’s Healthcare of Atlanta, Atlanta, GA

ThP 221 HDX-MS-guided drug discovery using the cancer driver Ras as a model system; Evgeniy V. Petroetchenko; Roopa Thapar; Edith Nagy; Jason B. Cross; Christoph H. Borchers; Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Cancer Center, Institute for Applied Cancer Science, Therapeutics Discovery Division, Houston, TX; Gerald Bronfman Department of Oncology, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; M.D. Anderson Cancer Center, Institute for Applied Cancer Science, Therapeutics Discovery Division, Houston, TX; Division of Experimental Medicine, McGill University, Montreal, QC; Department of Pathology, McGill University, Montreal, QC

ThP 222 Integration of HDX and TMS-q-ExFT-ICR MS/MS for the Structural Characterization of Native Proteins; Melby Fernandez Rojas; Kevin Jeanne Dit Fouque; Miguel Santos Fernandez; Francisco Alberto Fernandez Lima; Florida International University, Miami, FL; Florida International University, Miami, FL

ThP 223 HDX-MS reveals novel aspects of PI3KCB2 regulation by its extended N-terminus; Gillian Leigh Dornan; Klara Haas; Volker Hauke; Leibniz-Forschungsinstitut für Molekulare Pharmakologie, Berlin, Germany

ThP 224 HX-MS provides structural insights into the roles of mutations in structurally disordered regions of cancer-relevant proteins: Malvina Paparastosiu; Amanda L Waterbury; Hui Si Kwok; Geojay Lee; Allyson M Freedy; Cindy Su; Will Hawkins; Andrew Reiter; Samuel M Hoenig; Michael E Vinyard; Brian B Liu; Steven A Carr; Broad Institute, Cambridge, MA; Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA

ThP 225 Hydrogen/Deuterium Exchange of a Polylkotide Synapse During Its Catalytic Cycle; Josh Salem; Rebecca Taylor; Kristina Hakansson; University of Michigan, Ann Arbor, MI; University of Michigan-Ann Arbor, Ann Arbor, MI

ThP 226 Mapping interactions of staph enterotoxin B in neutralizing serum; Clint Vorauer; Camila Boniche-Ailaro; Bettina Fries; Mike Guttmann; University of Washington, Seattle, WA; Stony Brook University, Stony Brook, NY

ThP 227 Capsid-genome rearrangements drive asymmetric RNA egress and virus disassembly by integrative structural mass spectrometry and cryo-EM; Ganesh S Anand; Varun Venkatkrishnan; Sean Breet; The Pennsylvania State University, University Park, PA

ThP 228 Rapid and High-Throughput Screening of 3 Cannabinoids in Cell Culture Medium Using the Echo® MS system; Pengyi Hou; Dandan Si; Zhimin Long; Lihai Guo; SCIEX, Beijing, China; SCIEX, Shanghai, China

ThP 229 SP3-enabled high coverage multiplexed cysteine chemoproteomics; Flowreen Shikwana; Alexandra C. Turmon; Miranda Villanueva; Cindy Truong; Kenianni Bauckus; UCLA, Los Angeles, CA

ThP 230 The S-Trap for Clean and Robust Automated Sample Preparation in Bottom-Up Proteomics; Stefan Loroch; John P Wilson; Medical Proteome-Center, Ruhr-University, Bochum, Germany; Protiif, LLC, Fairport, NY

ThP 231 High-throughput label-free opioid receptor binding assays using automated desorption electrospray ionization mass spectrometry (DESI-MS); Yantai Feng; Nicolas M. Moreau; Kai-Hui Huang; Graham Cooke; Purdue University, WEST LAFAYETTE, IN

ThP 232 Development of a high-throughput MALDI-TOF MS biochemical screen for inhibitors of an
aminopeptidase; Leonie Mueller1; Simon Peace2; Melanie Leveridge3; Matthias Trost4; Rachel Peltier-Heap5; Maria Emilia Dueñas1; 1Newcastle University, Newcastle upon Tyne, United Kingdom; 2GSK, Medicinal Chemistry, Stevenage, United Kingdom; 3GSK, Screening, Profiling and Mechanistic Biology, Stevenage, United Kingdom; 4GSK, Discovery Analytical, Stevenage, United Kingdom

**ThP 233** Automated Data Analysis and Robust Quality Control for Affinity Selection Mass Spectrometry; Matthew Green1; Juan Florez2; Malwina Michalak1; Stephan Steigelt1; Stephan Heyse1; Genedata, Cambridge, United Kingdom; 2Genedata, Basel, Switzerland; 3Genedata, Munich, Germany

**ThP 234** Untargeted LC-MS metabolomics screening of 500,000 serum samples identifies novel biomarkers for cancer, cardiovascular, and liver diseases; Boris Sarvin1; Mark Vernik2; Avi Shoshan1; Eldad Kepten1; Carmel Shor1; Ori Kronfeld1; Avishai Gavish1; Shiria Shamah-Niv1; Tomer Shliom1; 1MetaSight Diagnostics LTD, Rehovot, Israel; 2Faculty of Biology and Computer Science, Technion—Israel Institute of Technology, Haifa, Israel

**ThP 236** A Rapid and Accurate Ejection Mass Spectrometry for High Throughput Analysis of Pharmaceutical Targets; Hang Hu1; Ophelia Ukaegbu1; Joseph Gouker1; Stephanie Chun1; Wai Ling Cheung-Lee1; Karla Camacho Soto1; Hsing-I Ho1; Amanda Marie Makarewicz2; Stephanie Galanis2; Xiajuan Wen2; David G. McLaren2; Kevin P. Bateman2; Chang Lu4; Thomas R. Covey2; Erik L. Regalado2; Emmanuel Appiah-Amponsah1; Merck & Co., Inc., Rahway, NJ; 2Merck & Co., Inc., West Point, PA; 3SICE, Concord, ON

**ThP 237** High throughput characterization of polyamide hydroxylase activity using open port sampling interface mass spectrometry; John F. Cahill1; Vilmos Kertesz1; Patricia Saint-Vincent1; Hannah Valentino1; Erin Drufva1; Joshua K. Michener1; Oak Ridge National Laboratory, Oak Ridge, TN

**ThP 238** A rapid workflow for high-throughput FFPE-based proteomics; Ganesh Pujari1; Kiron Mangalapalli1; M. Cristine Charlesworth1; Benjamin Madden1; Amy Josephine French1; Gurvene Sachdeva1; Eugenio Daviso2; Ulrich Thomann3; Patrick McCarthy4; Sameer Vasatgardakar4; Deb Bhattacharyya4; Akhilesh Pandey5; Mayo Clinic, Rochester, Minnesota; 2Covaris, Lexington, MA; 3Oregon State University, Corvallis, OR; 4Baylor College of Medicine, Houston, TX

**ThP 239** Building spectral libraries to enable large-scale quantitative proteomic studies in human plasma; Jian Wang1; Hareandra Gutar1; Yingxiang Huang1; Seth Just1; Shadi Ferdosi1; Xiaoyan Zhao1; Andrew Nichols1; Lee S Cantrell1; Alexey Stukalov1; Iman Mohtashemi1; Ting Huang1; Lucy Williamson1; Gabriel Castro1; Eltaher Elgeriat1; Ryan BJen1; Khaleeh Matomedchabobi1; Daniel Hornburg1; Asim Siddiqui1; Serafin Batzoglou1; 1Seer, Inc., Redwood City, CA

**ThP 240** Rapid Characterization of Unpurified Biotherapeutics through Online Buffer Exchange; Michael Poltash1; Weijing Lu2; Elsa Gorre1; Scott Kronewitter1; Rosa Viner1; Andrew Mahan1; Hirsh Nanda1; 1Janssen Pharmaceuticals, Spring House, PA; 2Thermo Fisher Scientific, San Jose, California

**ThP 241** High-throughput proteomics on a novel high-resolution accurate mass (HRAM) platform; Tabiwang N. Arrey1; Daniel Hermansson2; Jeff Op De Beeck3; Runsheng Zheng4; Xuetei Sun5; Paul Jacobs6; Nicolea Eugen Damoc7; Vlad Zabrouskev8; 1Thermo Fisher Scientific, Bremen, Germany; 2Thermo Fisher Scientific, San Jose, California; 3Thermo Fisher Scientific - Belgium, Ghent, Belgium; 4Thermo Fisher Scientific, Germering, Germany; 5Thermo Fisher Scientific, Sunnyvale, CA

**ThP 242** The development of Acoustic Ejection Mass Spectrometry as a high-throughput, label-free platform for cell-based profiling of metabolic processes; Amy Burton1; Justin T Munro2; Michelle Pemberton1; Julie Quayle3; Joseph Kozole4; Roland Annan4; 1Discovery Analytical, Screening, Profiling, and Mechanistic Biology, Stevenage, United Kingdom; 2Discovery Analytical, Screening, Profiling, and Mechanistic Biology, GlaxoSmithKline, Stevenage, United Kingdom; 3Discovery Analytical, Screening, Profiling, and Mechanistic Biology, GlaxoSmithKline, Collegeville, PA

**ThP 243** Integration of Desorption Electrospray Ionization and 2D-MS/MS for High Throughput Experimentation; Eric T. Dziekonski1; Thomas C. Sams1; Lucas J. Szalwinski1; 1Oregon State University, Corvallis, OR; 2Purdue University, WEST LAFAYETTE, IN

**ThP 244** High-Throughput Mass Spectrometry Enables Rapid Genome Engineering; Alessandra Paul1; Affinity Biosciences, San Bruno, CA

**ThP 246** Ion pre-accumulation in bent flatop boosts MS2 sensitivity and peptide identifications in an Orbitrap Expsiror 480 mass spectrometer; Florian Harking1; Julia Kragebring1; Hamish Stewart2; Pedro Navarro2; Konstantin Ayzikov1; Dmitry Grinfeld2; Alexander Harder2; 1GSK, Medicinal Chemistry, Discovery Innovation Center, Corvallis, OR; 2Oregon State University, Corvallis, OR

**ThP 250** High-throughput metabolic screening using encoded 96-plex tags; Michael R Armbuster1; Scott F Grady1; Christopher K Arnatt1; James L Edwards1; 1Saint Louis University, St. Louis, MO

**ThP 251** High-Depth Multiplexed Drug Profiling with the Orbitrap Ascend; Steven R. Shuken1; Graeme C. McAlister2; William D. Barshop3; Jessica D. Canterbury1; David Bergens4; Jingjing Huang5; Romain Huguet6; Joao A. Paulo6; Amanda E Lee6; Vlad Zabrouskev7; Steven P Gygi6; Qing Yu7; 1Department of Cell Biology, Harvard Medical School, Boston, MA; 2Thermo Fisher Scientific, San Jose, California
THURSDAY POSTERS

ThP 254 Subcellular Resolution Biochemical Imaging Method
Combining Electron Microscopy with Vacuum
Electrospray Beams. John Santman 1; Peter A Kottke 1;
Andrei G Fedorov 1; 1Georgia Institute of Technology, Atlanta, GA

ThP 255 Hadamard transform AP-MALDI imagery with a
digital micro-mirror array. Jun J Hu; Ningbo University, Ningbo,
China

ThP 256 Maximizing the Spatial Information of IR-MALDESI
Mass Spectrometry Imaging of Zebrafish Using a Top-
Hat Beam and Variable Step Size. Alena N Joiniant 1;
David C Muddiman 1; 1FTM Laboratory for Human Health
Research, Department of Chemistry, Raleigh, NC

ThP 257 Improvements in a Multi-Reflecting ToF Mass
Spectrometer to Enhance Mass Spectrometry Imaging
Specificity. Emmanuelle Claude 1; William Johnson 1; Joel
Keeler 1; Emma Marsden-Edwards 1; Martin Palmer 1;
Waters Corporation, Wilmslow, United Kingdom; 2Waters
Corporation, Milford, MA

ThP 258 Response Surface Methodology for Optimization of
nano-DESI Imaging using Orbitrap Instruments: Felix
Friedrich 1; Ingela Laneckoff 1; Uppsala University, Uppsala,
Sweden

ThP 259 Development of ambient mass spectrometry imaging
using laser ablation electrospray ionization separated
by gas transportation for analyses of intracellular
molecules. Riku Hirata 1; Hirono Hazama 1; Kunio
Awasu 1; 1Graduate School of Engineering, Osaka
University, Suita, Japan; 2Global Center for Medical
Engineering and Informatics, Osaka University, Suita,
Japan

ThP 260 ibTOF: Sensitive imaging of light elements at
nanometer resolution. Valentine Riedo-Grimaud 1; Lex
Pillatson 1; James Whittby 1; Michael Grössl 1; Steffen
Bräkling 1; Fotwerk AG, Thun, Switzerland

ThP 261 Comprehensive Assessment of MALDI-2 IMS
Performance on Human and Murine Tissues. Kameron R
Molloy 1, 2; Madeline E Colley 1, 2, 3; Lukasz G Migs 1, 2;
Allison B Esselman 1, 2, 4, 5; Martin Dufresne 3, 4, 5, 6;
Jeffrey M Spragginis 1, 2, 3, 4, 5; 1Department of Chemistry,
Vanderbilt University, Nashville, TN; 2Mass Spectrometry
Research Center, United Kingdom; 3Department of Chemistry,
Fukushima University, Fukushima, Japan; 4Department of Biochemistry,
Vanderbilt University, Nashville, TN; 5Delt Center for Systems and Control,
Delft University of Technology, Delft, Netherlands; 6Department of Cell and Developmental Biology, Vanderbilt University,
Nashville, TN

ThP 262 Pososecond Infrared Laser Desorption – Rapid
Evaporative Ionisation Mass Spectrometry for
Molecular Pathology and Imaging. Daniel Simon 1, 2, 3;
Ronan Battle 2; Yuchen Xiang 2; Stefania Maneta-
Stavrakaki 2; Lauren Ford 2; Robert T Murray 2; Josephine
Bunch 2; Zoltan Takats 1, 2; Rosalind Franklin Institute,
Harwell, Didcot, United Kingdom; 3Imperial College London,
London, United Kingdom; 4National Physical Laboratory,
Teddington, United Kingdom; 5Institute for Biomedical
Engineering, Delft University of Technology, Delft, Netherlands; 6Department of Pediatrics, Vanderbilt University Medical Center,
Nashville, TN

ThP 263 Coupling AP-SMALDI MS imaging technology with
Orbitrap Exploris MX mass detector; Domenic
Dreisbach 1; Carolin M Morawietz 1; Karl Christian Schäfer 1;
Kerstin Strupat 1; Bernhard Spengler 1, 2; 1Transmit GmbH,
Giessen, Germany; 2Justus Liebig University Giessen,
Institute of Inorganic and Analytical Chemistry, Giessen,
Germany; 3Faculty of Chemistry, University of Duisburg-Essen,
44139 Essen, Germany; 4Institute of Inorganic and Analytical
Chemistry, Justus Liebig University Giessen, Germany;
5TransMIT GmbH, Giessen, Germany

ThP 264 In-capillary dielectric barrier discharge post-ionization
for MALDI MSI of metabolites and lipids. Syen Heles 1, 2;
Bernhard Spengler 1; Sabine Schulz 1; Julian Schneemann 1;
Karl-Christian Schäfer 1; 1Leibniz Institute for Analytical
Sciences - ISAS - e.V., 44139 Dortmund, Germany; 2Faculty of Chemistry, University of Duisburg-Essen, 44139
Essen, Germany; 3Institute of Inorganic and Analytical
Chemistry, Justus Liebig University Giessen, Germany;
4TransMIT GmbH, Giessen, Germany

ThP 265 HiPLEX-HC MALDI imaging of FFPE Kidney tissue at
5µm utilizing microGRID on timTOF fex MALDI-2;
Connor West 1; Joshua Fischer 1; Corinna Henkel 1; Gargey
B. Yagnik 1; Mark Lim 1; 1Bruker Scientific, LLC, Billerica,
MA; 2Bruker Daltonics GmbH & Co.KG, Bremen, Germany;
3BamberGen, Inc., Billerica, MA

ThP 266 Dual-LIT Instrumentation for MS/MS Imaging and
Single-Cell Lipidomics. Zheng Ouyang 1; Xiangyu Guo 1; Aojie Zhang 1; Zhijun Cai 1; Wenpeng Zhang 1;
1Tsinghua University, Department of Precision Instrument,
Beijing, China

ThP 267 Development of a High Throughput Microscope-Mode
Secondary Ion Mass Spectrometry Imaging. Elena
Castellani 1, 2; Yifeng Jia 1; Anya Eyres 1, 3; Natasha Smith 1;
Michael Burl 1; Josephine Bunch 2, 5; Zoltan Takats 2, 4, 5; Mark
Brouard 1; Felicia M Green 2; 1University of Oxford, Dept.
of Chemistry, Oxford, United Kingdom; 2Rosalind Franklin
Institute, Harwell, Didcot, United Kingdom; 3National
Physical Laboratory, Teddington, United Kingdom; 4Imperial
College, London, United Kingdom

ThP 268 High resolution MALDI imaging mass spectrometry of
mouse fetuses to assess markers of neural tube
defects after maternal opioid exposure; Dustin A
Barnette 1; Richard Beger 1; Pravin R. Kaldhone 1; Joseph
Hanig 1; J. Edward Fisher 1; Dan Mellon 1; Grace Lee 1; Amy
Inselman 1; E. Ellen Jones 1; 1National Center for Toxicological Research, Jefferson, AR; 2Center for Drug
Evaluation and Research, Silver Spring, MD; 3Elevate
Therapeutics, Salt Lake City, UT

ThP 269 Changes in spatial distribution of brain N-glycans in
acute stress-induced mouse models using MALDI mass
spectrometry imaging (MSI); Hyun Jun Jang 1; Hyeyeon
Kang 1; Boyoung Lee 1; 1Institute for Basic Science, Daejeon,
South Korea

ThP 270 Mass spectrometry imaging reveals lipidomic changes
in skeletal muscles due to muscle hypertrophy; Naoko
GOTO-INOUYE 1; Nihon University, Fukushima, Japan

ThP 271 Traumatic brain injury and MSI-AP-MALDI:map of small
metabolites in the different brain regions; Angela Marika
Siciliano 1; Laura Brunelli 1; Giulia De Simone 1; Aurelia
Morabito 1; Francesca Pischitella 1; Federico Molo 1; Elisa R.
Zanier 1; Roberta Pellini 1; Enrico Davoli 1; 1Istituto di
Ricerche Farmacologiche Mario Negri IRCCS, Milano, Italy

ThP 272 In situ lipidomics of Staphylococcus aureus bone
infection using MALDI imaging mass spectrometry;
Christopher J Good 1; 1; Casey E Butrico 1; 1; Elizabeth K
Neumann 1; 1; Madeline E Colley 1; 1; Katherine N Gibson-
Corley 1; Luka D G Migs 1; 1; Cant Van De Plas 1; 1; James E
Cassap 1, 2, 3, 4, 5, 6; Jeffrey M Spragginis 1, 2, 4, 9; Richard M
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ThP 273 Quantifying Multiple Anti-tuberculosis Drugs in
Infected Mouse Tissue by MALDI Mass Spectrometry
Imaging; Michael Tucker 1; Florent Grèlard 1; Landry Blanc 1;
Véronique Dartevelle 1; Nolasco Deshayes 1; 1Institute of
Clinical Sciences, Bordeaux, Bordeaux, France; 2Hackensack Meridian Health Center for Innovation & Nutrition, Nutley, NJ
**ThP 274** Laser ablation inductively coupled plasma mass spectrometry imaging reveals how gold nanoparticle surface charge influences their distribution and excretion pathways; Jeerapat Dounchawee1; Laura J Castellanos1; Kristen Sikora1; Xianzhi Zhang1; Yuanchang Liu1; Vincent M. Rotello1; Richard W. Vachet1; University of Massachusetts Amherst, Amherst, MA

**ThP 275** Mass Spectrometry Imaging of Brain Fatty Acids and Behavioral Studies on Prenatal Cannabis Exposure and Omega-3 Fatty Acid Diet Supplementation; Samantha L. Cousineau1; Mohammed H. Sarkihaya1; Marta De Felice1; Aleksandra Doktor1; Steven R. Laviollette1; Daniel B. Hardy1; Ken K.-C. Yeung1; University of Western Ontario, London, ON

**ThP 276** Spatiotemporal Profiling of the Lipidome, Proteome, and Phosphoproteome of PLK1 Inhibited Colorectal Cancer Spheroids; Emily R. Sekera1; Brian D. Fries1; Amanda B. Hummon1; The Ohio State University, Columbus, OH

**ThP 277** Visualization of the spatial distribution of flavonoids and phenolic acids in the tuber root of Tetrastigma hemsleyanum using AP-MALDI-MSI; Junling Dun1; Hongyuan Hao1; Taohong Huang1; Yan Lin1; Shimadzu (China) Co., Ltd., Shanghai, China; Tongde Hospital of Zhejiang Province, Hangzhou, China

**ThP 278** Mass Spectrometry Imaging Studies of Metabolites in Mice Heart Affected With Chagas Disease; Dan Chen1; University of Oklahoma, department of chemistry and biochemistry, Norman, OK

**ThP 279** On-tissue visualization and quantification of steroid hormones using MALDI-2 in animal models of benign prostatic hyperplasia; Hannah N. Miles1,2,3; Ana Lucilia Bautista-Ruiz1,2,3; Teresa T. Liu1,2; William A. Ricker1,2,3; Lingjun Li1,2,3; UW-Madison School of Pharmacy, Madison, WI; Department of Urology, University of Wisconsin-Madison, Madison, WI; George M. O’Brien Center, University of Wisconsin-Madison, Madison, WI; School of Pharmacy, University of Wisconsin-Madison, Madison, WI; Department of Chemistry, University of Wisconsin-Madison, Madison, WI

**ThP 280** Distribution of active pharmaceutical ingredients in Forsythia Suspensa and quality control with mass spectrometry imaging; Zhenhe Chen1; Kaoru Nakagawa2; Jian Su3; Keisuke Shima1; Yongli Liu1; Rong Lei1; Jing Dong1; Hao Yuan1; Xiaolei Wang1; Satoshi Kasamatsu1; Lei Cao1; Xiaodong Li1; Shimadzu China Innovation Center, Beijing, China; Healthcare Solution Unit, Solutions Center of Excellence, Shimadzu Corporation, Kyoto, Japan; Hebei Institute for Drug and Medical Device Control, Shijiazhuang, China; MS Business Unit, Life Science Business Department, Shimadzu Corporation, Kyoto, Japan

**ThP 281** On-tissue Derivationatization for Mass Spectrometry Imaging of Fatty Acids with Enhanced Detection Sensitivity in Alzheimer’s Disease Brain; Malik Ebbini1; Hua Zhang1; Peng-Hsuan Huang1; Lingjun Li1,2; School of Pharmacy, University of Wisconsin-Madison, Madison, WI; Department of Chemistry, University of Wisconsin-Madison, Madison, WI

**ThP 282** Mapping the distribution of sterols in the mouse brain - integrating mass spectrometry imaging with the Allen Mouse Brain Atlas; Nico Verbeek1; Maria José Q Manta1; Eytan Yufec, Alice Ly1; William J Griffiths2; Marc Claessen1; Yuqin Wang1; Aspect Analytics, Genk, Belgium; Swansea University Medical School, Swansea, United Kingdom

**ThP 283** In Situ Free Radical Epoxidation with Laser Desorption Ionization for Mass Spectrometry Imaging of Fatty Acid Isomers; Huimin Ye1; Ruijun Jian1; Wenpeng Zhang1; Yu Xia1; Guangyao Zheng1; Tsinghua University, Beijing, China; National University of Singapore, Singapore, Singapore; St George’s University Medical School, London, United Kingdom

**ThP 284** Whole-body imaging of drugs and metabolites in mice by Desorption Electrospray Ionization Mass Spectrometry Imaging; Christian Janelti1; University of Copenhagen, Copenhagen, Denmark

**ThP 285** High spatial resolution TIMS MALDI-2 imaging of Dhc/l-KO rice reveal changes in cholesterol biosynthesis; Ethan Yang1; Azad Eshghi1; Amy L2; Libin Xu2; Shannon Cornett1; Bruker Daltonics, Billerica, MA; University of Washington, Seattle, WA

**ThP 286** MALDI Mass Spectrometry Imaging of 13C6-Glucose Uptake Measured in TCA Metabolites from Glioblastoma Mouse Brain; Joshua L Fischer1; Kari Wilder-Romans1; Ethan Yang2; Savannah R Snyder1; Katherine Stumpo1; Angeline Lin3; Zilong Zhao4; Jie Xu5; Daniel R. Wahl1; Bruker Daltonics, Billerica, MA; University of Michigan Ann Arbor, Ann Arbor, MI

**ThP 287** Investigating the effect of a COX inhibitor on early pregnancy in a mouse model using imaging mass spectrometry; Stefania Gitta1; Eva Szabo2; Laszlo Mark1; Institute of Biochemistry and Medical Chemistry, University of Pecs, Pecs, Hungary

**ThP 288** Evaluating the Effect of Collagen Degradation on Clostridiods difficile Infection in Murine Cecum via Imaging Mass Spectrometry; Paul Zerebinski1; Joshua Soto-Oçasa1; Jonathan T. Specker1; Joseph P. Zackular2,3; Boone M. Prentice1; University of Florida, Chemistry Department, Analytical Chemistry Division, Gainesville, FL; Division of Protective Immunity, Children’s Hospital of Philadelphia, Philadelphia, Pennsylvania; National Institute of Pathology and Laboratory Medicine, Perelman School of Medicine, University of Pennsylvania, Philadelphia, Pennsylvania

**ThP 289** In-Vitro Diagnostic Imaging of HepaRG Spheroids by DESI-Tandem Quadrupole MS; Mark Towers1; Lisa Reid1; Joanne Bailantyne1; Alicia Rosell-Hidagio1; Kirsten Headspith1; Waters Corporation, Waltham, United States; University of Technology, Delft, Netherlands

**ThP 290** Spatiotemporal study of lipid biosynthesis in the mutant seeds of Ara ginea with imaging mass spectrometry; Young-Jin Lee1; Iowa State University, Ames, IA

**ThP 291** A new multimodal desorption electrospray ionisation workflow enabling visualisation of lipids and biologically relevant elements in a single tissue section; Melanie Bailey1; Catia D S Costa1; Janella M De Jesus1; Josephine Bunch1; University of Surrey, Guildford, United Kingdom; Gyropyrox Ltd, Alderley Park, United Kingdom

**ThP 292** Mass spectrometry imaging of immune response in human papillomavirus-associated versus carcinogen-driven head and neck squamous cell carcinoma; William M. Temple Andrews1; Aleksandra Ogurtsova2; Mike Mikula1; Ogechi Nwankwo1; Liz Engle1; Carole Fakhy2; R. Alex Harbison1; Maureen Kane1; University of Maryland School of Pharmacy, Baltimore, MD; Johns Hopkins Hospital, Baltimore, MD

**ThP 293** Exploring a Human-Relevant Mouse Model for Detecting and Quantifying Medical Therapeutics for Organophosphate Toxicity in the Brain using MALDI-MSI; Samantha Carrier1,2; Benjamin Wadsorth1; C. Linn Cadieux1; Caitlin M. Tressler1; Oak Ridge Institute of Science Education, Oak Ridge, TN; U.S. Army Medical Research Institute of Chemical Defense, Gunpowder, Maryland; Johns Hopkins University School of Medicine, Baltimore, MD

**ThP 294** Assessing methods and performance for glycan imaging of human tissues; David T. Reeves1,2; Martin Dufresne1,3; Madeline E. Colley1,3; Lukasz G. Migas2; Audra M. Judd1; Jamie L. Allen1,2; Raf Van De Plas2; Jeffrey M. Spraggs1,2,3; Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; Department of Biochemistry, Vanderbilt University, Nashville, TN; Delta Center for Systems and Control, Delft University of Technology, Delft, Netherlands
**ThP 295** Multilevel human secondary lymphoid immune system compartmentalization revealed by complementary multiplexing and mass spectrometry imaging; Benjamin L. Oyster; Jefferon Valencia-Davila; Erin M. Myers; Adam Molyvdas; Kalliopi Ioannidou; Kyle March; David Ambrozak; Laurence De Leval; Giulia Fabozzi; Amina Woods; Richard Koup; Constantinos Petrovas; NIH, Gaithersburg, MD; National Institute of Allergy and Infectious Diseases, Bethesda, MD; Lausanne University Hospital, Lausanne, Switzerland

**ThP 296** Mapping distribution of an alkalamin in tissue for restoration of an immune-permissive microenvironment; Danielle Votley; Natalie Fowlkes; Maria Sophia Stenkamp; Erin H Seeley; Erikk Cressman; MD Anderson Cancer Center; Houston, TX; University of Texas at Austin, Austin, TX

**ThP 297** High Resolution Molecular Mapping of Alzheimer’s disease and Cerebral Amyloid Angiopathy (CAA) with MALDI IMS and IHC; Cody R Marshall; Claire F Scott; Lissa Ventura-Antunes; Wilber Romero-Fernandez; Alena Shostak; Lukasz G Miga2; Martin Dufresne; Nathan H Patterson; Raf Van De Plas; Matthew S Schrag; Jeffrey M Spraggins; Chemcal Physical Biology Program, Vanderbilt University School of Medicine, Nashville, TN; Biomolecular Multimodal Imaging Center, Vanderbilt University, Nashville, TN; Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; Department of Neurology, Vanderbilt University, Nashville, TN; Cerebral Amyloid Angiopathy Clinic, Vanderbilt University Medical Center, Nashville, TN; Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; Department of Biochemistry, Vanderbilt University, Nashville, TN; Department of Chemistry, Vanderbilt University, Nashville, TN

**ThP 298** Multi-Reflecting Time-of-Flight Mass Spectrometry Imaging of an Osteosarcoma Tumour Model to Inform Drug Development; Sophie M. Pearce; Neil A. Cross; Laura M. Cole; David P. Smith; James L. Language; Emmanuelle Claude; Lucy E. Flint; Richard Goodwin; Malcolm R. Glenn; Sheffield Hallam University, Sheffield, United Kingdom; Sheffield Hallam University, Sheffield, United Kingdom; Waters Corporation, Wilmslow, United Kingdom; AstraZeneca, Cambridge, United Kingdom

**ThP 299** MALDI-2 MSI of temozolomide distribution and metabolic dysregulation within a murine patient-derived xenograft model of glioblastoma; Krishna P.L. Bhat; Nancy Milam; Silvana Varenbrink; Eugene M. Lebenzon; Brendan Pradeaux; MD Anderson Cancer Center, Division of Pathology Lab-Medicine, Department of Pathology, Houston, Texas; University of Texas Medical Branch at Galveston, Galveston, Galveston, TX; Department of Neurobiology, Galveston, TX

**ThP 300** TOPICAL DELIVERY OF ANTIFUNGAL DRUGS WITH NANO-VESCULATI: FORMULATIONS CHARACTERIZED BY DESI-MSI; Ravit Yakobi; Elka Touitou; Hiba Natsheh; Katya Margulis; The Hebrew University of Jerusalem, Jerusalem, Israel

**ThP 301** Localization of Molecular Changes Due to Ionizing Radiation Exposure in a Model Tissue by Mass Spectrometry Imaging; Yixuan Wu; Franklin E. Leach III; University of California, Los Angeles, CA

**ThP 302** Spatiotemporal Phenotypic Analysis of a Teinturier Grape Cultivar with Atmospheric Pressure Matrix-assisted Laser Desorption Ionization (AP-MALDI) Mass Spectrometry Imaging; Vishal Mahale; Sujita Chatterjee; Nasiruddin Shaikh; Madhuri Gupta; Konstantin Novoselov; Eugene Moskovets; Kaushik Banerjee; Nitinda Bhattacharya; Venkateswarlu Panchagnula; Mass Tech. Inc., Columbia, MD; Barefeet Analytics Private Limited, Pune, India; IAC-National Research Centre for Grapes, Pune, India

**ThP 303** Enhanced molecular coverage, resolution and speed for in-situ pharmaceutical tablet MSI analysis by combining DESI and MALDI using multi-reflecting Q-Tof; Emmanuelle Claude; Wei Rao; Laurent Buitel; Noelle Elliott; Tristan Renaud; Joanne B Ballantyne; Waters Corporation, Wilmington, United Kingdom; Technology Servier, Orleans, France; Waters corp, milford, MA

**ThP 304** Spatial proteomics at subcellular resolution enabled by integration of deep UV ablation with nanoPOTS sample preparation; Piliang Xiang; Andrey Liyu; Yumi Kwon; Dehong Hu; William Chisler; Sarah Williams; Dušan Velčikovič; Lye Meng Mark; Ulijana Pavesic; Ying Zhu; Pacific Northwest National Laboratory, Richland, WA; Genentech Inc, San Francisco, CA

**ThP 305** Three-dimensional proteome mapping of human pancreatic islet microenvironment defines cell type localizations at 50-μm resolution; Yumi Kwon; Sarah M Williams; Jing Chen; Geremy C Olais; Dehong Hu; Lye Meng Mark; Ulijana Pavesic; Donald J Moore; Ernesto S Nakayasu; Martha Campbell-Thompson; Clayton Mathews; Ying Zhu; Wei-Jun Qian; Pacific Northwest National Laboratory, Richland, WA; University of Florida, Gainesville, FL; Genentech Inc., South San Francisco, CA

**ThP 306** Identifying modules of co-regulated metabolites through large-scale analysis of human metabolicomics data in METASPACE; Tim D Rose; Kevin Titlec; Sergii Mamedov; Lucas Maciel Vieira; Sergio Triana; Theodore Alexandrov; Structural and Computational Biology Unit, European Molecular Biology Laboratory, Heidelberg, Germany; Broad Institute of MIT and Harvard, Cambridge, MA; Institute for Medical Engineering and Science, MIT, Cambridge, MA; Department of Chemistry, MIT, Cambridge, MA; Ragon Institute of MGH, MIT and Harvard, Cambridge, MA; Metabolomics Core Facility, Heidelberg, Germany; Molecular Medicine Partnership Unit, Heidelberg, Germany; Bio Studio, Bioinnovation Institute, Copenhagen, Denmark

**ThP 307** Tumor heterogeneity of glioblastoma analyzed via SpatialOMX and HIPLEX-IHC MALDI Imaging; Corinna Henkel; Signe Frost Frederiksen; Katherine A. Stumpo; Matthias Szesny; Jörg W. Bartsch; Melanie C. Föll; Olivier Schilling; Bruker Daltonics GmbH & Co.KG, Bremen, Germany; Bruker Daltonics, Billerica, MA; Department of Neurosurgery, University of Marburg, Marburg, Germany; Institute for Surgical Pathology, Medical Center, University of Freiburg, Freiburg, Germany; Faculty of Medicine, University of Freiburg, Freiburg, Germany

**ThP 308** Tetramodal Chemical Imaging Delineates the Lipid-Amyloid Peptide Interplay at Single Plaques in Transgenic Alzheimer’s Disease Models; Junyue Ge; Srinivas Koutarapu; Durga Jha; Henrik Zetterberg; Kaj Biennow; Jörg Hanrieder; University of Gothenburg, Gothenburg, Sweden; Sahlgrenska University Hospital, Gothenburg, Sweden; University College London, London, United Kingdom; UK Dementia Research Institute at University College London, London, United Kingdom; Hong Kong Center for Neurodegenerative Diseases, Hong Kong, China; University of Wisconsin, Madison, WI

**ThP 309** Optimized Combination of MALDI MSI and Immunofluorescence; Cateyln C Ridge; Elizabeth K. Neumann; UC Davis, Davis, CA

**ThP 310** Large-Scale Interlaboratory Comparison of Imaging Mass Spectrometry Protocols for Spatial Untargeted Metabolomics: Veronika Saharakova; Måns Ekeloft; Lachlan Stuart; Lucas M. Vieira; Martin R Molenar; Alberto Baiolli; Katja Czarnikowska; Tobias Rauscha; Dennis Jakob; Mary King; Max Müller; Crystal Pace; Fernanda E. Pinto; Nicole Strittmatter; Jens Soltwisch; Dušan Veličkovič; Janina Oetjen; Christopher Anderton; Livia
S. Eberlin13; Richard Goodwin9; Christian Janfelt9; Manuel Liebeck4; David C. Muddiman1; Bernhard Spengler4; Klaus Dreisewerd15; Carsten Hopf14, 15; Theodore Alexandrov11, 16; 14, 16; 1, 16; 1, 16; Structural and Computational Biology Unit, European Molecular Biology Laboratory, Heidelberg, Germany; 1Department for BioMedical Research, University of Bern, Bern, Switzerland; 2CeMOS - Center for Mass Spectrometry and Optical Spectroscopy, Mannheim, Germany; 3Max Planck Institute for Marine Microbiology, Bremen, Germany; 4University of Texas at Austin, Austin, TX; 5Justus Liebig University Giessen, Institute of Inorganic and Analytical Chemistry, Gießen, Germany; 6Department of Chemistry, North Carolina State University, Raleigh, NC; 7Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark; 8AstraZeneca, Cambridge, United Kingdom; 9Institute of Hygiene, University of Münster, Münster, Germany; 10Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, Washington; 11Bruker Daltonics GmbH & Co. KG, Bremen, Germany; 12Department of Surgery, Baylor College of Medicine, Houston, TX; 13Medical Faculty of Heidelberg University, Heidelberg, Germany; 14Mannheim Center for Translational Neuroscience (MCTN), Medical Faculty Mannheim, Heidelberg University, Mannheim, Germany; 15Metabolomics Core Facility, Heidelberg University, Mannheim, Germany; 16Molecular Medicine Partnership Unit, Heidelberg, Germany; 17BioStudio, Biobinnovation Institute, Copenhagen, Denmark

**ThP 315**

**Mobility-Modulated Sequential Dissociation of Multiple Precursors (SDIMP) for Highly Multiplexed MS/MS Imaging**

Yao Qian1; Xiaoxiao Ma; Zheng Ouyang1; 1Department of Precision Instrument, Tsinghua University, Beijing, China

**ThP 316**

**Direct detection of lipid changes on cultured cells using imaging secondary ion mass spectrometry following chemical and/or biological perturbation.**

John Fletcher, University of Gothenburg, Gothenburg, Sweden

**ThP 317**

**Advancing the Construction of High Spatial Resolution 3-D Multimodal Molecular Atlases with the Aid of Data-Driven Image Fusion:**

Olof Gerurd Isberg1, 2; Melissa A. Farrow1, 3, 4; Lukasz G Migas; Madeline Colley1, 5; Jamie L. Allen1, 6; Haichun Yang7; Mark P. De Caestecker1; Raf Van De Plas1, 2, 3, 4; Metabolomics Core Facility, Heidelberg, Germany; 1Department of Biochemistry, Vanderbilt University, Nashville, TN; 2Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; 3Department of Biochemistry, Vanderbilt University, Nashville, TN; 4Department of Pathology, Microbiology, and Immunology, Vanderbilt University Medical Center, Nashville, TN; 5Delt Center for Systems and Control, Delft University of Technology, Delft, Netherlands; 6Department of Pediatrics, Vanderbilt University Medical Center, Nashville, TN; 7Department of Medicine, Vanderbilt University, Nashville, TN

**ThP 318**

**Scalable multimodal workflow for spatial glycan analysis of archival formalin-fixed paraffin-embedded (FFPE) human tissue using MALDI, MSI-TOF, and spatial transcriptomics:**

Ke Xuan Low1; Yue Song; Xiaowei Liu1; Marc Bosse1; Richard R Drake1; Peggi M. Angel1; Sean Bendall2; Mike Angelo1; 1Stanford University, Stanford, CA; 2Medical University of South Carolina, Charleston, SC

**ThP 319**

**Exploring MALDI-MSI with Higher Metabolite Coverage and Its Application in Spatial Metabolomics:**

Jia Yi1; Joe L. Fowles1; Leah P. Shriner1; Gary J. Patti1; 1Washington University in St. Louis, St. Louis, MO

**ThP 320**

**Micro-scaffold Assisted Spatial Proteomics (MASP) with Substantially Improved Spatial Resolution and Throughput forWhole Tissue Mapping:**

Shihua Huo1; Min Ma1; Shuo Qian1; Ming Zhang1; Jie Pu1; Xiaoyu Zhu1; Sailie Rasam1; Jun Qu1; 1University at Buffalo, Buffalo, NY; 2Roswell Park Comprehensive Cancer Institute, Buffalo, NY

**ThP 321**

**Ablent Biomolecular Imaging in the Omentum of Breast Disease:**

Hai Yan J Wang1; Chung-Yin Huang3; Kuo-Chen Wei3; 1Kuokian University; 2National Sun Yat-Sen University, Kaohsiung City, Taiwan; 3Neuroscience Research Center, Chang Gung Memorial Hospital, Taoyuan, Taiwan; 4Department of Neurosurgery, New Taipei Municipal Tucheng Hospital, New Taipei City, Taiwan; 5Department of Neurosurgery, Chang Gung Memorial Hospital, Taoyuan, Taiwan; 6School of Medicine, Chang Gung University, Taoyuan, Taiwan; 7Department of Surgery, Kaohsiung Chang Gung Memorial Hospital, Kaohsiung, Chang Gung University College of Medicine, Kaohsiung, Taiwan

**ThP 322**

**Dissecting Immunometabolism of Dilated Cardiomyopathy (DCM) on delta-sarcoglycan deficient hamster model with thoracic Imaging Mass Spectrometry (IMS):**

Makio Okamura1; Shinichi Yamaguchi2; Takushi Yamamoto2; Ryo Inoue2; Laura Yuriko González-Teshima; Keisuke Hakamada3; Kisaki Amemiya4; Kenji Minatoya5; Hidetoshi Masumoto; Satoru Noguchi; Ichizo Nishino6; Hatusue Ueda7; 1Masaya Ikekawa1; 2Department of Life and Medical Sciences, Doshisha University, Kyotanabe-city, Japan; 3 Shimadzu Corporation, Kyoto-city, Japan; 4Faculty of Agriculture, Selsun University, Hikarata-city, Japan; 5Department of Life and Medical Sciences, Doshisha University, Kyotanabe-city, Japan; 6AstraZeneca, Cambridge, United Kingdom; 7University of Cambridge, Cambridge, United Kingdom; 8The Institute of Cancer Research, London, United Kingdom; 9National Physical Laboratory, London, United Kingdom; 10AstraZeneca, Cambridge, United Kingdom
Bioinformatics, National Central University, Taoyuan, Taiwan; 2Department of Biomedical Sciences and Engineering, Institute of Systems Biology and Bioinformatics, National Central University, Taoyuan, Taiwan

End to End Interpretable Deep Learning Workflow for Untargeted Metabolomics: Mao Yu1, Rohit Tripathy2, Brian Hoffmann1, Yi Li3, Vivek Philip1, 1The Jackson laboratory, Farmington, CT; 2The Jackson Laboratory, Bar Harbor, ME

A workflow to track and normalize the abundance of unknown and known metabolites across LC/MS methods: Ethan Stanciliff1, Michaela Schweiger-Haber1, Gary J. Patti1, 1Washington University in Saint Louis, Saint Louis, MO

Skyline Processing Workflow for Lipidomics Using High Resolution Ion Mobility Mass Spectral Data with Mobility Aligned Fragmentation: Lauren C Royer1, Rachel Harris1, Daniel Debord1, 1MOBI Lion Systems, Inc, Chadds Ford, PA

Deep lipidsomics strategy for evaluation of cancer therapy: Haoyue Zhang1, Yikun Liu2, Donghui Zhang1, Wenpeng Zhang1, Zheng Ouyang1, 1Tsinghua University, Beijing, China

Enzymatic Dysregulation Estimation using Lipid Network Analysis: Tim D Rose1, 1; Nikolai Köhler1, 1; Lisa Falk1, 2; Lucie Kilschat1, 2; Olga E Lazareva2, 2; Josch K Pauling1, 1, 1; LipiTUM, Technical University of Munich, Germany; 2EMBL, Heidelberg, Germany; 3German Cancer Research Center (DKFZ), Heidelberg, Germany

PAMDA: Publicly Available Metabolomics Dataset Alignment and Analysis of Human Urine Measured by RPLC-MS: Han Habra1, Yamal Simon1, Tytus D. Mak1, 1NIST, Gaithersburg, MD

Fragmentation Site Prediction for Non-Targeted Metabolomics using Graph Neural Networks: Yannek Nowatzky1, 1Philippe Benner1, 1; Thilo Muth1; 2Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, Germany

MS/MS-centric data processing with SIRIUS 6: Kai Dürkop1, 1; Markus Fleischauer1, 1; Marcus Ludwig1, 1; Martin Andre Hoffmann1, 1; Fleming Kreßschmer1, 1; Sebastian Böcker1, 1; Friedrich-Schiller-University Jena, Jena, Germany

Lipid-class specific internal standard normalization of HilIC-MS/MS data embedded into untargeted data processing and interactive exploration: Edward Rudt1, Viola Jeck1, 1; Konstantin Schwarze1, 1; Ansgar Korf2; 2Matthew R. Lewis2, 2; Heiko Hayen1, 1, 1; Nikolaus Kessler1, 1; 1Institute of Inorganic and Analytical Chemistry, Münster, Germany; 3Bruker Daltonics GmbH & Co. KG, Bremen, Germany

Interactive Design and Application of MassCLQ Queries after Preprocessing for the Annotation of PFAS in LC-TIMS-PASEF data: Andrea Kiehne1, 1; Silke Bodendiek1, 1; Sofie Weinkouff1, 1; Mingxun Wang1, 1; Heiko Neuweiger1, 1; Nikolaus Kessler1, 1; 1Bruker Daltonics GmbH & Co. KG, Bremen, Germany; 2Department of Computer Science and Engineering, University of California Riverside, Riverside, CA

LipiDetective: a Deep Learning Framework for the Detection of Lipid Species in Mass Spectra: Vivian J Wuerl1, 1; Nikolai Köhler1, 1; Florian Molnar1, 1; Michael Wilting1, 1, 1; Josch K Pauling1, 1; 1Technical University of Munich, Freising, Germany; 2Helmholtz Zentrum München – German Research Center for Environmental Health, Neuherberg, Germany

The Evolving Open Access Metabolomics Resource MetaboLights: Claire C O’Donovan1, 1; Callum Martin1, 1; Ozgur Yurekten1, 1; Felix Amalados1, 1; Mark Williams1, 1; 1EMBL-EBI, Hinxton, United Kingdom

Incorporation of metabolite identification confidence into pathway analysis when processing untargeted metabolomics data improves enriched pathway discovery: Blake E. Sells1, 1; Ethan Stanciliff1, 1; Jacob S. Bedia1; Michaela Schweiger-Haber1, 1; Leah P. Shrives1; Gary J. Patti1; 1Washington University in St. Louis, St. Louis, MO
ThP 345 High-fidelity and high-performance LC-MS metabolomics data processing using asari; Shuzhao Li; 2; Amnah Siddiqua; 1; Maheshwar Thapa; 1; Shujian Zheng; 1; Jackson Laboratory, Farmington, CT; 2University of Connecticut School of Medicine, Farmington, CT

ThP 346 MSFragr: A versatile Python package for visualizing mass spectrometry data; Shauva Chanaan; 1; John T. Prince; 1; Enveda Biosciences, Boulder, CO

ThP 347 Combining MS2 and MS3 fragmentation spectra for the annotation of complex sphingolipids; Brandon Y. Lieng; 1; Jeremy K. Chan; 1; Nicholas S. Ly; 1; Hennes L. Røst; 1; J. Rafael Montenegro-Burke; 1; Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, ON

ThP 348 Glycoprotein analysis benefits from direct feature extraction and compound identification via correlation of experimental and accurately simulated Orbitrap mass spectra; Konstantin Nagornov; 1; Anton N. Kozhinov; 1; Sergey Vakhрушев; 1; Yuriy O. Tsybin; 1; Spectroswiss, Lausanne, Switzerland; 1University of Copenhagen, Copenhagen, Denmark

ThP 349 Reproducibility and challenges in analysis of large urine metabolomics datasets; Stephen Barnes; 1; Landon S. Wilson; 1; Taylor F. Berryhill; 1; Shaoyang Su; 2; University of Alabama at Birmingham, Birmingham, AL; 1Augusta University, Augusta, Georgia

ThP 350 SpectraSpector: An implementation of MassQL for rapid querying of MS data; Dylan J. Johnson; 1; Alan K Jarmusch; 1; Integrative Bioinformatics Support Group, National Institute of Environmental Health Sciences, National Institutes of Health, Durham, North Carolina; 1Metabolomics Core Facility, Immunity, Inflammation, and Disease Laboratory, Division of Intramural Research, National Institute of Environmental Health Sciences, National Institutes of Health, Durham, North Carolina

ThP 351 Library-scale assessment of spectral quality of MS/MS spectra; Christoph A. Ketterer; 1; J Taylor; 1; Tobias Kind; 1; Pelle Simpson; 1; Sarah E Haynes; 1; David Healey; 1; Enveda Biosciences, Boulder, CO

ThP 352 Ground-truth evaluation of high dimensional feature calling methods; J Taylor; 1; Alex A. Kislukhin; 1; Daniel Treen; 1; Tobias Kind; 1; Sarah E Haynes; 1; David Healey; 1; John T. Prince; 1; Enveda Biosciences, Boulder, CO

ThP 353 High-dimensional feature/adduct linking with a noise-tolerant, sparse cosine similarity measure; Daniel G.C. Treen; 1; John T. Prince; 1; Enveda Biosciences, Boulder, CO

ThP 354 Noise Filtering in Non-targeted Metabolomics; Iqbal Mahmud; 1; Akika Patel; 2; Lin Tan; 1; Sara A Martinez; 2; Bao Tran; 1; Bo Wei; 2; Rajesh Abraham; 2; Bradley Brown; 1; John Weinstein; 1; Philip L Lorenzo; 1; MD Anderson Cancer Center, Houston, TX; 1Rice University, Houston, TX

ThP 355 MS/MS Spectral Alignment Enables Structural Modification Site Localization; Mohammad Reza Zare Shahnehe; 1; Mingxun Wang; 1; University of California, Riverside, Riverside, CA; 1University of California Riverside, Riverside, CA

ThP 356 Automated Multiple Reaction Monitoring(MRM)-profiling and ozone electrospray ionization (OESI)-MRM Informatics Platform for High-throughput Lipidomics; Connor H Beveridge; 1; Sanjay Iyer; 1; Caitlin E. Randolph; 1; Gaurav Chopra; 1; Purdue University Department of Chemistry, West Lafayette, IN; 1Purdue University, Dept. of Chemistry, West Lafayette, IN

ThP 357 Updates in the MSFragger search engine: facilitating bulk-cell and single-cell proteomics data analysis; Fengchao Yu; 1; Daniel A. Polasky; 1; Andy T. Kong; 1; Guo Cui Teo; 1; Kevin L. Yang; 1; Alexey I. Nesvizhskii; 1; University of Michigan, Ann Arbor, MI

ThP 358 Quantification of peptideions in data from middle-down peptide mass spectrometry experiments with ProteoformQuant; Arthur Girmaud; 1; Frederik Haugaard Holck; 1; Ole Narrgaard Jensen; 1; Veit Stefan Schwämmle; 1; University of Southern Denmark, Odense, Denmark

ThP 359 Estimating False Discovery Rate During Real-Time Library Search Acquisitions; William Barshog; 1; Chris McGann; 1; Devin K Schwepp; 1; Jesse D. Canterbury; 1; Thermo Fisher Scientific, San Jose, California; 1University of Washington, Seattle, WA

ThP 360 AutoMod: a new solution for uncovering protein post-translational modifications; Hui-Yin Chang; 1; Jie-Wei Chiu; 2; Yi-Fan Chen; 3; Shuo-fu Chen; 4; Chia-Feng Tsai; 5; Department of Biomedical Sciences and Engineering, Institute of Systems Biology and Bioinformatics, National Central University, Taoyuan, Taiwan; 1Institute of Systems Biology and Bioinformatics, National Central University, Taoyuan, Taiwan; 1Interdisciplinary Program of Engineering, National Central University, Taoyuan, Taiwan; 1Department of Oncology, Taipei Veterans General Hospital, Taipei, Taiwan; 4Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA

ThP 361 A Crustacean Neuropeptide Spectral Library for Application in Data-Independent Acquisition Peptidomics Workflows; 1Puren Li; 2; Min-Mei; 1; Kellen Delaney; 1; Ashley Phetsathanh; 1; Lingjun Li; 1; University of Wisconsin-Madison, Madison, WI

ThP 362 CONGA: Combining open and narrow searches with group-wise analysis; Jack Freestone; 1; William Noble; 1; Uri Keich; 1; University of Sydney, Sydney, Australia; 1University of Washington, Seattle, WA

ThP 363 An XIC-centric approach for improved identification, quantification, and reproducibility in proteomic data analyses; Guanghui Wang; 1; Zheng Zhang; 1; Yi Liu; 1; Meghan C. Burke; 1; Sergey L. Sheetlin; 1; Stephen E. Stein; 1; NIST, Gaithersburg, MD

ThP 364 Generating spectral libraries using experimental target spectra and ProSift predicted decoy spectra; Robert W Seymour; 1; Andy Lin; 1; Pacific Northwest National Laboratory, Richland, WA

ThP 365 Information content assessment of peptide fragmentation spectra using deep learning models; Zahra Elhamraoui; 1, 2; Eva Borras; 3; Mathias Wilhelm; 1; Eduard Sabidó; 1, 3; 1Center for Genomic Regulation, Barcelona, Spain; 2Universitat Pompeu Fabra Barcelona, Barcelona, Spain; 3Technical University of Munich, Freising, Germany

ThP 366 Improvement of noncanonical peptide identification using local RNA expression value in MHC-I immunopeptidomics; Seunghyuk Choi; 1; Seunghyun Han; 1; Eunok Paek; 1; Hanyang University, Seoul, South Korea

ThP 367 ProSift-PTM: One model to predict them all; Wassam Gabriel; 1; Vitor Sterlinchi; 1; Omar Shouman; 1; Rodeina Mohand; 1; Daniel P. Zolg; 1; Ludwig Austenbacher; 1; Bernhard Kuster; 1; Mathias Wilhelm; 1; Computational Mass Spectrometry, Technical University of Munich, Freising, Germany; 1Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany

ThP 368 High-throughput Automated Muropeptide Analysis (HAMA) Reveals Peptidoglycan Composition of Gut Microbes; Ya-Chen Hsu; 1, 2; Ping-Rui Lin; 1, 2; Ying-Chih Hsu; 2; Department of Chemistry, National Taiwan University, Taipei, Taiwan; 1Department of Molecular Genetics, Erasmus University Medical Center, Rotterdam, Netherlands

ThP 369 SpecGlobX: a fast tool for aligning mass spectra in large proteomics datasets, capturing dissimilarities arising from multiple complex peptides modifications; Grégoire Prunier; 1, 2; Mehdi Cherkaoui; 1, 2; Olivier Langella; 1; Grégoire Prunier; 1; PROBE research infrastructure, BIBS facility F44316, Nantes, France; 1, 2INRAE UR1268 Polybiospectroscopy, Technical University of Munich, Freising, Germany; 1Institut des Sciences Moléculaires et de la Mise en Valeur du Lait, Université Paris-Saclay,无偿, CNRS
AgroParisTech, GQE - Le Moulon, PAPPSO, F-91190, Gif-Sur-Yvette, France

ThP 370
Precise and accurate real-time de novo sequencing of timsTOF data with the Novor algorithm on the PaSER platform, Rui Zhang¹, Qixin Liu², Mingjie Xie³, Dennis Trede⁴, Tharan Srikrumar⁴, Jonathan Krieger⁵, Bin Ma⁶, George Rosenberger⁶; ¹Rapid Novor Inc.; Kitchener, ON; ²Bruker Daltonics GmbH & Co. KG, Bremen, Germany; ³Bruker Ltd., Milton, ON; ⁴Bruker Switzerland AG, Fällanden, Switzerland; ⁵University of Tennessee, Knoxville, TN; ⁶Oak Ridge National Laboratory, Oak Ridge, TN

ThP 371
An assessment of the replicability and sample number requirements of differential expression analysis in bottom-up proteinomes, Steven Tavis¹, Diana Ramirez¹, Matthew J Keller¹, Frank Löffler¹, Robert L Hettich¹,²; ¹University of Tennessee, Knoxville, TN; ²Oak Ridge National Laboratory, Oak Ridge, TN

ThP 372
An integrative proteomics result viewer for FragPipe; Kai Li¹, Fengchao Yu², Daniel Polasky³, Alexey I. Nesvizhskii³; ¹University of Michigan, Ann Arbor, MI

ThP 373
Multiplexed peptide identification via iterative database search; Chen Qian¹; Seungjin Na¹; Eunok Paek¹; ¹Hanyang University, Seoul, South Korea

ThP 374
MS²Rescore 3.0: A modular and user-friendly platform for AI-assisted resoring of peptide identifications; Ralf Gabriels¹,²; Arthur Declercq¹,²; Robbin Bouwmeester¹,²; Sven Degrove¹,²; Lennart Martens¹,²; VIB-UU Center for Medical Biotechnology, Ghent, Belgium; ¹Department of Biomolecular Medicine, Ghent University, Ghent, Belgium

ThP 375
MS²Rescore and Sage enable open modification immunopeptidomics searching; Arthur Declercq¹,²; Robbin Bouwmeester¹,²; Aurélie Hirschler³; Christine Carapito³; Sven Degrove¹,²; Lennart Martens¹,²; Ralf Gabriels¹,²; VIB-UU Center for Medical Biotechnology, Ghent, Belgium; ¹Department of Biomolecular Medicine, Ghent University, Ghent, Belgium; ²Laboratoire de Spectrométrie de Masse BioOrganique (LSMBO) IPHC UMR 7178, Université de Strasbourg, France

ThP 376
Spectroscope: validating peptide spectrum matches by real time visualization of their neighborhoods with an interactive web interface; Long Wu¹; Ayman Hoque²; Henry Lam³; ¹HKUST, Hong Kong, China

ThP 377
De novo sequencing of random frog skin peptides with the Twister algorithm; Kira Vyatkina¹,²,³,⁴, Irina D. Vasilieva¹; Tatyana Y. Samagina¹; Albert T Lebedev²; ¹SPb Academy of Medical Sciences, Saint Petersburg, Russia; ²Saint Petersburg State University, St Petersburg, Russia; ³Saint Petersburg Electrotechnical University "LETI", St Petersburg, Russia; ⁴National Research Center on Addictions, Branch of V. Sertsyn NRMCN, Moscow, Russia; ¹Lomonosov Moscow State University, Chemistry department, Moscow, Russia; ²Federal Republic of Russia

ThP 378
Real-Time de novo sequencing of peptide antigens using PaSER™ for 'Run and Done' 4D-immunopeptidomics; Kirti Pandey¹; Rui Zhang², Qixin Liu²; Mingjie Xie³; Dennis Trede⁴; Tharan Srikrumar⁴; Jonathan Krieger⁵; Bin Ma⁶; George Rosenberger⁶; Anthony W. Purcell⁶; ¹Monash University, Clayton, Australia; ²Rapid Novor Inc.; Kitchener, ON; ³Bruker Daltonics GmbH & Co KG, Bremen, Germany; ⁴Bruker Ltd., Milton, ON; ⁵Bruker Switzerland AG, Fällanden, Switzerland; ⁶Oak Ridge National Laboratory, Oak Ridge, TN

ThP 379
Algorithm Development for Analysis of Human O-GlcNAcylated Protein using LC-MS/MS; Dasom Ahn¹; Jin Young Kim²; Heeyoun Hwang³; ¹Korea Basic Science Institute, CheongJu-si, South Korea; ²Korea Basic Science Institute, Cheoungui, South Korea

ThP 380
Investigating the Lipidome of ATP10d Corrected Murine Models Using LC-IM-MS with High Resolution Ion Mobility; David C. Koomen¹; Jody C. May²; Alexander J. Mansur³; Todd T. Graham⁴; John A. McLean⁵; ¹Vanderbilt University, Nashville, TN

ThP 381
Noncovalent Copper Complexation to Differentiate Drug Enantiomers by Conventional and High Throughput Development; Zongyuan Chen¹; Josh McBee¹; Miriam Fico²; ¹University of Colorado, Boulder, CO; ²University of Utah, Salt Lake City, UT

Resolution Ion Mobility-Mass Spectrometry; Benjamin K Blakley¹; Emanuel Zilbut¹; Allison R Reardon¹; Jody C. May¹; John A. McLean¹; ¹Vanderbilt University, Nashville, TN

ThP 382
Characterizing the Molecular Composition of Polysorbates by High Resolution Ion Mobility-Mass Spectrometry (HRIM-HRMS); Kyle E Lira²; Allison R Reardon¹; Jody C. May¹; John A. McLean¹; ¹Vanderbilt University, Nashville, TN

ThP 383
Pushing the Boundaries of Multidimensional Separations: Coupling 2D Chromatography with High-Resolution Structures for Lossless Ion Manipulations (SLIM) IM-MS; Ralph Aderoth²; Diana C. Velosa³; Shon P. Neal³; Christopher D. Chouinard³; ¹Clemson University, Clemson, SC; ²Florida Tech, Melbourne, FL

ThP 384
Brain metastasis of lung adenocarcinoma: gangliosidosis investigation by ion mobility tandem mass spectrometry; Mirela Sarbú¹; David W. Clemen²; Željka Vukelic³; Alina D. Zamfir³; ¹National Inst for R&D in Electrochemistry, Bucharest, Romania; ²Faculty of Medicine, University of Zagreb, Zagreb, Croatia; ³National Inst for R&D in Electrochemistry and Condensed Matter, Timisoara, Romania

ThP 385
LC-TIMS-MS based assay for profiling and quantitation of bile acid in human bile. A novel method; Ahsan Hameed¹,²; Mukul Dutt³; ¹Monash University, Clayton, VIC; ²University of Arkansas for Medical Sciences, Little Rock, AR; ³National Institute of Health, Bethesda, MD

ThP 386
Autonomous multi-pass and IMSn acquisitions on the Cyclic IMS platform; Jakub Ujma¹; Kevin Giles¹; Jose De Corral¹; Keith Richardson¹; David Langridge¹; Dale Cooper-shepherd¹; ¹Waters Corporation, Wilmslow, United Kingdom; ²Waters Corporation, Milford, MA

ThP 387
Coupling droplet microfluidics to cyclotron mobility mass spectrometry for the identification of isomeric small molecules; Laura I Penabá¹; Devin M. Makey¹; Robert T. Kennedy¹; Brandon T Ruotolo¹; ¹University of Michigan-Ann Arbor, Ann Arbor, MI

ThP 388
Applying Ultraviolet Photodissociation to a Low-Pressure Drift Tube Orbitrap Mass Spectrometer to Enhance the Structural Characterization of Intact Native Proteins; Jamie P. Blakely¹,²; James D. Polasky¹,²; Nathan W. Buzitis¹,²; Brian H. Clowers¹,²; ¹Max Planck Institute for Multidisciplinary Sciences, ÖSTERSUND, Germany; ²Bruker Daltonics, San Jose, CA

ThP 389
Separation of C18:1 Fatty acid Isomers using Cyclic Ion Mobility Mass Spectrometer; Ahsan Hameed¹; Hailemariam Abra Assresse²; Renny S Lan¹; Mario G Ferruzzi³,²; ¹Arkansas Children’s Hospital Nutrition Center, Little Rock, AR; ²University of Arkansas for Medical Sciences, Little Rock, AR; ³Department of Pharmacology and Toxicology, University of Arkansas for Medical Sciences, Little Rock, Arkansas

ThP 390
Ion mobility of crosslinked peptide-RNA (oligo)nucleotides as a parameter for improved identification of crosslinks; Sergey Moshkovskii¹; Olexandr Dybykov¹; Timo Sachsenberg¹; Ralf Pflanz¹; Monika Raabe¹; Oliver Kohlbacher¹; Henning Urlaub¹; ¹Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany; ²University of Tübingen, Tübingen, Germany; ³University Medical Center Goettingen, Goettingen, Germany

ThP 391
SLIM Ion Mobility-IMS-Based Screening for Drugs of Abuse in Urine on a High-Throughput Development System; Zongyuan Chen¹; Josh McBee¹; Miriam Fico²; ¹University of Colorado, Boulder, CO; ²University of Utah, Salt Lake City, UT
Frederick G. Strathamann; Daniel Debord; *MOBILion Systems, Inc., Chadds Ford, PA

**ThP 392**

Amyloid formation of metabolites: Understanding the transformation of cysteine into amyloid-like fibrils and cystine crystal; Thanh D Do; Damilola S. Olawutoba; Miranda N. Limbach; *University of Tennessee, Knoxville, TN

**ThP 393**

Diagnostic Lipid Biomarkers discovery for Alzheimer’s Disease using High-Resolution Ion Mobility Mass Spectrometry; Orobola E. Olaide; Kimberly Y Kartowikromo; Junwei Wang; Yuyan Yi; Jingyi Zheng; Amal K Kaddoumi; Ahmed M Hamid; *Auburn University, Auburn, AL

**ThP 394**

Top/Middle-Down Characterization ofo- Synuclein Glycoforms; Kevin Jeanne Dit Fouque; Samuel A. Miller; Eldon Hard; Matthew R. Pratt; Francisco Alberto Fernandez Lima; *Florida International University, Miami, FL; 1University of Southern California, Los Angeles, CA

**ThP 395**

Rapid screening of Bispecific Antibodies and Antibody Impurities using trap-ions in-solution Ion Mobility Induced Unfolding coupled with IM-MS; Ruwan Kurulugama; Christian Klein; Harsha P. Gunawardena; *Agilent Technologies, Santa Clara, CA; 2Janssen Research & Development, Spring House, PA

**ThP 396**

Fast Separation and Quantitation of α-, iso-α-, and β-acids via Differential Ion Mobility Spectrometry; Emir Nazdrajić; Christian Ierandi; Scott Hopkins; *University of Waterloo, Waterloo, ON; 2Waterline Innovation, Waterloo, Ontario; 3Centre for Eye and Vision Research, Hong Kong, Hong Kong

**ThP 397**

Differentiation of isomeric, non-separable carbohydrates using Tandem Trapped Ion Mobility Spectrometry—Mass Spectrometry (tandem-TIMS/MS); Jusuna Lee; Fanny C Liu; Christian Bleiholder; *Florida State University, Tallahassee, FL

**ThP 398**

Improving the annotation of bile acids in fecal samples using a Liquid Chromatography-Ion Mobility-High Resolution Mass Spectrometry method; Dimitra Diamanditou; 1, 2 Christina Virgiliou; 1 Olgia Begou; 1, 2 Richard Seitz; 1 Carsten Baessmann; 1 Helen Gika; 1, 2 Georgios Theodoridis; 2 1 Aristotle University of Thessaloniki, Thessaloniki, Greece; 2Bioquant AUTH, Center for Interdisciplinary Research and Innovation, Thessaloniki, Greece; 3Bruker Scientific, Billerica, MA; 4Bruker Daltonics GmbH & Co. KG, Bremen, Germany

**ThP 399**

Imaging of Isomeric Metabolites in Mouse Brain with a nano-DESI timsTOF system; Syeda Nazifa Wali; Luxue Jiang; Julia Laskin; *Purdue University, WEST LAFAYETTE, IN

**ThP 400**

In-depth identification and accurate quantification of mitochondrial and lysosomal crosstalk proteins; Byoung-Kyu Cho; 1 Young Ah Goo; 1, 2, 3 1 MTAC, MGI, Washington University School of Medicine in St. Louis, St. Louis, MO; 2Department of Biochemistry and Molecular Biophysics, Washington University School of Medicine in St Louis, St. Louis, MO; 3Department of Genetics, Washington University School of Medicine in St Louis, St. Louis, MO

**ThP 401**

Confident identification of N-glycopeptides from standard glycoproteins using a cyclic ion mobility mass spectrometry system; Sayantani Chatterjee; 1 Joshua A. Klein; 1 Joseph Zaia; 1, 2, 3 Department of Biochemistry, Center for Biomedical Mass Spectrometry, Boston University Chobanian & Avedisian School of Medicine, Boston, MA; 4Bioinformatics Program, Boston University, Boston, MA

**ThP 402**

 Influence of MS acquisition and integration parameters on isotope ratio determinations; Huihui Yao; Haihong Zhou; David McLaren; Hao Chen; Stephen Previs; 1 Merck & Co, Inc., Kenilworth, New Jersey; 2New Jersey Institute of Technology, Newark, NJ

**ThP 403**

Reimport of carbon from cytosolic and vacuolar sugar pools into the Calvin–Benson cycle explains photosynthesis labeling anomalies; Yuan Xu; 1 Thomas Wieloch; 2 Joshua A. M. Kaste; 1 Yair Shachar-Hill; 1 Thomas D. Sharkey; 1 *Michigan State University, East Lansing, MI; 2Umeå University, Umeå, Sweden

**ThP 404**

LC-MS method to determine Coenzymes (CoA) Flux; Vasanta Puttoni; 1 Abu Hena Mostafa Kamal; 3 Chandara Shekar Reddy Ambati; 2 Nagireddy Puttoni; 2 *Baylor College of Medicine, Houston, TX; 3Baylor College of Medicine, Houston, Texas

**ThP 405**

Determination of mouse liver HSD17B13 protein half-life following metabolic labeling with deuterium oxide and quantitation with high resolution mass spectrometry; Thomas Angel; *AUBURN, AL

**ThP 406**

Fully labeled carbon-13 mice: an expanded view of the mammalian metabolome and its dynamics; Annelaure Damont; 1 Anaïs Legrand; 1 Kathleen Rousseau; 1 Laurent Bellanger; 2 Jean-Jacques Leguy; 3 Christophe Junot; 3 François Fenaille; 1 Eric Ezan; 2 CEA-INRA, Laboratoire Innovations en Spectrométrie de Masse pour la Santé (LI-MS); DRF/ Institut Joult/ DMTS, SPI, MetabolHub, CEA Saclay - Université Paris Saclay, Gif sur Yvette, France; 3Université Paris-Saclay, CEA, INRAE, Département Médicaments et Technologies pour la Santé (DMTS), SPI, Bagnols-sur-Cèze, France; 4UMR 7265 CEA-CNRS-Université Aix Marseille, DRF/Institut de Biosciences et Biotechnologies d’Aix-Marseille (BIAM), plateau PHYTOTECH, Cité des Energies, Saint-Paul-lez-Durance, France

**ThP 407**

A combined stable isotope infusion method to assess therapeutic efficacy in primary hyperoxaluria patients; Dewi Van Harskamp; Sander F. Garrels; Jaap W. Groothoff; Michiel J.S. Oosterveld; Johannes B. Van Goudoever; Henk Schierbeck; 1 Amsterdam UMC location University of Amsterdam, Department of Clinical Chemistry and Pediatrics, Laboratory Genetic Metabolic Diseases, Emma Children’s Hospital., Amsterdam, Netherlands; 2Amsterdam UMC location University of Amsterdam, Department of Pediatric Nephrology, Emma Children’s Hospital, Amsterdam, Netherlands; 3Amsterdam UMC location University of Amsterdam, Department of Pediatric Nephrology, Emma Children’s Hospital, Amsterdam, Netherlands; 4Amsterdam UMC location University of Amsterdam, Department of Pediatrics, Emma Children’s Hospital, Amsterdam, Netherlands; 5Amsterdam UMC location University of Amsterdam, Department of Pediatrics, Emma Children’s Hospital, Amsterdam, Netherlands

**ThP 408**

Steady-state and dynamic operation of photoreceptor metabolism: integrating 13C metabolic flux analysis and ion size measurements; Xinyu Fu; Berkley J Walker; 1, 2 1 Department of Energy-Plant Research Laboratory, Michigan State University, East Lansing, MI; 2Department of Plant Biology, Michigan State University, East Lansing, MI

**ThP 409**

13CO2 labeling for monitoring lipid biosynthesis in Lemma minor with MALDI-MSI; Vy T Tat; 1 Andrew E. Paulson; Young Jin Lee; 1 Iowa State University; Ames, IA

**ThP 410**

Defining nutrient inputs that fuel globulostoma metabolism in vivo using stable-isotope tracing metabolomics; Andrew J Scott; 1 Pietro Morlacchi; 2 Costas Lysiotis; 1 Daniel R. Wahl; 1 University of Michigan-Ann Arbor, Ann Arbor, MI; 2Agilent Technologies, Lexington, MA

**ThP 411**

A new StageTips method based on an innovative sorbent for fast and efficient peptide fractionation in proteomic studies; Kaynoush Naraghi; 1 Mana Shafeii; 1 Michel Arotçarena; 1 Florine Hallez; 1 Cerina Chhuon; 2 Chiara Guerrera; 2 Sami Bayoudh; 2 AFFINISEP, Le Houlme, France; 2Affinisep USA LLC, Miami, FL; 3INSERM -US24 SFR Necker Proteome, Paris, France

**ThP 412**

Optimization of solid phase extraction pretreatment for urinary DNA adducts by high resolution mass spectrometry; Alexandra Keid; 1 Carolina Möller; 2 Yuan-Jhe Chang; 3 Mu-Rong Chao; 4 Jazmine Virzi; 2 Laura Deloso; 2 Theresa Evans-Nguyen; 1 Chiung-Wen Hu; 3
THURSDAY POSTERS

Marcus Cooke1; 1Department of Chemistry, University of South Florida, Tampa, Florida; 2Oxidative Stress Group, Department of Molecular Biosciences, University of South Florida, Tampa, Florida; 3Department of Occupational Safety and Health, Chung Shan Medical University, Taichung, Taiwan; 4Department of Occupational Medicine, Chung Shan Medical University Hospital, Taichung, Taiwan; 5Department of Public Health, Chung Shan Medical University, Taichung, Taiwan

ThP 413 Deep proteome coverage of human plasma in a fast, reproducible and easy-to-perform fashion: combining the novel ENRICH-IST workflow with fractionation; Sebastian H. Johansson1, 2; Visitors of the Walter and Eliza Hall Institute of Medical Research, Department of Medical Biology, University of Melbourne, Melbourne, Australia; Walter and Eliza Hall Institute of Medical Research, Technology and Biology Division, The Walter and Eliza Hall Institute of Medical Research, shenzhen, China

ThP 414 The spatial proteome study based on micro-FFPETissues using LCMSampling: Hao Chen; Beijing Genomics Institute, Shenzhen, China

ThP 415 Automated Sugaring-Out Assisted Liquid-Liquid Extraction and Determination of Neonicotinoids in Honey Samples using a Robotic Autosampler and LC-MS/MS Platform; Fred Foster1; Megan Harper2; Nicole Kfouri1; Jaqueline Whitecavage1; Gerstel, Inc., Linthicum, MD

ThP 416 Mature Fully Automated Peptide Mapping; Jason L. Richardson1; Zhongqi Zhang1; Anjen, Thousand Oaks, CA

ThP 417 Easy and Robust Automated Sample Preparation and Extraction for LC-MS/MS Bioanalytical Workflows; Jonathan Danaceau1; Mary Trudeau1; Meagan Callis2; Steven Lai2; Waters Corporation, Milford, MA; 3Waters corp, milford, MA

ThP 418 The effects of DDM on proteomic data in routine usage; Kajaping Yuan1; Renata Moravcova1; Jason C. Rogalski2; Leonard J. Foster2; Proteomics Core Facility, UBC, Vancouver, BC; 2Department of Biochemistry and Molecular Biology, UBC, Vancouver, BC

ThP 419 Advanced sample preparation in LC/MS bioanalysis using new solid phase extraction; Toshikazu Minehata1; Ai Tsutsui1; Hajian Ari; Keiko Shiren1; Satoshi Yamaki1; SHIMADZU Corporation, Kyoto, Japan; Shimadzu Global Lab Consumables Co., Ltd., Beijing, China; 1, 2Advanced Technology and Biology Division, The Walter and Eliza Hall Institute of Medical Research, Melbourne, Australia; 2Department of Medical Biology, University of Melbourne, Melbourne, Australia; 3Population Health Division, The Walter and Eliza Hall Institute of Medical Research, Melbourne, Australia; 4Faculty of Health and Medical Sciences, The University of Adelaide, Adelaide, Australia; 5Faculty of Health and Medical Sciences, The University of Adelaide, Adelaide, Australia

ThP 420 β-Galactosidase spike-in as a strategy for normalisation in large-scale plasma DIA proteomics; Vinit Vaihbhai1, 2; Samantha J Emery-Corbin1; 2; Megan Penno3; 2; Humana M Youssef1, 2; Helena Oakley1; Jennifer J Cooper1; Leonard C Harrison1; 2; John M Wentworth1; Andrew I Webb3; Laura F Dagley2; Jing Li1, 2; Advanced Technology and Biology Division, The Walter and Eliza Hall Institute of Medical Research, Melbourne, Australia; 2Department of Medical Biology, University of Melbourne, Melbourne, Australia; 3Population Health Division, The Walter and Eliza Hall Institute of Medical Research, Melbourne, Australia; 4Faculty of Health and Medical Sciences, The University of Adelaide, Adelaide, Australia; 5Faculty of Health and Medical Sciences, The University of Adelaide, Adelaide, Australia

ThP 421 A complete and automated end-to-end sample preparation strategy for high-throughput and standardized proteomics with high sensitivity; Dorte B. Bekker-Jensen1; Florian Harking2; Magnus Husefeldt3; Mortiz Heusel1; Lasse Falkenberg1; Jesper V. Olsen1; Nicolai Bache1; 1Evoseq Biosystems, Odense, Denmark; 2University of Copenhagen, Copenhagen, Denmark

ThP 422 Standardized, high-throughput platform for automated, rapid, and extensive plasma proteome characterization; Claudia Martelli1; Fabian Wendt1; Andreas Schmidt1; Katrin Hartinger1; Gary Kruppa2; Nils A. Kulak2; Manuel Bauer2; 1Bruker Switzerland AG, Fällanden, Switzerland; 2Bruker Daltonics GmbH & Co. KG, Bremen, Germany; 3Preomics GmbH, Martinsried, Germany; 4Bruker S.R.O., Brno, Czech Republic

ThP 423 Extraction and Quantitation of Per and Polyfluoroalkyl Substances (PFAS) in Bioanalytical Matrices Determined using UHPLC-MS/MS: Adam Senior1; Kyle Bevan2; Lee Williams1; Geoff Davies3; Alan Edgington1; Helen Lodder1; Russell Parry4; Charlotte Hayes5; Lucy Lund1; Zainab Khan1; Claire Desbrow1; Dan Menasco1; 1Biotage GB Limited, Cardiff, United Kingdom

ThP 424 Streamlined and semi-automated MS-based proteomics pipeline from protein extraction to real-time data analysis by coupling BeatBox, PreON and PaSER platforms; Measmo Abreha1; Jasmin Johansson1; Zehan Hu1; Jonathan Krieger1; Katharina Limm1; Katrin Hartinger1; Nils A. Kulak2; Preomics Inc, Islands, NY; 1Preomics GmbH, Planegg/Martinsried, Germany; 2Bruker Ltd, Milton, ON L9T 6P4

ThP 425 Optimized proteolytic digestion workflows for maximizing protein identification while reducing enzyme usage by an order of magnitude; Ivo A Hendriks1; Michael L Nielsen2; 1Novo Nordisk Foundation Center for Protein Research, University of Copenhagen, København, Denmark

ThP 426 A comparison of silica SPE techniques - a novel hybrid composite versus traditional loose packed; James Edwards; Porvair Sciences, Wrexham, United Kingdom; J. G. Finneran, Vineland, NJ

ThP 427 An optimized sample preparation workflow for rare cell subpopulation proteomics: from cell collection to sample injection; Christopher Kume1; Sylvia Tielen2; Maximilian Fléron3; Dominique Bawir4; Laurent Nguyen4; Gauthier Eppe1; Gabriel Mazzucchelli1, 2; 1Laboratory of Mass Spectrometry, MolSys Research Unit, University of Liège, Liège, Belgium; 2Laboratory of Molecular Regulation of Neurogenesis, GIGA Stem Cells, University of Liège, Liège, Belgium; 3GIGA Proteomics Facility, University of Liège, Liège, Belgium

ThP 428 Analysis of PFAS in Breast Milk: An Alternative Sample Prep; Tina Chambers1; Jennifer Cottine Hitchcock1; 1Agilent Technologies, Santa Clara, CA

ThP 429 Evaluation of Chemical Structure of SPE Reverse Phase Sorbents in StageTips on Total Number of Protein and Peptide Identifications; Michael Apokaudzu1; Xiaohui Zhang1; Xiaolu Lin1; 1CDS Analytical, Oxford, PA

ThP 430 A three-in-one End-to-End Automated Sample Preparation and LC/MS Metabolomics, Lipidomics, and Proteomics Workflow for Plasma: Genevieve C. Van De Bittner1; Karen E. Yannell1; Mark Sartain1; Wendi A. Hale1; Cate Simmermaker1; Dustin Chang1; 1Agilent Technologies, Inc, Santa Clara, California; 2Agilent Technologies, Inc, Lexington, Massachusetts, USA

ThP 431 Innovation Development of Comprehensive Dimensional Profiling and Lossless Extraction Technology of the Multi-Residue Pesticides Analysis in TCm using LC/MS/MS: Bo Chen1; Yue Song1; Yu-Chia Lin1; Shan-An Chan1; 1Agilent Technologies, Shanghai, China; 2Great Engineer Technology Corp., Taipei, Taiwan; 3Agilent Technologies, Taipei, Taiwan

ThP 432 Building a universal proteins sample preparation platform using low-cost liquid handling robotics and 3D-printing; Benedikt C. Clemens1; Eric F. Zaniewski1; Johanna Kreuzer1; Soroush Hajizadeh1; Wilhelm Haas1; 1Massachusetts General Hospital, Boston, MA

ThP 433 Classification of Bacterial Species from Whole Cell Lysates Using Two-Dimensional Tandem Mass Spectrometry and Open-Source Supervised Machine Learning; L. Edwin Gonzalez1; Yanyang Hu2; Donna M Wang3; Eric T. Dziekonski2; R. Graham Cooks3; 1Purdue University, West Lafayette, IN; 2Purdue University, WEST LAFAYETTE, IN

ThP 434 Optimization of Lipid Extraction for Untargeted Lipidomic Analysis Using Liquid Chromatography/Mass Spectrometry: Ashraf M. Omar1; Qibin Zhang1; 2; 1Center for Translational Biomedical Research, University of North Carolina at Greensboro,
North Carolina Research Campus, Kannapolis, NC; 2Department of Chemistry & Biochemistry, University of North Carolina at Greensboro, Greensboro, NC

ThP 435 Elucidating the Lipidomic Dynamics of Lentiviral Production and Infection. Joshua A Roberts1; Elena Goodbody2; Christopher Boddy2; Jean-Simon Dillal2; Jeffrey C Smith3; 1Carleton University, Ottawa, ON; 2Centre for Cancer Therapeutics, Ottawa Hospital Research Institute, Ottawa, ON; 3University of Ottawa, Ottawa, ON

ThP 436 Unlocking the Secrets of mRNA LNP Components Under Extreme Conditions with TIMS-TOF Technology. Michael Girgis; George Mason University, Fairfax, VA

ThP 437 Evaluation of Aqueous-Acetonitrile Based Mobile Phase for Untargeted Analysis of Polar Metabolome and Lipidome: Gioraggia Isaac1; Robert Plumb1; 1Waters Corporation, Milford, MA

ThP 438 Don’t Be Ear-ritated: Kendrick Mass Defect-facilitated Determination of Triacylglycerides in Exearac: Allix M. Coon1; Gavin Setzen1; Rabi A. Musah1; 1University of Albany, State University of New York, Albany, NY; 2Albany ENT & Allergy Services, Albany, NY

ThP 439 Improved the detection and identification of labile lipids using Xevo™ G3 QTof Mass Spectrometer: Nyasha C Munjoma1; Steven La2; Lisa Reid1; Jayne Kirk2; Lee Getings2; Richard Lock1; 1Waters Corporation, Wilmslow, United Kingdom; 2Waters Corporation, Milford, MA

ThP 440 Discovery Lipidomics and Mapping of Exogenous Fatty Acid Incorporation into the HeLa Lipidome Using LC-IMS/MS and LC-IMS/MS/MS. Johannes Morstein1; Andrew Baker1; 1University of California San Francisco, San Francisco, CA; 2Waters, Inc., Pleasanton, CA

ThP 441 How Acute Exercise Alters Rat’s Lipidomic Profile of Liver: David A Gaul1; Samuel G Moore2; Xueyun Liu1; 1Department of Animal and Veterinary Sciences, Sejong University, Seongnam, South Korea

ThP 442 Variations in Lipid Profiles in the Serum Coronas Produced around Liposomal Drugs with Different Surface Properties: Gwi Ju Jang1; Heejou Joung1; Sang Yun Han1; 1Department of Pharmacy, Gachon University, Seongnam, Korea

ThP 443 Untargeted 2D-LC-Mass Spectrometry using SWATH-DIA-Based Workflow for the Characterization of Lipid Profiles in Plasma Samples: Laura Gisela Gonzalez-Iglesias1; Gerard Hopfgartner1; Renzo Picenoni1; Guenter Boehm1; 1LSMS, Department of Inorganic and Analytical Chemistry, University of Geneva, Geneva, Switzerland; 2C GAME Analytics AG, Zwingen, Switzerland

ThP 444 Comprehensive lipidome profiling facilitates the discovery of targetable metabolic vulnerabilities in Group 3 medulloblastoma: Jeremy K. Chan1; William D. Gwynne1; Andrew T. Quaile1; 1Department of Medicine, Vanderbilt University, Nashville, Tennessee; 2Department of Pharmacology, Vanderbilt University, Nashville, Tennessee; 3Department of Chemistry, Vanderbilt University, Nashville, Tennessee

ThP 445 Untargeted lipidomics analyses of exosomes from malaria parasite-infected red cells: Sina Feizbaksh Bazargani1; Timothy Hamerly2; Borja Lopez-Gutierrez2; Rhoel R Dinglasan3; Timothy J. Garrett4; 1University of Florida, Gainesville, FL; 2University of Florida, Gainesville, Florida

ThP 446 Lipid composition of serum-derived small extracellular vesicles could discriminate rectal cancer patients with different status of regional lymph node metastasis: Lukasz Marczak1; Katarzyna Dubkwicz1; Marcin Zeman2; Monika Pietrowska1; Anna Wojakowska1; 1Institute of Bioorganic Chemistry Polish Academy of Sciences, Poznan, Poland; 2Maria Sklodowska-Curie National Research Institute of Oncology, Giwiczice, Giwiczice, Poland

ThP 447 Lipidomic Analysis of Human Serum of Pancreatic Cancer Patients with Focus on Less Abundant Lipid Classes by HILIC-UHPLC/MS: Ondřej Peterka1; Alessandro Maccelli2; Robert Jiráško1; Zuzana Vašíková1; Jakub Idkowiak1; Denise Wolrab1; Roman Hrstka1; Michal Holčapek1; 1University of Pardubice, Pardubice, Czech Republic; 2Masaryk Memorial Cancer Institute, Brno, Czech Republic

ThP 448 The inhibition of TGFß changes the profiles of collagen crosslinks and lipids in tumor: Qiang Ling1; Alessandra Castiglioni2; Yagai Yang3; Shannon Turley1; Rafael Cubas2; Wendy Sandoval2; 1Genentech, SSF; 2Genentech Inc, South San Francisco, CA

ThP 449 Development of an MRI-based phospholipid profiling method in human plasma using an inert C18 column: Masaki Yamada1; Naoko Nagano2; Yutaka Umakoshi1; 1SHIMADZU Corporation, Kyoto, Japan

ThP 450 High-throughput UHPLC-TIMS-based lipidomics: Sub-5 min screening of plasma, cells, stool and tissues: Eduard Sommer1; Fabrizio Mercai1; Pietro Campiglia1; 2Erica Forsberg1; 1University of Salerno, Fisciano (SA), Italy; 2Bruker Daltonics, Billerica, MA

ThP 451 Inorganic arsenic treatments alter lipidomic profiles of Escherichia coli: Brett T Sather1; Hunter Faussel1; Scott Spurzem1; Garrett Gill1; Cole Kayser1; Anya Knowlton1; Georgia Eastham1; Sydney Peterson1; Brian Bothner1; 1Montana State University, Bozeman

ThP 452 Lipidomics on a High Fat Diet mouse model indicate alterations in lipid metabolism arising from aerobic exercise and calories restriction: Thomai Mouskettara1; 1, 2Christina Virgiliou1; 1, 2Ioannis I. Moustakas2; 3Eric Halls2; Carsten Baessmann2; Helen Gika1; 1Aristotle University of Thessaloniki, Thessaloniki, Greece; 2Biomic AUT, Center for Interdisciplinary Research and Innovation, Thessaloniki, Greece; 3Medical School, National and Kapodistrian University of Athens, Athens, Greece; 4Bruker Daltonics, Billerica, MA; 5Bruker Daltonics GmbH & Co. KG, Bremen, Germany

ThP 453 Lipidomics analysis reveals changes in the regulation of lipid metabolism in a surgical bone defect model: Dhirukshika S. W. Palagama1; Matthew J Kwiatkowski1; Phillip M Rzeczycki1; Thomas A Owen1; Maria I Morano1; Miguel A Gjon1; Paul D Kennedy2; Stephen D Barrett1; 1Cayman Chemical Company, Ann Arbor, MI; 2Bruker Daltonics, San Jose, CA

ThP 454 Coupling MaxPeak HPS UHPLC and PASEF-enabled lipidomics to maximize performance for multimodal analysis of small human biospecies: Madeline E Colley1, 2; Katerina V Djambazova1, 2; Lukasz G Migas1; Martin Dufresne1, 2, 3; Jamie L. Allen1, 2, 3; Angela R. S. Kruse1, 2, 3, 4; Richard M Capiolli1, 2, 3, 4, 5; Pat Van Drunen1, 2, 3, 4, 5; Jeffrey M Spraggens1, 2, 3, 4, 5; 1Vanderbilt University; Department of Biochemistry, Nashville, Tennessee; 2Mass Spectrometry Research Center, Vanderbilt University, Nashville, Tennessee; 3Department of Cell and Developmental Biology, Vanderbilt University, Nashville, Tennessee; 4Delt Center for Systems and Control, Delft University of Technology, Delft, Netherlands; 5Department of Medicine, Vanderbilt University, Nashville, Tennessee; 6Department of Pharmacology, Vanderbilt University, Nashville, Tennessee; 7Department of Chemistry, Vanderbilt University, Nashville, Tennessee

ThP 455 4D-lipidomics for the in-depth characterization of cardiolsins in Barth Syndrome patient hearts using VIP-HESI and timsTOF mass spectrometry: Sven Wolfgang Meyer1; Yorrick R.J. Jaspers2; Bauke V. Schomakers2, 3; Jan Bert Van Klinken2, 3, 4; Eric Wever2, 3; Regner Boddy2; Stephan Kemp2; Frédéric M. Vaz2, 3; Riekelt H. Houtkooper2; Michel Van Weeghel1; 1Bruker Daltonics GmbH & Co. KG, Bremen, Germany; 2Laboratory Genetic Metabolic Diseases, Amsterdam UMC, University of Amsterdam, Amsterdam; 3Amsterdam Gastroenterology Endocrinology Metabolism, Amsterdam, Netherlands; 4Robust Metabolomics, Amsterdam UMC, Amsterdam, Netherlands; 5Department of Human Genetics, Leiden University Medical Center, Leiden, Netherlands
ThP 456 Establishment of a global metabolomics method for Arabidopsis thaliana using high-sensitivity MS/MS on the ZenoTOF 7600 system; Jinmei Chen$^{1}$; Dandan Si$^{2}$; Zhimin Long$^{1}$; Lilai Guo$^{1}$; $^{1}$SCiEX, Shanghai, China; $^{2}$SOICT, Beijing, China

ThP 457 Classification of Beef Using Metabolomics: Zhentian Lei$^{1}$; Saurav Sarma$^{2}$; Carol Lorenzen$^{3}$; Jade Cooper$^{4}$; Lloyd Sumner$^{5}$; $^{1}$University of Missouri, Columbia, MO; $^{2}$Bayer Crop Science, St. Louis, MO; $^{3}$Oregon State University, Corvallis, OR; $^{4}$Texas A&M University, College Station, TX; $^{5}$University of Missouri-Columbia, Columbia, MO

ThP 458 Advantages of a novel high resolution accurate mass analyzer for metabolite identification in untargeted metabolomics studies; Siegrun Mohring$^{1}$; Bashar Amer$^{2}$; Susan Bird$^{3}$; Nicolaie Eugen Damoc$^{4}$; Martin Zeller$^{5}$; Alexander Tiegel$^{1}$; $^{1}$Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; $^{2}$Thermo Fisher Scientific, San Jose, California

ThP 459 A Multi-Omics Approach to Investigate Interactions between Elizabethkingia anophelis and Zika Virus; Junyao Wang$^{1}$; Omme Fatema Sultana$^{2}$; Maria Onyango$^{3}$; Yehia Mechref$^{4}$; $^{1}$Texas Tech University, Lubbock, TX

ThP 460 Development of Chemical Isotope Labeling LC-Orbitrap-MS for Comprehensive Analysis of small peptides; Zhan Chen$^{1}$; Liang Li$^{2}$; $^{1}$University of Alberta, Edmonton, AB

ThP 461 Targeted and untargeted metabolomics of mucopolysaccharidases model in mouse liver by LC-MS/MS; Nathaniel Ghafari$^{1}$; Iskren Menkovski$^{2}$; Pamela Lavoie$^{3}$; Michel Boutin$^{4}$; Christiane Aury-Blais$^{5}$; Lekha Sleno$^{6}$; $^{1}$University of Quebec in Montreal, Montreal, QC; $^{2}$Department of Pediatrics, Division of Medical Genetics, Faculty of Medicine and Health Sciences, Sherbrooke University, Sherbrooke, QC; $^{3}$University of Quebec in Montreal (UQAM), Chemistry department, Montreal, QC

ThP 462 Utilizing Tandem Mass Spectrometry and Computational Methods to Elucidate Fragmentation Mechanisms for Kyurenine Metabolites; Madisin Hayes$^{1}$; Esther Mbuna$^{2}$; Jaya Paudel$^{3}$; Dr. Benjamin Bythew$^{1}$; $^{1}$Ohio University, Athens, OH

ThP 463 Non-targeted metabolomics investigation suggests female is more vulnerable to chronic variable stress leading to depression in association with insulin resistance; Seulgi Kang$^{1}$; Boyeon Bae$^{2}$; Woonhee Kim$^{3}$; Jimin Nam$^{4}$; Ke Li$^{5}$; Yua Kang$^{6}$; Chihye Chung$^{7}$; Jeongmi Lee$^{8}$; $^{1}$Sungkyunkwan University, Suwon, South Korea; $^{2}$Konkuk University, Seoul, South Korea

ThP 464 Understanding the impact of sourdough starter microbiomes on bread quality; Eva Kehohan$^{1}$; Jacqueline Chaparro$^{2}$; Josephine Wee$^{3}$; Charlene Van Buiten$^{4}$; Jessica Prendi$^{5}$; $^{1}$Colorado State University, Fort Collins, CO; $^{2}$Penn State University, Centre County, Pennsylvania

ThP 465 Impact of Toxoplasma gondii acute and chronic infection on organ metabolism in IL-1R$^{-/-}$ and WT mice; Mahbubeh Legani$^{1}$; Tzu-Yu Feng$^{2}$; Sarah E. Ewald$^{3}$; Laura-Isabel Molle$^{4}$; $^{1}$University of Oklahoma, Norman, OK; $^{2}$University of Virginia, Charlottesville, VA; $^{3}$University of Oklahoma, Department of Microbiology and Plant Biology, Norman, OK; $^{4}$University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK

ThP 466 A Novel Screening Approach for Comparing LC-MS Revered-Phase and HILIC Methods for Separations in Biological Matrices Using Amino Acid Examples; Conner McHale$^{1}$; Taylor Harmon$^{2}$; $^{1}$Advanced Materials Technology, Wilmington, DE

ThP 467 Metabolic profile variation of Fragaria ananassa induce by Anthrospora platensis addition, under condition of nutritional stress; Candy Andreina Montaño-Pérez$^{1}$; Cecilia-Rocio Juárez-Rosete$^{2}$; Juan José Ordaz-Ortiz$^{3}$; Javier-Cerman Rodríguez-Carpena$^{4}$; Gabriela Avila-Villarea$^{5}$; $^{1}$Maestria Intuminstitucional en Agricultura Protegida, CONACIT, Unidad Académica de Agricultura, Universidad Autónoma de Nayant, Tepic, Mexico; $^{2}$Unidad Especializada en I+D+i Calidad de Alimentos y Productos Naturales, Centro Nayarita de Innovación y Transferencia de Tecnología A.C., Tepic, Mexico; $^{3}$Unidad de Genómica Avanzada, Centro de Investigación y de Estudios Avanzados del Instituto Politécnico Nacional, CINVESTAV, (LANGEBO), Impulso, Mexico; $^{4}$Unidad Académica de Ciencias Químico Biológicas y Farmacéuticas, Universidad Autónoma de Nayant, Tepic, Mexico

ThP 468 Metabolomics of Colorectal Cancer for Human Serum Screening; Kinjal Bhatt$^{1}$; Marie-Alice Meuwis$^{2}$; Edouard Louis$^{3}$; Pierre-Hugues Stefanel$^{4}$; Jean Francois Focant$^{5}$; $^{1}$University of Liege, Liege, Belgium; $^{2}$Liege University Hospital, Liege, Belgium

ThP 469 System suitability testing of LC-IMS-HRMS for metabolomics applications; Sven Wolfgang Meyer$^{1}$; Illmari Kreds$^{2}$; Stefan Harsdorf$^{3}$; Patrick Groos$^{4}$; Jonas Wloka$^{5}$; Erica Forsberg$^{6}$; Matthew R. Lewis$^{7}$; $^{1}$Bruker Daltonics GmbH & Co. KG, Bremen, Germany

ThP 470 PlantMASST: a mass spectrometry tool for mining public datasets from plants; Paulo Wender Portal Gomes$^{1}$; Helena Mannochio-Russo$^{2}$; Simone Zuffa$^{3}$; Robin Schmid$^{4}$; Andrés Mauricio Caraballo-Rodríguez$^{5}$; Pieter C Dorrestein$^{6}$; $^{1}$Collaborative Mass Spectrometry Innovation Center, Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, San Diego, California

ThP 471 A metabolomics approach using Simultaneous Quantitation and Discovery (SQUAD) on high resolution accurate mass full MS1 level; Bashar Amer$^{1}$; Christian Klaas$^{2}$; Catharina Crone$^{3}$; Siegrun Mohring$^{4}$; Rahul Deshpande$^{5}$; Claire Dauly$^{6}$; Thomas Moehring$^{7}$; Susan S. Bird$^{8}$; $^{1}$Thermo Fisher Scientific, San Jose, CA; $^{2}$Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany

ThP 472 Mass spectrometry analysis of the effect of hemin on Pseudomonas aeruginosa alkyl quinolone production; Daniel J Breiner$^{1}$; Rachel Neve$^{2}$; Vanessa V. Phelan$^{3}$; $^{1}$CU Anschrift Skaggs School of Pharmacy and Pharmaceutical Science, Aurora, CO; $^{2}$University of Massachusetts Medical School, Worcester, MA; $^{3}$University of Colorado Anschutz Medical Campus, Aurora, CO

ThP 473 Integrated analysis of LC/MS and GC/MS data in NASH and NAFLD model mice; Yutaka Umakoshi$^{1}$; Tsutomu Matsubara$^{2}$; Chiho Kadono$^{3}$; Yuko Sakamoto$^{4}$; $^{1}$SHIMADZU Corporation, Kyoto, Japan; $^{2}$Osaka Metropolitan University, Osaka, Japan

ThP 474 An Innovation Solution of Functional Metabolomics Reveals the Central role of Pentose Phosphate Pathway in Resident Thymic Macrophages Infections; Tsung-Lin Tsai$^{1}$; Chia-Lin Hsu$^{2}$; Yue Song$^{3}$; Dai-Yong Huang$^{4}$; Shan-An Chan$^{5}$; Yanan Yang$^{6}$; $^{1}$Institute of Microbiology and Immunology, National Yang Ming Chiao Tung University, Taipei, Taiwan; $^{2}$Agilent Technologies, Shanghai, China; $^{3}$Agilent Technologies, Inc, Guangdong, China; $^{4}$Agilent Technologies, Taipei, Taiwan; $^{5}$Agilent Technologies, Santa Clara, CA

ThP 475 Feature-based molecular networking revealed Jasmnin sambac cell extract as a powerful mixture of antioxidant metabolites; Sara Cecchetti$^{1}$; Adriana De Lucia$^{2}$; Assunta Tortora$^{2}$; Antonio Colantuono$^{2}$; Gennaro Carotenuto$^{1}$; Annalisa Tito$^{3}$; Maria Chiara Monti$^{4}$; $^{1}$Department of Pharmacy, University of Salerno, Fisciano, Italy; $^{2}$Artefa Bioscience SpA, Naples, Italy

ThP 476 Characterization of the diurnal pattern of exhaled volatile fatty acids and enteric methane emissions of dairy cows; Stamatios Giannoukos$^{1}$; Zakirul Islam$^{2}$; Susanna Räisänen$^{3}$; Kai Wang$^{4}$; XiaQi Ma$^{5}$; Renato Zenobi$^{6}$; Mutian Niu$^{7}$; $^{1}$ETH Zurich, Zurich, Switzerland; $^{2}$ETH Zurich, Zurich, Switzerland; $^{3}$Agroscope, Bern, Switzerland; $^{4}$Advanced Materials Corporation, Tokyo, Japan; $^{5}$Advanced Materials Technologies, Wilmington, DE

ThP 477 Investigating systemic gut microbiome derived metabolites from IL18−/− mice as potential mechanisms in health and disease; Emily G Armitage$^{1}$; Alan Barnes$^{2}$;
Nicholas Groth Mørild; J. Miota Zarebska; Neil Loftus; Jonathan Swann; Tonia L Vincent; Shimadzu Corporation, Manchester, United Kingdom; Kennedy Institute of Rheumatology, University of Oxford, Oxford, United Kingdom; School of Human Development and Health, Faculty of Medicine, University of Southampton, Southampton, United Kingdom

ThP 478 Reproducibility Analyses of Metabolic Data; Xinjian Yan; Stephen E. Stein; National Institute of Standards and Technology, Gaithersburg, MD

ThP 479 Evaluation of a UPLC zwitterionic HILIC stationary phase for deep coverage and high throughput metabolomics; Rebecca J. Jones; Lia Ficaro; Tori Rodrick; Manor Askenazi; Yik Sui; Thomas H. Walter; Kerri M. Smith; Jonathan Turner; Drew R. Jones; NYU Langone Health, New York; Biomedical Hosting LLC, Arlington, MA; Waters Corporation, Milford, MA; MA

ThP 480 Untargeted metabolic analysis of acute lead exposure to Danio rerio embryos using LC-MS/MS; Gwendolyn O. Osinubi; Tyler K. Hunt-Smith; Hunter Fausset; Christina S. Merchol; Brian Bothner; Department of Chemistry and Biochemistry, Montana State University, Bozeman, Montana; Department of Microbiology and Immunology, Montana State University, Bozeman, Montana

ThP 481 Exploring the Effect of Yeast Strain and Hop Addition Time on the Metabolomics of Omega Yeast Beer; Clara Myer; Brian Bothner; Erik D. Tague; Christopher Bolcato; Amirmansoor Hakimi; Lance Shaner; Laura Burns; Omega Yeast, Chicago, Illinois

ThP 482 Understanding early metabolic response of Saccharomyces cerevisiae to different oxidants using quantitative metabolomics with Isotopic Ratio Outlier Analysis (IROA); Debashish Ghosh; Felice A. De Jong; Chris Beecher; Vladimir Shulavev; University of North Texas, Denton, TX; IROA Technologies, Chapel Hill, NC

ThP 483 Simultaneous Quantitation and Discovery (SQUAD) metabolomics: an intelligent combination of targeted and untargeted workflows using a novel mass spectrometer; Bashar Amer; Siegrun Mohring; Nicolaie Eugen Damoc; Tabiwang N. Arrey; Rahul Ravi Deshpande; Daniel Hemmson; Thomas Moehring; Susan Bird; thermo Fisher Scientific, San Jose, California; thermo Fisher Scientific, Bremen, Germany

ThP 484 Simultaneous Quantitation and Discovery (SQUAD) metabolomics workflow implementing parallel analysis on Thermo Ascend Trubrid instrument; Bashar Amer; Jingjing Huang; David Bergen; Rahul Ravi Deshpande; Vad Vladzibrouska; Thomas Moehring; Susan Bird; thermo Fisher Scientific, San Jose, California; thermo Fisher Scientific, Bremen, Germany

ThP 485 Evaluating the metabolic function of LuxS and Autoinducer-2 in Escherichia Coli; Lindsay P Brown; Shawna R. Campagna; University of Tennessee Knoxville Chemistry Dept., Knoxville, TN

ThP 486 Elucidating the progressive multiorgan metabolic response in the setting of mitochondrial myopathies using combined omics and in-vivo stable isotope tracing; Dawson Miller; Steven S Gross; Marilena D'aurello; Qiuying Chen; Well Cornell Medicine, New York, NY; Cornell University Medical College, New York, NY

ThP 487 Differentiating Lung Tumor Biology in Metabolomes using Matched Flash Frozen and Fixed Tissues; Vanessa Y. Rubio; Hayley D. Ackerman; John H. Lockhart; Nicole R. Hackel; Elsa R. Flores; John M Koomen; Moffitt Cancer Center, Tampa, FL

ThP 488 Metabolism investigation of poly-l-lysine induced cytotoxicity; Vahid Jahan; Kristine Aunina; Liva Vita Kaufmane; Fatemeh Rastegar Adib; Dagnija Loca; Kristaps Klavins; Riga Technical University, Riga, Latvia; Baltic Biomaterials Centre of Excellence, Headquarters at Riga Technical University, Riga, Latvia

ThP 489 A Simultaneous Quantitation and Discovery (SQUAD) Trubrid method template combining Ion Trap and Orbitrap analysis; Sunandini Yadla; Brandon Bills; Bashar Amer; Rahul Deshpande; Susan Bird; Vlad Zabrouskov; Elys Rodriguez; Uri Keshet; Oliver Fiehn; thermo Fisher Scientific, San Jose, CA; UC Davis, CA

ThP 490 Investigating the Impact of Flame Retardants on Stem Cell Differentiation by Untargeted Metabolomics; Whitney L Stutte; Yu-Chun Chiu; Melissa Gronске; Seth W. Kilman; North Carolina State University, Raleigh, NC

ThP 491 Nitroliotriacetic acid-conjugated magnetic nanoparticle affinity probe-based metabolomics: Mass spectrometry for porphyrin profiling; Elia Gizzaw Mernie; Mei-Chun Tsang; Rofeamor P Obena; Fu-Lien Huang; Tzu-Ming Liu; Yu-Ju Chen; Institute of Chemistry, Academia Sinica, Taipei, Taiwan; Institute of Chemistry, Academia Sinica, Taipei, Taiwan; Department of Chemistry, Taipei, Taiwan; Institute of Biomedical Engineering, National Taiwan University, Taipei, Taiwan; Institute of Translational Medicine, Faculty of Health Sciences, University of Macau, Macau, China; Department of Chemistry, National Taiwan University, Taipei, Taiwan

ThP 492 Interfacing chromatographic, mass spectrometry, and ionization techniques for a better profiling of endogenous and exogenous metabolites in human milk; Alyiah A. Remoroza; Yamil Simões; Concepcion A. Remoroza; William E. Wallace; Stephen E. Stein; Chengpeng Chen; University of Maryland - Baltimore County, Baltimore, MD; National Institute of Standards and Technology, Gaithersburg, MD

ThP 493 Identification of Xenobiotic Biotransformation Products Using Mass Spectrometry-based Metabolomics Integrated with a Structural Elucidation Strategy by Assembling Fragment Signatures; Yuan-Chih Chen; Pao-Chi Liao; National Cheng Kung University, Taiwan, Taiwan

ThP 494 Dynamic 13C isotopic labeling and metabolic flux analysis of two fast-growing cyanobacteria: a study with SWATH tandem mass spectrometry; Pramod P Wangikar; Damini Jaiswal; Minal Nenwani; Indian Institute of Technology Bombay, Mumbai, India

ThP 495 MetabOle structure elucidation and analysis enabled by a curated microbial bioscreening frame; Chris L Brown; Yelena Adelfinskaya; Yue Fu; Jesse Balcer; Krishna Kuppapan; Yannick Djoumou Feunang; Matt Chase; Elizabeth Ibeve; Serge Fotsos; Paul Graupner; David Robbins; Jeffery Gilbert; Corteva Agrisciences, Indianapolis, IN; Corteva Agrisciences, Indianapolis, IN; Purdue University, Lafayette, IN

ThP 496 Benchmarking the relationship between spectral and chemical similarity in the context of chemical classes and molecular networking; Yasin Eli Abiad; Wout Bittremieux; Robin Schmid; Simone Zuffa; Justin J Van Der Hoof; Mingxin Wang; Pieter C Dorrestein; Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, San Diego, CA; Campus Middelheim, University of Antwerp, Antwerpen, Belgium; IOCB Prague, Prague, Czech Republic; Wageningen University, Wageningen, Netherlands; University of California Riverside, Riverside, CA

ThP 497 Investigation of the zearealenone metabolism using Electrochemistry-MS: Electrochemical vs. in vivo and in vitro approaches; Jean-Pierre Cherve; Boguslaw Buszewski; Malgorzata Szulka-Mylnska; Antec Scientific, Alphen a/d Rijn, Netherlands; Nicolaus Copernicus University, Faculty of Chemistry, Torun, Poland

ThP 498 Novel real-time acquisition logic to prevent fragmentation of uninformative precursors; Pelle Reimor; Simon Simpson; Nikolaj Krasskau; Helko Neuwege; Enveda Biosciences, Boulder, CO; Bruker Daltonics GmbH & Co. KG, Bremen, Germany; Bruker Scientific, LLC, Billerica, MA
ThP 499  Topic modelling improves accuracy of feature assignment in untargeted metabolomic analysis of the cancer microbiome; Devanand M. Pinto1; Andrew Leslie1; Tracy McGaha1; Kenneth Chinsholm1; 2NR, Halifax, NS; 2Princess Margaret Cancer Centre, University Health Network, Toronto, ON.

ThP 500  Real time library search for the confident annotation of compound classes on Thermo Ascend Tribrid instrument; Rahul Ravi Deshpande1; Bashar Amer1; Jingjing Huang1; David Berger1; Thomas Moehring1; Susan Bird1; 1Thermo Fisher Scientific, San Jose, California; 2Thermo Fisher Scientific, Bremen, Germany.

ThP 501  Phytoto-metabolomics of Phlogacanthus curvifolius by using an integrative LC-ESI-QTOF/MS/MS and GC-Q-TOF-MS approach: Evaluation of Antioxidant activity and enzyme inhibition potential; Srikanth Ponneganti1; National Institute of Pharmaceutical Education and Research Guwahati (NIPI-G), Guwahati, India.

ThP 502  Multiomics Profiling Shows Acetyl-CoA Carboxylase Inhibition Reveals T cell Life; Name: Diane Wallace1; Jess Thaxton2; 3Brian P. Risenberg1; Katie Hurst2; Elizabeth Hunt2; 4Brandie Ehrmann1; 1Department of Chemistry, University of North Carolina at Chapel Hill, Chapel Hill, NC; 2Lineberger Comprehensive Cancer Center, University of North Carolina at Chapel Hill, Chapel Hill, NC; 3Department of Cell Biology & Physiology, University of North Carolina at Chapel Hill, Chapel Hill, NC; 4Department of Cell Biology & Physiology, University of North Carolina at Chapel Hill, Chapel Hill, NC.

ThP 503  Application of a UPLC-QTOF/MS/MS Metabolomics Approach to Identify Yellow Rice Wine with Different Aging Times: Huimin Chen1; Jiangang Hu1; Zong Yang1; Bingjie Liu2; Lihai Guo3; SICIEX, Nanjing, China; 1Shaoxing Testing Institute of Food and Drug, Shaoxing, China; 2SICIEX, Shanghai, China.

ThP 504  Untargeted metabolomics of human urine from the hPOP consortium: profiling variations by gender, age, body mass index, ethnicity and nutrition; Myriam Mireault1; Lekha Steno1; 1University of Quebec in Montreal (UQAM), Chemistry department, Montreal, QC.

ThP 505  Comprehensive metabolomic analysis of single-spheroids based on chemical isotope labeling liquid chromatography-mass spectrometry; Cyrune Catena1; Liang Li1, 2; 1University of Alberta, Edmonton, AB; 2The Metabolomics Innovation Centre (TMIC), Edmonton, Alberta.

ThP 506  Creation of the HoneyBe Metabolomics DataBase (HBDB); Armando Alcazar Magana1; Sofia Colaneres1; Jason C. Rogalski1, 2; 2Peter Awram1; 3Leonard L. Foster1; 1Life Sciences Institute, UBC, Vancouver, British Columbia; 2UBC, Vancouver, BC; 3Authentic Food Solutions, Vancouver, British Columbia; 4Department of Biochemistry and Molecular Biology, UBC, Vancouver, BC.

ThP 507  Development of Robust and Sensitive Chemical Isotope Labeling (CIL) LC-MS for Metabolomic Profiling of One Microbe: Alan Luo1; Zoino Li1, 2; 1The Metabolomics Innovation Centre, Edmonton, AB; 2University of Alberta, Edmonton, AB.

ThP 508  Enniatins and beauvericin emerging mycotoxins affect pigs’ metabolism; Emilien L Jamin1; 2Justin Oules1; 2Jean-François Martin1; 3Barbara Novak1; 4Dian Schatzmayer1; 5Isabelle P Oswald1; 6Oliver Puel1; 7Philippe Pinton1; 8Toxalim (Research Center in Food Toxicology), Toulouse university, INRAE, ENVT, INP-Purpan, Toulouse, France; 9MetaboHUB-MetaToul, National Infrastructure of Metabolomics and Fluxomics, Toulouse, France; 10DSM - BIOMIN Research Center, Technopark 1, Tullin, Austria.

ThP 509  Genome mining and untargeted metabolomics to discover secondary metabolites involved in ectomycorrhizas; Sangua Interactions; Sameer Mudhpar1; 2Manasa R. Appidi1; 3Rytas Vigalys1; 4Robert L. Heitich1; 5Lotus Lofgren3; 6Paul E. Abraham1; 2The University of Tennessee, Knoxville, Tennessee; 3Oak Ridge National Laboratory, Oak Ridge, TN; 4Duke University, Durham, NC.

ThP 510  Longitudinal multi-omics characterization of propyl gallate-mediated nephrotoxicity in beagles; Nathaly Reyes Garcés1; Weiken Sun1; St Mou1; Tim Hummer1; Xuejin Peng1; Alvaro Sebastian Vaca2; Erica Forssberg1; Matt Willett1; Anton L. Rosenbaum1; 2Kevin Contrepois1; 3AstraZeneca, South San Francisco, CA; 4AstraZeneca R&D, Gaithersburg, Maryland; 5Bruker Scientific, San Jose, CA; 6Bruker, San Jose, CA; 7Bruker Scientific, Billerica, MA.

ThP 511  Development of an Ion Chromatography Mass Spectrometry Platform and Spectral Library for Cancer Metabolomics; Sara A Martinez1; Lin Tan2; Bao Tran1; 1John Weinstein1; 2Philip Lorenzi1; 3The University of Texas MD Anderson Cancer Center, Houston, TX.

ThP 512  Signal Response Evaluation Cleans Untargeted Mass Spectrometry Data to Improve Data Interpretability; Kirsten E Overdahl1; Alex R. Jarmusch1; National Institute of Environmental Health Sciences, Research Triangle Park, NC.

ThP 513  A New Methodology Approach for Metabolomics Analysis of Rumen; Kailyn M Melo1; Janet Li1; Sang Weon Na1; Mi Zhou1; Le Luo Guan1; Liang Li1; Shuang Zhao1; 1The Metabolomics Innovation Centre, University of Alberta, Edmonton, AB; 2Department of Agricultural, Food and Nutritional Science, University of Alberta, Edmonton, AB.

ThP 514  Enhancing the mobility resolution for co-eluting compound classes during plasma characterisation using multi-sequence IMSn acquisitions.; Adam M King1; Christopher Jurtschenko2; Dale A. Cooper-Chepherd3; Martin Palmer4; Darren Hewitt3; Emma Marsden-Edwards3; Waters corporation, Wilmont, United Kingdom; 4Waters, Milford, MA; 5Waters Corporation, Wilmont, United Kingdom.

ThP 515  Secretory response of Aspergillus niger IOC 4687 subjected to copper stress; Silas De Almeida Perdigão Cota De Almeida1; Enrique Eduardo Rozas1; Claudia Augusto Ollier Nascimento1; Merielen Dias1; Maria Ana Mendes1; 1Dempest MS Lab, Chemical Engineering Department of Polytechnic School of University of São Paulo (USP), São Paulo, Brazil.

ThP 516  Production and Characterization of Hydrothermal Extracts of the Needles from Four Conifer Tree Species; Omolara O. Mofokwa1; Emelemi Eronen1; Marko Mákinen1; Jannne Jänis1; 1University of Eastern Finland, Department of Chemistry, Joensuu, Finland.

ThP 517  Biochemical phenotyping of null allele in human induced pluripotent stem cell-dervived cell lineages: Integrating genetics with metabolomics; Maheshwori Thapa1; Shujian Zheng1; Nello Oliveira1; Arti Taggar1; 2Ammah Siddiqua1; Minhao Gong1; Anahita Amini1; Justin McDonough1; Bill Skames1; 3Paul Robson1; 2Shuzhao Li1; 4The Jackson laboratory, Farmington, CT; 5University of Connecticut School of Medicine, Farmington, CT.

ThP 518  GC-MS Metabolomic Profiling of Honey Samples from Zambia and Botswana for Geographical Origin Classification; Kwenga F Sichilongo1; Tumelo Padiso1; Bonang B Nkoeane1; Godireneo Tatolo1; Ogaufi Modisane1; 1University of Botswana, Gaborone, Botswana.

ThP 519  Differences in metabolic profiles of patients with heart failure using high resolution GC-Q/TOF; Sofia Nieto1; Luis Valdiviez2; Oliver Fiehn2; 3Aglert Technologies, Inc., Santa Clara, CA; 2West Coast Metabolomics Center, University of California, DAVIS, CA.

ThP 520  Illuminating the Cellular and Molecular Response to Drug Treatment by Combining Bioenergetic Measurements with Untargeted Metabolomics; Mark Sartain1; Genevieve C. Van De Bittner1; Natalia Romero1; Yoonseok Kam2; Jana B. Petho1; Dianhong Zhang1; 4Aglert Technologies, Santa Clara, CA; 2Aglert Technologies, Lexington, MA.
**ThP 521** Flexible, Vendor-agnostic Assessment of Liquid Chromatography - Mass Spectrometry System Performance using MassQL; Heather Winter; Dylan J. Johnson; Alan K Jarmsuch; *1 Metabolomics Core Facility, Immunity, Inflammation, and Disease Laboratory, Division of Intramural Research, National Institute of Environmental Health Sciences, National Institutes of Health, Durham, North Carolina; 2 Integrative Bioinformatics Support Group, National Institute of Environmental Health Sciences, National Institutes of Health, Durham, North Carolina

**ThP 522** Artificial Intelligence (AI)-Powered Discovery in Large-Scale Non-Targeted Mass Spectrometry; Saumya Tiwari; Jeramie D. Waterous; Tao Long; Lori Glenwenkel; Igor Segota; Phil Worboys; Khoi Dao; Edmond Porcu; Andrew Leverentz; Tanya Nguyen; Kim Lagerborg; Vinay Bhupathy; Sean Ramsey; Mohit Jain; *1 Sapien Bioanalytics, San Diego, CA

**ThP 523** Microfluidic Sample-to-Analysis Platform Enables Dynamic Monitoring of Metabolic Pathways of T-Cell Activation by ESI-MS; Jenny L. Sullibrown; Gianna C. Bowles-Welch; Bryan Wang; Peter A. Kottke; Angela C. Jimenez; Yan Xu; Angela A. Sergievsky; Jiawei Ni; *1 University of Alberta, Edmonton, AB

**ThP 524** A Quantitative Assay for Measuring 1000 Metabolites in Plasma Samples; Lun Zhang; Jiamin Zheng; Mathew Johnson; Rupasri Mandal; David S. Wishart; *1 University of Alberta, Edmonton, AB

**ThP 525** Metabolomics-Based Elucidation of Streptococcus pneumoniae and its Response to Exposure with Burkholderia-derived Alkaloids; McKinley D Williams; James L Smith; Thomas D Horvath; Melinda A Engevik; Ravi S Orugunti; *1 Texas A&M University, College Station, TX; 2 Sano Chemicals, Bryan, TX; 3 Texas Children's Hospital, Houston, TX

**ThP 526** Using internal standards to honeize untargeted metabolomics data: lessons from an inter-laboratory ring trial; Charles R Evans; Emily Phillips; Yuqian Gao; David A Gau; Franki E Leach III; Brianna Garcia; Kevin Cho; Bradley Evans; Tong Shen; Shuzhao Li; Timothy J. Garrett; Gary J. Patti; Arthur Edison; Xuexia Du; Facundo Fernandez; Oliver Fleisch; Thomas O. Metz; *1 University of Georgia, Athens, GA; 2 Georgia Institute of Technology, Atlanta, GA; 3 Pacific Northwest National Lab, Richland, WA; 4 Petit Institute for Bioengineering and Bioscience, Atlanta, GA; 5 University of Georgia, Department of Chemistry, Athens, GA; 6 University of Georgia, Athens, GA; 7 Washington University in St. Louis, St. Louis, MO; 8 Donald Danforth Plant Science Center, Saint Louis, MO; 9 University of California Davis, Davis, CA; 10 Jackson Laboratory, Farmington, CT; 11 University of Florida, Gainesville, Florida; 12 Washington University in Saint Louis, Saint Louis, MO; 13 University of North Carolina at Charlotte, Charlotte, NC; 14 Pacific Northwest National Laboratory, Richland, WA

**ThP 527** Investigation of the Anti-Inflammatory Effect of Astragalus radix on Macrophages using UHPLC-QTOF/MS-based Metabolomic Profiling and Pathway Analysis; Akshay S Patil; Yan Xu; *1 Cleveland State University, Cleveland, OH; 2 Cleveland State University, Cleveland, OH

**ThP 528** Metabolomic analysis of Rhizopus microsporus IOC4668 fungus isolated from mining environment: Screening for protein biomarkers induced by copper; Merielien Dias; Silas De Almeida Perdigão Cota De Almeida; Enrique Eduardo Rozas Sanchez; Claudio Oller Do Nascimento; Ricardo Pinheiro de Souza Oliveira; Maria Anita Mendes; *1 Dempster MS Lab - Poli-USP, Sao Paulo, Brazil; 2 Faculdade de Ciências Farmacêuticas - USP, São Paulo, Brazil

**ThP 529** An LC-MS-based high throughput confirmative analysis of Glucose Transporter 1 (GLUT1) in human brain microvascular endothelial cells (BMECs); Yash Mehta; Dhavalkumar Patel; Iqra Pervaz; *1 Abraham Al-Ahmadi; 2 Texas Tech University Health Sciences Center, Amarillo, TX

**ThP 530** UPLC-ESI-MS/MS Method for the Quantitative Measurement of β-Methylamino-L-alanine in Biological Matrices; Farid Jim; Philip Brogan; Cidrik Brandani; Benjamin Blount; *1 Centers for Disease Control and Prevention, Chamblee, GA

**ThP 531** Quantitative histone proteoform analysis of the Mus Musculus brain throughout lifespan and with life extension, spatial, and cell type specificity; Bethany C. Taylor; Kari F. Poncha; *1 Verna & Mars McLean Department of Biochemistry and Molecular Biology, Baylor College of Medicine, Houston, TX

**ThP 532** Preliminary analyses from a planned cohort of 1,000 individuals: Cerebrospinal fluid proteomics from a multi-omic study of Alzheimer’s disease; Alexander W. Rookyard; Jayanta K. Chakrabarty; Anu Jain; Badri N. Vardarajan; Min Suk Kang; Lipi Das; *1 Emily G. Werth; 2 Marielba Zerlin-Esteves; Lawrence S. Honig; 3, 4 Lewis M. Brown; 3, 4 Richard Mayeux; 1, 2, 3, 4 Department of Biological Sciences, Quantitative Proteomics and Metabolomics Center, Columbia University, New York, NY; 2 Taub Institute for Research on Alzheimer’s Disease and the Aging Brain, Columbia University, New York, NY; 3 G. H. Sergievsky Center, Vagelos College of Physicians and Surgeons, Columbia University, New York, NY; 4 Department of Neurology, Columbia University, New York, NY

**ThP 533** LC-MS/MS analysis reveals region-specific and age-related changes of glycosphingolipids in rat brain; Tianqi Gao; Fanfan Huang; *1 Ashok Kumar; Thomas Foster; Zhongwu Guo; 1 Department of Chemistry, University of Florida, Gainesville, FL; 2 Department of Neurosciences, University of Florida, Gainesville, FL

**ThP 534** Customizing sequential metabolic profiling to followflow in human iPSC-derived neurons; Jiawei Ni; Ashley Frankenfield; Ling Hao; *1 The George Washington University, Washington, DC

**ThP 535** Development of a robust UPLC-MS/MS method for the analysis of polyamines in biofluids and tissues from neurodegenerative diseases; Michele Iannone; Liesbeth Vereyken; Farid Jadhav; *1 Elien Grajchen; 2 Sara Gorremans; 1, 2 Luc Ver Donck; 1, 2 Alexis Bretteville; 1 Diederik Moechars; 1 Rob J. Vreeken; 1, 2 Janassen Pharmaceutica NV, Beerse, Belgium; 2 Maastricht University, Maastricht, Netherlands

**ThP 536** Taking Charge: An integrative structural proteomics approach to characterize conformational behaviour of α-synuclein and effects of metal ion binding; Emily L Byrd; *1 Martin Wilkinson; 2 Dale A. Cooper-Shepherd; 2 Sheena E. Radford; 1 Frank Sobott; 2 The University of Leeds, Leeds, United Kingdom; 3 Waters Corporation, Stamford Ave, Altrincham Road, Wilmslow, United Kingdom

**ThP 537** Proteomic analysis and characterization of detergent-insoluble proteome in Alzheimer’s disease; Masihzor Zaman; Yingxue Wu; Ping-Chung Peng; *1 Shi Yang; 1, 2 Zhiping Wu; 3, 4 Zhen Wang; 3, 4 Suresh Poudel; 1, 2 Xusheng Wang; Junmin Peng; 1, 2 St Jude children research hospital, Memphis, TN
ThP 538 Brain derived peptide abundance correlations reveal molecular subtypes of sporadic Alzheimer’s disease; Deanna Plubell1; Gennifer Merrilhew2; Jea Park3; Chris Hsu4; Christine C. Wu5; Thomas J. Montine6; Michael J. MacCoss7; 1University of Washington, Seattle, WA; 2Stanford University, Stanford, CA

ThP 539 Whole Blood for Analysis of Neurodegenerative Disease Biomarkers; Wenxue Zha1; Kevin P. Gillespie1; Teerapat Rojjaikul1; Clementina Mesaros2; Ian Alexander Blair1; 1University of Pennsylvania, Perelman School of Medicine, Philadelphia, PA

ThP 540 Synaptic dysfunction in Neurodegenerative diseases – the road from MS characterization to biomarker markers in clinical routine; Ann Brinkmalm1; Hilin Kvartsberg2; Johanna Nilsson1; Gunnar Brinkmalm1; Henrik Zetterberg1; Nicholas Ashton1; Kaj Blennow1; 1University of Gothenburg, Molndal, Sweden

ThP 541 Proteomic analysis of apoE isoform effects in human iPSC-derived neurons using peptide-level analysis; Justin McKelvey1; Einar K Krogsgaer2; Nevan J Krogan3; 2Yadong Huang1; 2Danielle L Swayne1; 1UCSF, San Francisco, CA; 2Gladstone Institutes, San Francisco, CA

ThP 542 Mass spectrometry-based metabolomics reveals methoxychlor-induced Parkinson’s disease-like metabolic changes in C57BL/6 mice; Fuyue Wang1; Xiaoxiao Wang1; Zongwei Cai1; 1State Key Laboratory of Environmental and Biological Analysis, Hong Kong Baptist University, Hong Kong, Hong Kong SAR, China, Hong Kong, China

ThP 543 DESI-MS as a Complementary Tool for the Investigation of Biomarkers in Amyotrophic Lateral Sclerosis – A Pilot Study in Neurodegeneration; Irma Berrueta Razo1; Michael Eyres1; Ping Yip2; Laura Ajram3; Andrey Gagunashvili4; Andrea Malaspina5; 5Philippe Hart1; 1Medicines Discovery Catapult, Manchester, United Kingdom; 2Queen Mary University of London, East London, United Kingdom; 3University College London, London, United Kingdom

ThP 544 Characterizing and cataloguing protein changes in Alzheimer’s disease across three clinical stages of human post-mortem tissue; Evgeni Kanshin1; Mitchell Marta Arta2; Manon Thierry-Mieg1; Dominique F Leitner1; 1Man, May Askenuzi1; Thomas Wisniewski2; Eleanor Drummond3; Beatrix Lieberheide1; 1NYU Grossman School of Medicine, New York, NY; 2Biomedical Hosting LLC, Arlington, MA; 3University of Sydney, Sydney, Australia

ThP 545 Identification and quantification of amino acid isomerization-prone proteins in cell lysate: impact of structure and buffer conditions on protein aging; Thomas A Shoff1; Hoi Ting Wu1; Joseph Generaux2; Ryan R. Julian1; 1University of California, Riverside, Riverside, CA

ThP 546 Large-scale, deep plasma proteomics: An 1800 sample study of Alzheimer’s disease; Asim Siddiqui1; Harendra Guturu1; Matthijs De Geus2; Sudeshna Das3; Pia Kivisaak4; Seralim Batzoglou1; Steven E Arnold5; 1Seer, Inc., Redwood City, CA; 2Massachusetts General Hospital, Boston, MA

ThP 547 Proteomics method development for analysis of murine blood-brain barrier by spatially restricted in-vivo biotinylation; Jan Scheja1; Liang Jin1; Xue Wang1; Chenqi Hu2; Yu Tian2; Nadine Ruderisch3; 1AbbVie Bioresearch Center, Worcester, MA; 2Takeda Pharmaceuticals, Cambridge, MA; 3AbbVie, Cambridge, MA

ThP 548 N1-Methylenadenosine in RNA Contributes to Neurodegeneration Arising from CAG Nucleotide Repeat Expansion; Yuxiang Sun1; Hui Dai2; Xiaoxia Dai3; Jiekiyai Yin4; Xuyiyang Cui5; XiaoChuan Liu5; Gwendolyn Gonzales6; Jun Yuan7; Feng Tang8; Nan Wang9; Alexander Perlegos9; Nancy Bonini10; William Yang10; WeiLei Gu5; Yinheng Wang5; 1University of California, Riverside, RIVERSIDE, CA; 2University of California - Los Angeles, Los Angeles, CA; 3University of Pennsylvania, Philadelphia, PA; 4University of California, Los Angeles, Los Angeles, CA

ThP 549 eIFSA hypusination, boosted by dietary spermidine, protects from premature brain aging and mitochondrial dysfunction; Yongtian Liang1; Chengli Piao2; Christine B Beuschel3; David Toppe4; Laxmikant Kollipara5; Boris Bogdanov6; Marta Maglione7; Janine Lütkendorf7; Jason Chun Kit See7; Sheng Huang1; Tim O F Conrad8; Ulrich Kintscher1; 1Frank Madoe2; Fan Liu2; Albert Sickmann3; 4Stephan J Sigrist9; 1Institute for Biology Genetcs, Freie Universität Berlin, Berlin 14195, Germany; NeuroCure Cluster of Excellence, Charité Universitätsmedizin Berlin, Berlin 10117, Berlin, Germany; 1Institute for Analytic Sciences - ISAS - e.V., Dortmund 44139, Germany, Dortmund, Germany; 2Department of Chemical Biology, Leibniz-Forschungsinstitut für Molekulare Pharmakologie (FMP), 13125, Berlin, Germany; 3Institute for Mathematics and Computer Sciences, Freie Universität Berlin, Berlin 14195, Germany; Zuse Institute Berlin, Berlin 14195, Berlin, Germany; 4University of California Riverside, CA; 5AstraZeneca, Macclesfield, United Kingdom; 6University of Sydney, Sydney, Australia

ThP 550 An Integrated omics and data-independent acquisition approach to characterize and validate the role of extracellular matrix molecules in neurodegeneration; Joseph T. Ngo1; Margaret Downs2; Joseph Zaia2; Thor D. Stein3; Marveen K Sathi4; 1Boston University Chobanian and Avedisian School of Medicine, Boston, MA; 2Boston University, Boston, MA

ThP 551 A draft human brain proteome atlas for understanding the molecular basis of brain functions; QI Xiao1; Yuting Xie2; Jinlong Gao2; Hui Yang3; Zhengyi Yang4; Tianzi Jiang5; Ying Mao5; Yan Li6; Tiannan Guo7; 8Westlake University, Hangzhou, China; 3Westlake University, Hangzhou, China; 4Fudan University, Shanghai, China; 5Institute of Automation, Chinese Academy of Sciences, Beijing, China; 6Shanghai Jiao Tong University, Shanghai, China; 7Westlake university, hangzhou, China

ThP 552 A Novel 3D Imaging Pipeline for Analyzing Efficacy of Compounds on Amyloid-Plaque Dynamics in Pre-clinical Alzheimer’s Disease Animal Models; Gianna Ferron1; Anthony Knesis1; Stefan Linehan1; Tim Ragan1; Mike Sasser1; Katherine Stumpo1; Michael Easterling2; Mark Lim3; Gargi Yagnik4; 1Institute for Analytical Sciences - ISAS - e.V., 44139, Dortmund, Germany; 2TissueVision, Inc., Newton, MA; 3The Jackson Laboratory, Bar Harbor, ME; 4Bruker Daltonics, Billerica, MA; 5AmberGen, Inc., Billerica, MA

ThP 553 CHARACTERISATION OF OLIGONUCLEOTIDES WITH PHOSPHODIESTER OR PHOSPHOROTHIOATE LINKER BY NEGATIVE ION ESI TANDEM MS AND IMS

ThP 554 A Workflow for Purity Determination, Intact Mass Measurement and MS/MS Sequencing of Oligonucleotide Impurities Detected in Synthetic Oligonucleotides; Catalin E Doneanu1; Jonathan Fox2; Christopher Knowles2; Ying Qing Yu3; Waters Corporation, Milford, MA; 2Waters Corporation, Wilslow, United Kingdom; 3Waters, Milford, MA

ThP 555 Time-course continuous monitoring of digestion reactions increases the coverage afforded by strand-
cleavage approaches for the characterization of larger nucleic acids: Daniele Rolle1; Thomas Kenderdine1; Ghazaleh Yassaghi1; Chris Bell2; Daniele Fabris1,2; 1University of Connecticut, Storrs, CT; 2RyboDynamics, Manchester, Connecticut.

ThP 556 LC-MS/MS for Assessing DNA ADP-ribosylation; Ting Zhao1; Yun Xiong1; 1University of California, Riverside, Riverside, CA

ThP 557 High-resolution and sensitive LC-MS/MS method for the quantification of oligonucleotides; Dilipkumar Reddy Kandula1; Greg Roman1; Lei Xiong1; 1Sciei, Framingham, MA; 2SCIEX, Redwood city, CA

ThP 558 Development of DNA CUT-MS for sensitive quantification of damage-associated DNA modifications; Terry D Kim1; Ting-Yu Wang1; Tsui-Fen Chou1; Daniel R Semlow1; 1California Institute of Technology, Pasadena, CA

ThP 559 Nucleos1:0D: new search engine enabling the untargeted identification of RNA post-transcriptional modifications from tandem mass spectrometry analyses of nucleosides; Yannis Nicolas Francois1; Clarisse Gosset-Erard1,2; Jerome Pansanel1; Anthony Lechner4; Philippe Wolff1; Lauriane Kuhn1; Patrick Chaimbault1; 1Laboratoire de Spectrométrie de Masse des Interactions et des Systèmes (LSMIS) UMR 7140 (Unistra-CNRS), Université de Strasbourg, Strasbourg, France; 2Laboratoire de Chimie et Physique Approches Multi-échelles des Milieux Complexes (LCP-AMC), Université de Lorraine, METZ, France; 3Université de Strasbourg, IPHC, CNRS, UMR7178, Strasbourg, France; 4Architecture et Réactivité de l’ARN (ARN) UPR 9002, CNRS, Université de Strasbourg, Strasbourg, France; 5Plateforme Protéomique Strasbourg Espplanade FR 1589, CNRS, Strasbourg, France

Improved Characterization of Heavily Modified RNA Therapeutics via Electron-Beam Fragmentation Methods; Daniel Jacob Nesbitt1; Trenton M. Peters-Clarke1; Keaton L. Mertz3; Michael S. Westphall1; Trent J. Vaughn Miller2; 1Agilent Technologies, Lexington, MA; 2Division of Therapeutic Performance I, Office of Pharmaceutical Quality, Center for Drug Evaluation and Research, U.S. Food and Drug Administration, Silver Spring, MD; 3Division of Therapeutic Performance II, Office of Pharmaceutical Quality, Center for Drug Evaluation and Research, U.S. Food and Drug Administration, Silver Spring, MD

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ThP 561 Stationary Phase Effects in Hydrophilic Interaction Liquid Chromatographic (HILIC) Separation of Oligonucleotides; Scott Abernathy1; Patrick A. Limbach1; 1University of Cincinnati, Cincinnati, OH

ThP 562 Universal Mass Exclusion List for Enhanced Modification Mapping of RNA during LC-MS/MS analysis; Asif Rayhan1; Balasubrahmnamy Addapalli1; Patrick A. Limbach1; 1University of Cincinnati, Cincinnati, OH; 2University of Cincinnati, Cincinnati, OH

ThP 563 Studies on the stability and dissociation of tetramolecular RNA quadruplexes; Anna Planer1; Sarah Viola Heei2; Kathrin Breuker1; 1Institute of Organic Chemistry and Center for Molecular Biosciences Innsbruck (CMBI), University of Innsbruck, Innsbruck, Austria; 2Institute of Organic Chemistry and Center for Molecular Biosciences Innsbruck (CMBI), University of Innsbruck, Innsbruck, Austria

ThP 564 Oligonucleotide Characterization by Bio LC and Q-TOF; Yulan Bian1; David L Wong2; 1Agilent Technologies, Singapore, Singapore; 2Agilent Technologies, Santa Clara, CA

ThP 565 Software enabled oligonucleotide mapping analysis of Erythropoietin mRNA; Alexander Bunkowski1; Waltraud Evers1; Eckhard Belau1; Thomas Meid1; Lars Vorweg1; Stuart Pengeley1; Yun Yang2; Guillaume Tremintin2; Detlev Sukau1; Bruker Daltonics, Bremen, Germany; 2Bruker Daltonics, San Jose, CA

ThP 566 Optimized CID conditions for 24-75mer oligonucleotide MS/MS characterization; Stuart Pengelley1; Eckhard Belau1; Yeni Yung-Mu2; Dirk Wunderlich1; Timo Schierling1; Julia Schneider1; Detlev Sukau1; Bruker Daltonics, Bremen, Germany; 2Bruker Daltonics, San Jose, CA; 3Axolabs GmbH, Kulmbach, Germany

ThP 567 Auto MSMS and targeted MSMS for in-depth qualitative and quantitative analysis of oligonucleotide synthesis products and side products; Detlev Sukau1; Stuart Pengelley1; Julia Schneider1; Timo Schierling1; Arian Alving1; Eckhard Belau1; Konrad Winkels1; Lars Vorweg1; Alexander Bunkowski1; Bruker Daltonics, Bremen, Germany; 2Axolabs GmbH, Kulmbach, Germany; 3Bruker Daltonics, Billerica, MA

ThP 568 Synthetic modified oligonucleotides analysis using a matrix-assisted laser desorption/ionization high resolution mass spectrometer (MALDI-DIT-MS); Yuko Fukuyama1; Hideharu Shichii1; Masaki Murase1; Yoshibiro Yamada1; Sadanori Sekiya1; Shinichi Iwamoto1; Koichi Tanaka1; 1SHIMADZU Corporation, Kyoto, Japan

ThP 569 A simple robust method for synthetic therapeutic RNA. New chemistry, new quantitation; Kenneth Cogg1; Ulrik Mistarz2; Alexander Schwahn1; Keeley Murphy3; Min Du3; 1Thermo Fisher Scientific, Franklin, MA; 2Thermo Fisher Scientific, Sunnyvale, CA; 3Thermo Fisher Scientific, Cambridge, MA; 4Agilent Technologies, San Francisco, CA

ThP 570 Sequence determination of long therapeutic DNA combining restriction enzyme cleavage and mass spectrometry; Christian Sattler1; Arip Shahnavazi1; Shima Marandi1; Andela Juric1; Luisa Hoffmann1; Burak Ceylan1; Michael Ruehl1; 1BioSpring Gesellschaft für Biotechnologie mbH, Frankfurt am Main, Germany

ThP 571 Validation of HILIC-MS/MS Method for Quantitative Oligonucleotide Analysis; Md Rabiul Islam1; A M Abdullilah1; Cynthia Sommers2; Jason Rodriguez2; Deyi Zhang2; Darby Kozak2; Kui Yang2; 1Division of Complex Drug Analysis, Office of Testing and Research, Office of Pharmaceutical Quality, Center for Drug Evaluation and Research, U.S. Food and Drug Administration, Saint Louis, MO; 2Division of Therapeutic Performance I, Office of Research and Standards, Office of Generic Drugs, Center for Drug Evaluation and Research, U.S. Food and Drug Administration, Silver Spring, MD

ThP 572 5’ mRNA Analysis By Microchip CE-MS Using an Internal Cleavage Motif for RNase H Digestion; Adi M Kulkarni1; Robert L Ross2; Min Du2; Kate Yu1; 1908 Devices, Boston, MA; 2Thermo Fisher Scientific, Cambridge, MA

ThP 573 Raw Material Testing: Developing Methods for Quality Control of Phosphoramidites used in the Chemical Synthesis of Oligonucleotides; Chris Henry; 1Waters Corporation, Waltham, United Kingdom

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Liquid Chromatography and Differential Mobility Spectrometry – Mass Spectrometry Workflow for Glycoprotein characterization using Electrorn Capture and Conformation Induced Fragmentation of Full Glycoforms; Chantal Jacquel1; 2; Gérard Hopfgartner1; 2; University of Geneva, Geneva 4, Switzerland

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Peptide-Spectrum Match Rescoring for Post Translational Modifications and Cysteine proteomes with MBSBooster and FragPipe; Kevin L. Yang1; Fengchao Yu1; 2Daniel A. Polasky3; Vadim Demichev1; 2Alexander I. Nesvizhskii1, 3; 2Department of Computational Medicine and Bioinformatics, Ann Arbor, MI; 4Department of Pathology, University of Michigan, Ann Arbor, MI; 5Charité – Universitätsmedizin Berlin, Berlin, Germany

ThP 599

Pinpointing isomerized residue location in peptides with MS3 analysis; Hoi Ting Wu1; 2Ryan J. Julian1; 1University of California, Riverside, Riverside, CA

ThP 600

Proteome-wide profiling of hydroxylation with ProAlanase and trypsin in human cell line and tissue samples; Feixuan Wu1; 2Dylan Tabang2; Hannah N. Miles2; Sara Sackett2; William A. Ricke3, 5, 6; Jon Odorico2; Lingjun
ThP 601 High-throughput Peptide Mapping for analysis of post-translational modifications and sequence variants in early development of biotherapeutics: Vesela Encheva-Yokova; Sina Rafiee Mahmoudreza; Lukas Krasny; Karina Bora; James Graham; Lonza, London, United Kingdom

ThP 602 Glycosylation site mapping using highly efficient ECD in a Q-TOF: Joseph Meeuwsen; Mike Hare; Rebecca Wisniski; Valerie Bockman; m-MSion, Corvallis, OR; Agilent Technologies, Santa Clara, CA

ThP 603 Unlocking the Potential of Site-Localized PTMs: The Power of dia-PASEF and Robust Quantification Techniques: Justin Sing; Aparna Srinivasan; Hannes Röß; Department of Molecular Genetics, University of Toronto, Toronto, ON; Terrence Donnelly Centre for Cellular & Molecular Research, Toronto, Ontario; Department of Computer Science, University of Toronto, Toronto, Ontario

ThP 604 Mass spectrometric profiling of citrullination in proteome and matrisome during human pancreas maturation and type 1 diabetes: Hung-Yu Chiang; Bin Wang; Daniel M. Tremmel; Sara Dutton Sackett; Jon S. Odorice; Lingjun Li; School of Pharmacy, University of Wisconsin-Madison, Madison, WI; Biophysics Program, University of Wisconsin–Madison, Madison, WI; Department of Surgery, Division of Transplantation, School of Medicine and Public Health, Madison, Wisconsin; University of Wisconsin-Madison, School of Medicine and Public Health, Madison, WI; University of Wisconsin-Madison, School of Medicine and Public Health, Department of Urology, Madison, WI

ThP 605 Arginylation Discovery Using an Unbiased Bottom-Up Proteomic Technique: Joanna M. Gongora; Zongtao Lin; Faith M Robison; Xinguo Liu; Xyqiao (axe) Xie; Benjamin A. Garcia; Department of Biochemistry and Molecular Biophysics, Washington University in St. Louis, St Louis, MO

ThP 606 Identifying Isomerization of Aspartic Acid Residues in Neuropeptides: Samuel Okey; Elena V. Romanova; Jonathan V. Swedler; University of Illinois-Urbana Champaign, Urbana, IL; University of Illinois Urbana-Champaign, Urbana and Champaign, IL

ThP 607 Nrich(s): four strategies to delve into protein N-terminome: Seonjeong Lee; Cheouli Lee; Chemical and Biological Integrative Research Center, Korea Institute of Science and Technology, Seoul, South Korea; Division of Bio-Medical Science and Technology, KIST School, University of Science and Technology, Seoul, South Korea

ThP 608 A combined gas phase separation strategy to improve ADP-ribosylation sequencing depth: Taku Kasai; Shiori Kuraoka; Hideyuki Higashi; Masanori Aikawa; Sasha A. Singh; Center for Interdisciplinary Cardiovascular Sciences, Division of Cardiovascular Medicine, Department of Medicine, Brigham Women's Hospital, Harvard Medical School, Boston, MA; Center for Excellence in Vascular Biology, Cardiovascular Division, Brigham and Women's Hospital, Harvard Medical School, Boston, MA; Channing Division of Network Medicine, Department of Medicine, Brigham Women's Hospital, Harvard Medical School, Boston, MA

ThP 609 Improved performance of phosphopeptides characterization using online capillary electrophoresis coupling with ion mobility mass spectrometry (CE-IM-MS): Ling Ling; Fuxing Xu; Chuan-Fan Ding; Liang Wang; Kate Yu; Ningbo University, Ningbo, China; 908 Devices, Shanghai, China; 908 Devices, Boston, MA

ThP 610 Modification Specific Modelling in PeptideProphet Improves Validation of Rare PTM Containing Peptides in Complex Samples: David D. Streyberg; Alex Zelter; Nina Isoherranen; Michael R. Hoopmann; Luis Mendoza; Jimmy Eng; Eric W. Deutsch; Robert L. Moritz; Institute for Systems Biology, Seattle, WA; University of Washington, Seattle, WA

ThP 611 Analysis of 4-hydroxynonenal modifications in cellular retinoic acid binding protein 1 by intact protein and bottom-up mass spectrometry: Ayelet Zelner; Ellen Riddle; King CB Yabut; Benjamin Zercher; Alice Martynova; Michael J. MacCoss; Matthew F Bush; Nina Isoherranen; Department of Genome Sciences, University of Washington, Seattle, Washington; Department of Biochemistry, University of Washington, Seattle, WA; Department of Pharmacuetics, University of Washington, Seattle, WA; Department of Biochemistry, University of Washington, Seattle, WA; Department of Genome Sciences, University of Washington, Seattle, WA; Professor and Chair, Seattle, WA

ThP 612 Integrating Capillary Electrophoresis and Ultraviolet Photodissociation for the Characterization of Phosphorylation States in the Carboxy-Terminal Domain of RNA Polymerase II: Joseph H. Koetter; Jennifer Brodbelt; University of Texas at Austin, Austin, TX

ThP 613 Combining Multi-Enzymatic Limited Digestion and tryptic digest with Interpretable Machine Learning for identification and selection of PTMs-modified biomarker candidates: Raphaël La Rocca; France Baumann; Christopher Kune; Jean-Luc Balligand; Maximilien Fleron; Dominique Bawir; Gauthier Eppe; Gabriel Mazzucchelli; Laboratory of Mass Spectrometry, MoISys Research Unit, University of Liège, Liège, Belgium; Pole of Pharmacology and Therapeutics (FATH), Institut de Recherche Expérimentale et Clinique (IREC) and Department of Medicine, Cliniques Universitaires Saint-Luc, Université Catholique de Louvain, Bruxelles, Belgium; GIGA Proteomics Facility, University of Liège, Liège, Belgium

ThP 614 Direct determination of tyrosine sulfation sites in proteomic analysis: Menatallah M. Youssf; Carson W. Sot; Miriam F. Ayad; Lobna A. Hussein; Maha F. Abdel-Ghany; Kristina Hakansson; University of Michigan, Ann Arbor, MI; Faculty of Pharmacy, Ain Shams University, Cairo, Egypt

ThP 615 Evaluation of MS2 Versus MS3 TMT Quantitation for Phosphotyrosine, Acetyllysine, and Methylnarginine Peptides: Alissa J. Nelson; Jian Min Ren; Anthony Possemato; Vicky Yang; Matthew Stokes; CELL SIGNALING TECHNOLOGY, DANVERS, MA

ThP 616 Combination of the unique functions from timsTOF and ZenoTOF enables in-depth analysis of the glycophotome: Chi-Hung Lin; Mark Mani; Wen-Fang Chou; Yi (jimmy) Zeng; Philip Ma; Bruce Wilcox

ThP 617 FAIMS-LC/MS Reveals Structural Heterogeneity of Isolveuglandin-adducted Peptide Autoantigens: Daniel Roeth; Nathaniel Bloodworth; Wei Chen; David M. Patrick; David G Harrison; Markus Kalkum; City of Hope, Duarte, CA; Vanderbilt Institute for Infectious, Immunology, and Inflammation, Vanderbilt University Medical Center, Nashville, TN

ThP 618 Utilization of electron activated dissociation (EAD) on a new QTOF platform for comprehensive analysis of histone post-translational modifications: Emily Zahn; Richard M Searfoss; Yixuan (axe) Xie; Zongtao Lin; Francesca N De Luna Vitorino; Benjamim A.; Washington University School of Medicine, St. Louis, MO

ThP 619 Discovery of nitrotyrosine-containing proteins and peptides by antibody-based enrichment strategies;
Firdous Bhat1; Kiran K. Mangalaparthi1; Joel-Sean Hu1; Jane A. Peterson2; Husheng Ding1; Dong Gi Mun1; Akhilesh Pandey1,3; 1Department of Laboratory Medicine and Pathology, Mayo Clinic, Rochester, Minnesota; 2Mayo Clinic, Rochester, Minnesota; 3Center for Individualized Medicine, Mayo Clinic, Rochester, Minnesota

ThP 620 PASEF-DDA and one pot preparation of proteins for enrichment-free detection and quantitation of protein termini from pathogenic Mycobacteria; Daniel D Hui1; Owen A Collins1; Patricia A Champion1; Matthew M Champion1; 1University of Notre Dame, Notre Dame, IN

Rapid Automated Reaction Screening and Optimization by the Unchained Labs Junior Interfaced with Open Port Interface Mass Spectrometry; David Calabrese1; Nate Hoxie1; Pranav Bende1; Meghav Verma1; Cullen Klein1; John Janiszewski1; Alex Godfrey1; Sam Michael1; Chang Li1; Thomas R. Covey1; 1NIH/NCATS, Rockville, MD; 2SICERT, Concord, ON

A Comparative Analysis of LC-MS Based Workflows for Host Cell Process Analysis in Bioprocess Development; Sachini P Karunaratne1,2; Roger Lu1; Chris Chumssa1; Julia Ding1; 1Bristol-Myers Squibb, DEVA, MA; 2University of Kansas, Lawrence, KS

Combining intact glycoprofiling and cell culture media analytics for in-process monitoring of an automated high-throughput multi-parallel bioreactor system; Yun Aleynas1; Charles Prochaska1; Clint Lukia1; Guillaume Bechade1; Patrick Boyce1; Mark Wrona1; 1Waters Corporation, Milford, MA; 2Sartorius Stedim NA, Bohemia, NY; 3Waters Corporation, Milwosw, United Kingdom

Automating sub-unit mAb attribute screening for in-process monitoring of an automated high-throughput multi-parallel bioreactor; Nick Pitman1; Patrick Boyce1; Caitlin Hanna1; Samantha Ippoliti1; Yun W Aleyunas1; Charles Prochaska1; Clint Lukia1; Guillaume Bechade1; Magnus Wetterhall1; Mark Wrona2; Stephan M Koza2; Ying Qing Yu1; 1Waters Corporation, Milwosw, United Kingdom; 2Waters Corporation, Milford, MA; 3Sartorius Stedim NA, Bohemia, NY

Amino Acid Quantitation in Over 50 Mammalian Cell Culture Media with an Integrated E-MS Analyzer; Kenion H Blakeman1; Reagan Draper1; Zhanna Sheyner1; Ji Young Anderson1; Scott Miller1; 1908 Devices, Inc., Boston, MA

A Mass Spectrometry-Based Correlation Profiling Method for Investigating Disease Associated Alterations in Membrane Lipid-Protein Interactions; Liuyu Peng1; Richard G Lee1; Nichollas E Scott1; Aleksandra Filipovska1; Gavin E Reid1; 1University of Melbourne, Melbourne, Australia; 2Telethon Kids Institute, Neledlands, Australia

Parallel evaluation of ten biont ligases for proximity proteomics; William Hardy1; Rawan Kalloush1; Saya Sedighi1;2; Julia Itaygoryodsky1;3; Vesal Kasmaeifar1;3; Queenie Hu1; Reuben Samson1;2; Brendon Seale1; Zhen-Yuan Lin1; Cassandra Wong1; Alexey Nesvizhskii1,2; The-Claude Ginigra1,2;3; 1Lunenfeld-Tanenbaum Research Institute at Mount Sinai Hospital, Toronto, ON; 2Department of Molecular Genetics, University of Toronto, Toronto, ON; 3Department of Pathology, University of Michigan, Ann Arbor, MI; 4Department of Computational Medicine and Bioinformatics, Ann Arbor, MI

Complete structural characterization of patient-derived monoclonal autoantibodies associated with vaccine-induced thrombotic thrombocytopenia reveals the molecular mechanism of this pathology; Danill G Ivanov1; Son N Nguyen1; Si-Hung Le1; Yi Du1; Nikola Ivetic1; Ihsac Nazy2; Igor A Kallashov2; 1University of Massachusetts Amherst, Amherst, MA; 2Michael G. DeGroot School of Medicine, McMaster University, Hamilton, ON

Rapid profiling the glycosylation effects on cellular entry of SARS-CoV-2 using MALDI-MS with high mass detection; Yuye Zhou1;2; Congrui Tan1; Na Wu1; Renato Zenobi1; 1ETHZ, Zurich, Switzerland; 2KTH Royal Institute of Technology, Stockholm, Sweden

Native Mass Spectrometry for Determining the Effectiveness of Molecular Glues in Enhancing E3 Lipase-Protein Interactions for Targeted Protein Degradation; Xiaojing Huang1; William A. Donald1; 1UNSW, Sydney, Australia

Improve sensitivity, mass resolution and accuracy in micro-SEC-MS characterization of antibody-siRNA complexes; Jason X. Tang1; Zhongping Liao1; 1El Lilly & Company, Indianapolis, IN

Matrix-Assisted Laser Desorption/Ionization (MALDI) Studies for SARS-CoV-2 Drug Development; Congrui Tan1; Yuye Zhou1,2; Renato Zenobi1; 1ETH Zurich, Zurich, Switzerland; 2KTH Royal Institute of Technology, Stockholm, Sweden

Characterization of a Nucleotide-Binding Site at the C-Terminal Domain of Human TRAP1 by Native Mass Spectrometry and Free Electron Laser Spectroscopy; KTH Royal Institute of Technology, Stockholm, Sweden

Quantitative Shotgun Glycomics using Concentration-Independent (COIN) Native Mass Spectrometry; Duong T. Bui1; James Favel1; Elena N. Kitova1; Zhixiong Li2; Kelli A. McCord1; Edward N. Schmidt; selective ionization (VUPD); 1Hill, Chapel Hill, NC; 2Texas A&M University, College Station, TX; 3St. Jude Children's Research Hospital, Memphis, TN

Membrane Proteins Enrich Distinct Lipids from Natural Lipid Extracts; Yun Zhu1; Melanie Odenkirk1; Pei Qiao1; Jack P. Ryan1; Tianti Zhang1; Samantha Schrecke1; Ming Zhou1; Mike Marty2; Erin Baker1; Arthur Lagowski1; 1Texas A&M University, College Station, TX; 2University of North Carolina at Chapel Hill, Chapel Hill, NC; 3Baylor College of Medicine, Houston, Texas

Accurate golden standards and statistical models for co-fractionation mass spectrometry-based protein complex discovery; Youngwoon Lee1; Pengcheng Yang1; Jun Xie1; Daniel Zeylmanski1; 1Purdue University, WEST LAFAYETTE, IN

Insights Into the Structure and Function of Polyglutamine Disease Target DNAJB6 Using Native Mass Spectrometry; Devin M. Makey1; Oleta T. Johnson2; Laura I. Penabd1; Jason E. Gestwicki1; Robert T. Kennedy1; Brandon T. Ruotolo1; 1University of Michigan, Ann Arbor, MI; 2University of California San Francisco, San Francisco, CA

Automated High-throughput Online Native MS Screening for Proteins and Protein Complexes; Scott Kronewitter1; Olufemi Adeyemi1; Paul Gazis1; Ping Yip1; Weijing Liu1; Albert Konijnenberg1; Rosa Viner1; 1ThermoFisher Scientific, San Jose, CA; 2ThermoFisher Scientific, San Jose, CA; 3Thermo Fisher Scientific, Boston, MA; 4Thermo Fisher Scientific, Austin, TX

Quantifying Interactions of Methylglucose Lipopolysaccharides (MGLP) with Fatty Acids Ligands Quantifying Interactions of Methylglucose Lipopolysaccharides (MGLP) with Fatty Acids Ligands; Elena Kitova1; Duong T. Bui1; Ann Arbor, MI; 2University of Texas at Austin, Austin, TX; 3St. Jude Children's Research Hospital, Memphis, TN

Insights Into the Structure and Function of a Nucleotide Derivative siRNA for Proteins and Protein Complexes; Alcides Qiao1; 1ThermoFisher Scientific, San Jose, CA; 2ThermoFisher Scientific, San Jose, CA; 3Thermo Fisher Scientific, Boston, MA; 4Thermo Fisher Scientific, Austin, TX
### THURSDAY POSTERS

| ThP 642 | Comprehensive Proteomic Interrogation of the SHOC2-MRAS-PP1C Complex: Robert A. Dippolito 1, Matthew Drew 1, Kelly Sneed 1, Dominic Esposito 1, Frank McCormick 1, 2; Kavli Institute for Nanoscience Discovery, Oxford, United Kingdom | ThP 653 | Application of Crosslinking-based technology in Quantitative Analysis of PHD2 Interactome: Haijung Yuan 1, Xinyu (cindy) Hou 1, Xiaorang (sherry) Wang 2, Yao Gong 1, Lan Huang 1, Yue Chen 1, University of Minnesota, Minneapolis, MN; 2University of California Irvine, Irvine, CA |
| ThP 643 | Native mass spectrometry uncovers the role of Ca2+ and lipid binding on synaptotagmin 1 oligomerisation and function: Sophie A. S. Lawrence 1, 3, Tanrick J. El-Baba 1, 2; Jack L. Bennett 1, 2, 4; Frederick National Laboratory for Cancer Research, Frederick, MD; 3Helen Diller Family Comprehensive Cancer Center, University of California, San Francisco, CA | ThP 654 | Native mass spectrometry unveils the details behind the GroEL allosteric functioning mechanism: He M Sun 1, Thomas Walker 1, Arthur Laganowsky 1, Hays Ry 1, 2 David H. Russell 1, 2Texas A&M University, College Station, TX |
| ThP 644 | Structure and DNA binding of single-strand annealing proteins by native MS: Zhaiho Qi 1, 2; Charles E. Bell 1, 2, Vicki H. Wysocki 1, 2; Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH; 1Resource for Native Mass Spectrometry Guided Structural Biology, Columbus, OH; 2Department of Biological Chemistry and Pharmacology, Columbus, OH | ThP 655 | Characterization of ligand – bond protein complexes using collisional-induced dissociation in tandem ion mobility spectrometry/mass spectrometry (tandem-TIMS/MS): Oluleni Samuel Arayobo 1, 2, Fanny C Liu 1, Christian Bleihder 1, 3Florida State University, Tallahassee, FL |
| ThP 645 | Mass spectrometric analysis of acoustically activated microdroplet mediated lipid-protein complex formation: Chayenne P. Sircher 1, 2, Ashton Taylor 1, Theresa Evans-Brizendine 1; Laboratory of Protein Science, Technology and Research (A*STAR), Singapore, 1University of Southern Denmark, Odense, Denmark; 2Russian Academy of Sciences, Moscow, Russia | ThP 660 | Exploring the potential of negative ion mode proteomics: an MS/MS-free approach using minute time scale analysis: Pelayo Alvarez Penanes 1, Vladimir Gorskiov 1, Mark V Ivanov 1, Mikhail V Gorskov 1, Frank Kieltsch 1, 2; University of Southern Denmark, Odense, Denmark | |
| ThP 646 | Quantifying protein co-assembly using Native Mass Spectrometry: Viktoria Sadowska 1, Justin Bencich 1, Dominik Saman 1; Department of Chemistry, University of Oxford, Oxford, United Kingdom | ThP 661 | Rapid identification of human alloantibody binding structure to human leukocyte antigen allele HLA-A*11 by cross-linking mass spectrometry: Zheng Ser 1, Yue Gu 1, Jiawei Yap 1, Yanting Lim 1, Shi Mei Wang 1, Nicholas RJ Gascogne 1, Paul A Macary 1, Bedrich Sobot 1, 2; Institute of Molecular and Cell Biology (IMCB), Agency for Science, Technology and Research (A*STAR), Singapore, Singapore; 1Department of Microbiology and Immunology, Yong Loo Lin School of Medicine, National University of Singapore, Singapore, Singapore; 2Singapore, Singapore | |
| ThP 647 | A microscale proximity-dependent biotinylation procedure for low cell input samples using protease-resistant streptavidin on a magnetic substrate: Brendon Seale 1, Reuben Samson 2, Ikas Gerber 1, Cassandra Wong 2, Anne-Claude Gingras 2, 3; Lufenen-Tandenbaum Research Institute at Mount Sinai Hospital, Sinai Health, Toronto, ON; 2University of Toronto, Toronto, ON; 3ReSyn Biosciences, Pretoria, South Africa | ThP 662 | Real-Time Bottom-Up Characterization of Protein Mixtures Enabled by Online Microdroplet-Assisted Enzymatic Digestion (MAED): Chih-Chen Hsu 1, 2, Chih-Lin Chen 1, 2, Fengqiang Wang 1, 2, 3, 4, 5; Department of Chemistry, National Taiwan University, Taipei, Taiwan | |
| ThP 648 | Measuring the Energies of Lipid Binding to Specific Sites on Membrane Proteins with Native MS and Mutant Cycles: Hir unay Li 1, Rosalind Ang 1, Fengqiang Wang 1, Hongxia Wang 1, 2, 3, 4, 5; University of California Irvine, Irvine, CA | ThP 663 | An in-depth plasma proteomics workflow powered by a Novel HRAM mass spectrometer: Amiransoor Hakimi 1, 2; Tabiawang N. Arrey 1, 2, Jeff Op De Beeck 1, 2, Bernard Delanghe 1, Sally Webb 1, Nicolaie Eugen Damoc 3, 4, 5; Thermo Fisher Scientific, San Jose, CA; 6Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; 7Thermo Fisher Scientific - Belgium, Ghent, Belgium | |
| ThP 649 | Building a contaminant repository for proximity proteomics: Julia Kitaygorodsky 1, 2, Vesal Kasmaefal 1, 2, Geoffrey Hesketh 1, 2, Ugo Dionne 1, 2, Reuben Samson 1, 2, William Hardy 1, Rawan Kalloush 1, Maria sedigi 1, Queenie Hu 1, Brendon Seale 1, Zhen-Yuan Lin 1, Cassandra Wong 1, Alexey I. Nesvitzhski 1, Anne-Claude Gingras 2, 3; Lufenen-Tandenbaum Research Institute at Mount Sinai Hospital, Sinai Health, Toronto, ON; 2Department of Molecular Genetics, University of Toronto, Toronto, ON; 3Department of Biochemistry and Molecular Biology, Dalhousie University, Halifax, NS; 4Department of Pathology, University of Michigan, Ann Arbor, MI | ThP 650 | Proximity labeling – mass spectrometry as a tool to define DDX3X interactomes and R-loop regulators: Thomas Beer 1, Hui Shen 1, Michael C. Owens 2, Qingqing Yan 1, Philip Fullridge 1, Kavitha Sarma 1, Kathy Fange Liu 1, Hsin-Yao Tang 1; The Wistar Institute, Philadelphia, PA; 2Department of Biochemistry and Biophysics, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA | |
| ThP 651 | Quantifying Binding of Multiple Protein-ssDNA Homologs Eliminates Ambiguity from Protein-Ligand Binding Measurements: Anthony Blue 1, Alex i Sadowska 1, Caroline Doherty 1, 2, 4, 5; Baylor University, Waco, TX | ThP 664 | A Fast and EfficientArginine-Specific Protease for Proteomic Applications: Chris Hofsfield 1, Jessica Wolffarth 1, Jennifer Guergues 1, Ethan Strauss 1, Michael M. Rosenblatt 1, Marijeta Urh 1, 2, 3, 4, 5; Promega Corporation, Madison, WI; 6University of South Florida, Tampa, FL | |
| ThP 652 | Integrated Probabilistic Scoring of Protein-Protein Proximity Data Illuminates the Function of Dark Kinases: Isaac B Plutzer 1, Dhaval P. Bhatt 1, Emily M. Wilkerson 1, Dennis Goldfarb 1, M. Ben Major 1; Washington University School of Medicine, St. Louis, MO | ThP 665 | Improving Depth of Coverage and Detection of Low-Level Host Cell Proteins in Biotherapeutic Development |
**THURSDAY POSTERS**

**ThP 664** Extracellular vesicles surfaceome profiling using a DTSSP cross-linking reagent and LC-ion-mobility mass spectrometry; Hiroyuki Katayama1; Taketo Kato2; Palihawadana Amungama3; Ranran Wu4; Yining Cai2; Fuchung Hsiao5; Johannes Fahrmann5; Jody Vyukoulak5; Sam Hanash1; The University of Texas, Department of Clinical Cancer Prevention, Houston, TX; 2Division of Thoracic Surgery, Nagoya University, Nagoya, Japan

**ThP 665** New and improved data acquisition schemes enabled by new functionalities of Real-Time Library Search on Orbitrap Tribrid instruments; Peter Mowldes1; Jenny Ho2; William Barshop1; Sebastian Gallien1; Jesse Canterbury1; Thermo Fisher Scientific, Edinburgh, United Kingdom; 2Thermo Fisher Scientific, Edenburgh, United Kingdom; 3Thermo Fisher Scientific, Hemel Hempstead, United Kingdom; 4Thermo Fisher Scientific, San Jose, CA; 5Thermo Fisher Scientific, Courtabeuf, France; 6Thermo Fisher Scientific, San Jose, CA

**ThP 666** A high-throughput plasma proteomics with high Resolution Data Independent Acquisition Method Across Multiple Orbitrap Mass Spectrometers; Rebecca Kiss1; Gabriel Castro2; Purvi Tandel2; Lucy Williamson3; Khatereh Motamedchaboki4; Eltaher Elgierari5; 6Seer Inc, Redwood City, CA; 7Seer, Inc, Redwood City, CA

**ThP 667** Comparing SP3 and SP4 Sample Preparation Techniques with a Sodium Dodecyl Sulfate-Assisted Digestion for Proteomic Profiling of MCF7 Subcellular Fractions; Jessica M Conforti1; Charli S. Worth1; Amanda M. Ziegler2; Joseph H. Taube3; Elyssie J. Frazier4; Baylor University, Waco, TX

**ThP 668** ADDoVenom: mass spectrometry at the heart of the development of a more effective innovative snakebite therapy based on virus-like particles; Fivos Gadiotis1; Dominique Blain2; Stefanie Menzies2; Nicholas R. Casewell2; Loic Quentin1; 1Laboratory of Mass Spectrometry, MolSys Research Unit, University of Liège, Liège, Belgium; 2GIGA Proteomics Facility, University of Liège, Liège, Belgium; 3Centre for Snakebite Research and Interventions, Liverpool School of Tropical Medicine, Pemboke Place, United Kingdom

**ThP 669** How sweet it is: Leveraging the nuclear envelope glycome for the automated extraction of proteins from cell nuclei; Julia E Robbins1; Christopher Ashwood1; Erin Brodenick1; Andrea Gutierrez2; Daniela Ganzani3; Lindsay K Pino3; Alexander J Fink1; 1The University of Texas, Department of Biochemistry and Molecular Genetics, University of Texas, Austin, TX; 2Miami Children's Research Hospital, Miami, FL; 3Children's Hospital of Eastern Ontario Research Institute, University of Ottawa, Ottawa, ON, Canada; 4Department of Internal Medicine, University of Manitoba, Winnipeg, MB; 5Department of Biochemistry and Medical Genetics, University of Manitoba, Winnipeg, MB; 6CancerCare Manitoba Research Institute, Winnipeg, MB

**ThP 670** A novel high-throughput plasma workflow facilitating fast and robust plasma proteome profiling; Katrin Hartinger1; Katharina Limm1; Zehan Hu1; Xaver Wurzenberger1; Sebastian H. Johannsson1; Nils A. Kulak1; PreOmincs GmbH, Planegg-Martinsried, Germany

**ThP 671** A high throughput 96 samples-per-day (SPD) workflow to quantify more than 7500 proteins from cells and complex samples; Jan Linnemann1; Giada Marino1; Felix Jose1; Till Kindel2; Mathieu Cyrille3; Xavier Meniche2; Florian Flennkenthaler1; Carleen M Kluger4; Ivan Silbern1; Thomas Wild1; Barbara Kracher1; Andreas Tebbe1; Nagarjuna Nagaraj5; 6Evotech München GmbH, Neuried, Germany; 7EVOTEC, Toulouse, France

**ThP 672** An Optimized Methodology of High-Throughput Shotgun Immunoproteomics for Antigen Identification; Nicholas A. Shortreed1; Anjali J. Panicker1; Kiran K. Mangalapurath1; Jun Zhong1; Akhilesh Pandey1; Leigh G. Griffiths1; 1Mayo Clinic, Rochester, MN

**ThP 673** Increasing the depth of single shot proteomics with enhanced data acquisition and processing strategies using a new Orbitrap Tribrid MS; David Bengen1; Jingjing Huang2; David Horn3; Daniel Hermanson4; Graeme C McAlister4; Romain Huguet4; Bernard Delanghe5; Vlad Zabrouskov5; 1Thermo Fisher Scientific, San Jose, California; 2Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; 3VICT Valco Instruments, Houston, TX

**ThP 674** A high-throughput and robust multi nanoparticle-based label-free mass spectrometry workflow for deep plasma proteomics at scale; Vé der J Garcia1; Biao Li1; Tianyu Cai1; 1University of Houston, Houston, TX; 2University of Texas Health Science Center at Houston, Houston, TX; 3VICT Valco Instruments, Houston, TX

**ThP 675** Early responses of human corneal and conjunctival epithelial cells to hyperosmotic stress; Guoping Qin1; Yunxin Fu2; Shara Duong1; Jennifer Copeland1; Chengzhi Yang2; 1University of Houston, Houston, TX; 2University of Texas Health Science Center at Houston, Houston, TX; 3VICT Valco Instruments, Houston, TX

**ThP 676** An Optimized Methodology of High-Throughput Shotgun Immunoproteomics for Antigen Identification; Nicholas A. Shortreed1; Anjali J. Panicker1; Kiran K. Mangalapurath1; Jun Zhong1; Akhilesh Pandey1; Leigh G. Griffiths1; 1Mayo Clinic, Rochester, MN

**ThP 677** A high throughput 96 samples-per-day (SPD) workflow to quantify more than 7500 proteins from cells and complex samples; Jan Linnemann1; Giada Marino1; Felix Jose1; Till Kindel2; Mathieu Cyrille3; Xavier Meniche2; Florian Flennkenthaler1; Carleen M Kluger4; Ivan Silbern1; Thomas Wild1; Barbara Kracher1; Andreas Tebbe1; Nagarjuna Nagaraj5; 6Evo- tech München GmbH, Neuried, Germany; 7EVOTEC, Toulouse, France

**ThP 678** Streamlined 2-min proteolytic digestion using a broad-specificity enzyme for super-fast relative and absolute quantitative proteomics; Helen Jiang1; Humberto Gonçarzowak-Jorge2; Ying Lao3; Victor Spicer3; John Wilson4; Andreas Roos4; 5René Zahedi4; 6, 7, 8Manitoba Centre for Proteomics and Systems Biology, Winnipeg, MB; 8Leibniz-Institut für Analytische Wissenschaften-ISAS e.V., Dortmund 44139, Germany, Dortmund, Germany; 9Profiti, LLC, Fairport, NY; 4Department of Neuropediatrics, Developmental Neurology and Social Pediatrics, Centre for Neuromuscular Disorders in Children, University Hospital Essen, Essen, Germany; 5Children’s Hospital of Eastern Ontario Research Institute, University of Ottawa, Ottawa, ON; 3Department of Internal Medicine, University of Manitoba, Winnipeg, MB; 6Department of Biochemistry and Medical Genetics, University of Manitoba, Winnipeg, MB; 4CancerCare Manitoba Research Institute, Winnipeg, MB

**ThP 679** Improvements in real-time dynamic single-molecule protein sequencing increase proteome coverage; Badri Singh1; Manjula Pandey2; Kathren Fink Croce3; Kenneth Skinner1; Maria Charron4; Haidong Huang5; Khanh D.Q. Nguyen6; Caixia Li7; Juan Felipe Beltran3; Brian D. Reed8; 1Quantum-Si, San Diego, CA

**ThP 680** Deep neuron-specific proteome profiling of AAV-mediated mice brain by two-step purification; Xue Zhang1; Huan Sun2; Yun Jiao3; Zhiping Wu4; Junmin Peng5; 1St Jude Children's Research Hospital, Memphis, TN; 2St. Jude Children's Research Hospital, Memphis, TN; 3St. Jude Children Research Hospital, Memphis, TN; 4St. Jude Children's Research Hospital, Memphis, TN; 5St. Jude Children's Research Hospital, Memphis, TN

**ThP 681** How sweet it is: Leveraging the nuclear envelope glycome for the automated extraction of proteins from cell nuclei; Julia E Robbins1; Christopher Ashwood1; Erin Brodenick1; Andrea Gutierrez2; Daniela Ganzani3; Lindsay K Pino3; Alexander J Fink1; 1The University of Texas, Department of Biochemistry and Molecular Genetics, University of Texas, Austin, TX; 2Miami Children's Research Hospital, Miami, FL; 3Children's Hospital of Eastern Ontario Research Institute, University of Ottawa, Ottawa, ON, Canada; 4Department of Internal Medicine, University of Manitoba, Winnipeg, MB; 5Department of Biochemistry and Medical Genetics, University of Manitoba, Winnipeg, MB; 6CancerCare Manitoba Research Institute, Winnipeg, MB

**ThP 682** A high throughput 96 samples-per-day (SPD) workflow to quantify more than 7500 proteins from cells and complex samples; Jan Linnemann1; Giada Marino1; Felix Jose1; Till Kindel2; Mathieu Cyrille3; Xavier Meniche2; Florian Flennkenthaler1; Carleen M Kluger4; Ivan Silbern1; Thomas Wild1; Barbara Kracher1; Andreas Tebbe1; Nagarjuna Nagaraj5; 6Evo- tech München GmbH, Neuried, Germany; 7EVOTEC, Toulouse, France

**ThP 683** Streamlined 2-min proteolytic digestion using a broad-specificity enzyme for super-fast relative and absolute quantitative proteomics; Helen Jiang1; Humberto Gonçarzowak-Jorge2; Ying Lao3; Victor Spicer3; John Wilson4; Andreas Roos4; 5René Zahedi4; 6, 7, 8Manitoba Centre for Proteomics and Systems Biology, Winnipeg, MB; 8Leibniz-Institut für Analytische Wissenschaften-ISAS e.V., Dortmund 44139, Germany, Dortmund, Germany; 9Profiti, LLC, Fairport, NY; 4Department of Neuropediatrics, Developmental Neurology and Social Pediatrics, Centre for Neuromuscular Disorders in Children, University Hospital Essen, Essen, Germany; 5Children’s Hospital of Eastern Ontario Research Institute, University of Ottawa, Ottawa, ON; 3Department of Internal Medicine, University of Manitoba, Winnipeg, MB; 6Department of Biochemistry and Medical Genetics, University of Manitoba, Winnipeg, MB; 4CancerCare Manitoba Research Institute, Winnipeg, MB

**ThP 684** A high-throughput and robust multi nanoparticle-based label-free mass spectrometry workflow for deep plasma proteomics at scale; Vé der J Garcia1; Biao Li1; Tianyu Cai1; 1University of Houston, Houston, TX; 2University of Texas Health Science Center at Houston, Houston, TX; 3VICT Valco Instruments, Houston, TX
**THURSDAY POSTERS**

**ThP 685**

Recovery, Identification and Quantitation of Low Starting Protein Quantities for Bottom-up MS Analysis in the ProTrap. Victoria Miller; Jessica L. Nickerson; Jean-François Noël; Sara Lashees Little; Angela Giraldo; Hugo Gagnon; Alliums Corporation, Halifax, NS; PhenomenX Biosciences Inc., Sherbrooke, QC.

**ThP 686**

High throughput total protein sequencing via multiprotease microdroplet digestion on commercially available ESI sources. Mathew Ellenberger; Anastasia Lindahl; Geltor, Emeryville, CA.

**ThP 687**

A simplified high throughput cell-based assay for increased proteomic coverage of cardiomyocytes. Saeed Seyedmohammad; Cedars Sinai Medical Institute, Los Angeles, CA.

**ThP 688**

Shredder: a new way to sequence. Alexandre Zougmann; John Wilson; University of Leeds, Leeds, United Kingdom.

**ThP 689**

Automated Container-less Cell Processing Method for Single-cell Proteomics. Cory J. Matsumoto; Xiniao Shao; Marko Bogosavljevic; Liang Chen; Yu Gao; University of Illinois at Chicago, Chicago, IL.

**ThP 690**

Development of a 3D-Printed Ionization Source for Single-Cell Analysis. Qinlei Liu; Sandra Martinez-Jarquin; Wenjie Ge; Renato Zenobi; Department of Chemistry and Applied Biosciences, ETH Zurich, Zurich, Switzerland.

**ThP 691**

An Optimized Workflow for TMT Based Single Cell Proteomics. Ruqi Jian; Tiffany Trinh; Lihua Jiang; Michael Snyder; Stanford University, Stanford, CA.

**ThP 692**

Single-cell lipidomics by miniature dual-LIT mass spectrometry system. Zhijun Cai; Ningxi Li; Simin Cheng; Xiaoxiao Ma; Zheng Ouyang; Tsinghua University, Beijing, China.

**ThP 693**

Label-free single-cell proteomics made easy. Ximena Sanchez-Avila; Madraon Johnston; Xiaofeng Xie; Thy Truong; Kei Webber; Nathaniel A. Axtell; Verónica Puig-Sanvisens; Ryan T. Kelly; Brigham Young University, Provo, UT; HP Inc., Corvallis, Oregon.

**ThP 694**

Assessing quantitation strategies for single-cell equivalent protein amounts. Krishnatej Nshitala; Adrian Neil; Alex Demarco; Ralf B Schittenhelm; Monash Proteomics & Metabolomics Facility, Biomedicine Discovery Institute, Monash University, Melbourne, Australia; Department of Biochemistry and Molecular Biology, Biomedicine Discovery Institute, Monash University, Melbourne, Australia; Dept. of Mechanical and Aerospace Engineering, Monash University, Melbourne, Australia.

**ThP 695**

Online solid phase microextraction-capillary zone electrophoresis-tandem mass spectrometry system for single-cell proteomics. Jorge Colon-Rosado; Liangliang Sun; Michigan State University, East Lansing, MI.

**ThP 696**

Extending coverage in multiplexed single-cell proteomics. Jingjing Huang; Benjamin Furtwangler; Nil Uresin; Graeme C McAlister; Wang Xiao; Mike Goodwin; Jeff Op De Beeck; Natalie Van Landuyt; David Bergen; Vlad Zabrouska; Romain Huguet; Bo Persson; Enine M. Schoof; Thermo Fisher Scientific, San Jose, California; Copenhagen University, Copenhagen, Denmark; Thermo Fisher Scientific - Belgium, Ghent, Belgium; Technical University of Denmark, Copenhagen, Denmark.

**ThP 697**

Improving single-cell proteome profiling depth using single-site proteases. Marion Pang; Jeff Jones; Nicole Kubat; Ting-Yu Yang; Basu Ou; Yanping Qiu; Tsu-Fen Chou; Michael L. Roukes; California Institute of Technology, Pasadena, CA.

**ThP 698**

Accelerated Liquid Chromatography Gradient Generation with Constant-Pressure Elution Improves Sensitivity and Throughput for Single-Cell Proteomics. Ryan Kelly; Xiaofeng Xie; Thy Truong; Yiran Liang; Madisyn Johnston; Kei Webber; Brigham Young University, Provo, UT.

**ThP 699**

Investigating the Metabolism of Heterogeneity of Cancer Single-Cell Using Functional Single-Cell Selection and nLC Combined with Multinozzle Emitter Mass Spectrometry. Cheng Kai-Wen; Su Pin-Rui; Chien Miao-Ping; Hsu Cheng-Chih; Department of Chemistry, National Taiwan University, Taipei, Taiwan.

**ThP 700**

A Novel Design for Cheap Robust Pre-Formed Step Gradient LC System. Sige Huang; Kei Webber; Xiaofeng Xie; Thy Truong; Ryan Kelly; Brigham Young University, Provo, UT.

**ThP 701**

High Field Asymmetric Waveform Ion Mobility Spectrometry enhances sensitivity for single cell proteomic analyses. Eric Bonneil; Jiali Peng; Michael Belford; Cornelia Boeser; Jean-Jacques Dunyach; Etienne Caron; Aaron Wheeler; Pierre Thibault; Institute of Research in Immunology and Cancer, Université de Montréal, Montreal, QC; Institute of Biomedical Engineering, University Of Toronto, Toronto, ON; Thermo Fisher Scientific, San Jose, California; CHU Sainte Justine Research Center, Montreal, QC; Department of Chemistry, Université de Montréal, Montreal, QC.

**ThP 702**

Single Cell Proteome using novel Glass-Oil-Air-Droplet chip and its application on embryo development. Liu Zhu; Catherine C. L. Wong; Department of Biochemistry and Biophysics, Peking University Health Science Center., Beijing, China; Peking-Tsinghua Center for Life Sciences, Beijing, China; Department of Medical Research Center, State Key Laboratory of Complex Severe and Rare Diseases, Peking Union Medical College Hospital, Chinese Academy of Medical Science & Peking Union Medical College, Beijing, China.

**ThP 703**

Detection and Quantification of Viral Proteins in Infected Cells by Single Cell Proteomics. Akos Vegvari; Soham Gupta; Ujwial Neogi; Jimmy E Rodriguez; Roman A Zubarev; Karolinska Instituted, Stockholm, Sweden.

**ThP 704**

Comparison of two sampling modes for single-cell metabolomics reveals alterations in senescent cells. Catia Marques; Francesca Castoldi; Liangwen Liu; Federico Pirotrello; Ingela Lanekoff; Uppsala University, Uppsala, Sweden; Stockholm University, Stockholm, Sweden; Uppsala University, Uppsala, Sweden.

**ThP 705**

Top-down proteomic analysis of amount-limited samples and single cells using ultra-narrow bore open-tubular nanoflow liquid chromatography columns. Michael Gregus; Yunfan Gao; Somak Ray; Alexander R. Ivanov; Northeastern University, Boston, MA.

**ThP 706**

Seamless integration of chip-based single-cell sample preparation with high-throughput liquid chromatography and diaPASEF acquisition improves sensitivity and reproducibility. Claudia Ctoerteck; Anjali Seth; Michael A. Gillette; Namrata D. Udeshi; Steven A. Carr; Broad Institute of MIT and Harvard, Cambridge, MA; Cellion SANS, Lyon, France; Massachusetts General Hospital, Boston, MA.

**ThP 707**

Highly Streamlined Chip-DIA Strategy for Microscale Phosphoproteomics from Small Cell Population to Single Cell; Gul Muneer; Sofani Tafesse Gebreyesus; Ciao Syuan Chen; Tzu Tsung Lee; Hsiung Lin Tu; Yu Ju Chen; Institute of Chemistry, Academia Sinica, Taipei, Taiwan.

**ThP 708**

Lipid signatures and inter-cellular heterogeneity of naïve and lipopolysaccharide-stimulated human microglia-like cells. Max Alexander Mueller; Norman Zweig; Bernhard Spengler; Maria Weinert; Sven Heiles.
ThP 709
High sensitivity top-down proteomics toward single cell analysis; Zhan Gao1; Jake A Melby2; Kalina J Reese2; Mallory C Wilson2; Daiqiao Wang3; Ying Ge2; 1UW-MADISON, Madison, WI; 2UW-Madison, Madison, WI; 3Newomics, Berkeley, CA

ThP 710
Optimization of targeted proteomics for single glomerulus measurements; Chris Hsu1; Lilian R. Heil1; Philip M Remes2; Ping Yip2; Jesse D. Canterbury3; Christine C. Wu1; Mariya T. Sweetwynne1; Michael J. MacCoss1; 1University of Washington, Seattle, WA; 2Thermo Fisher Scientific, San Jose, California

ThP 711
Combining single-cell mass spectrometry and transferable meta-learning framework to predict cell phenotypes; Yunpeng Lan1; Tra D. Nguyen1; Songyuan Yao1; Yihan Shao1; Zhibo Yang1; 1University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK

ThP 712
Improving protein quantification for single cell proteomics; Hannah Boekweg1; Alexander Solivais1; Daisha Van Der Watt2; Sarah Furnsley3; Aniswa R. Mongane4; Michael R. Shortreed5; Sam Payne1; 1Brigham Young University, Provo, UT; 2University of Wisconsin-Madison, Madison, WI

ThP 713
Nano-LC-MS based lipidomics for Single Cell Applications; Rahul Ravi Deshpande1; Bashar Amer1; Amirnassor Hakimi1; Jeff Op De Beeck2; Thomas Moehring3; Susan Bird4; 1Thermo Fisher Scientific, San Jose, California; 2Thermo Fisher Scientific, Bremen, Germany

ThP 714
Short and Long-term Stability of Aromatic Amines in Human Urine; Shriha Mazumder1; Rayaj A. Ahamed1; Tiffany H. Seyler1; Lanqing Wang1; 1Centers for Disease Control and Prevention, Atlanta, GA

ThP 715
Quantification of boronic acids at pg/mL levels of sensitivity; Jack Steed1; SICIEx, Macclesfield, United Kingdom

ThP 716
Sensitive quantification of the protein targeting chimera (PROTAC) TL 13-112 in rat plasma using an LC-MS/MS workflow; Ebru Seilen1; Rahul Baghla1; Eshani Nandita2; 1SICIEx, Redwood City, CA; 2SCIEx, Bangalore, India

ThP 717
Internal Standard Quantiﬁcation of Cardiotonic Steroid Telocinobutelogan in Rat Urine using UHPLC-Orbitrap-MS; Sabriti Lamichhane1; Dhihlani Faleel1; Steven T. Haller2; David J. Kennedy2; Dragan Isaiovic1; 1University of Toledo, Toledo, OH

ThP 718
A sensitive method for the quantification of formoterol in human plasma; Santhosh Pillai1; Lakshmanan Deenadayalan1; Rahul Baghla1; Elliott Jones2; Eshani Nandita2; 1SICIEx, Bangalore, India; 2SCIEx, Redwood City, CA

ThP 719
Low-level quantification of 10 mutagenic nitrosamine impurities in Pioglitazone hydrochloride using accurate mass spectrometry; Eshani Nandita1; Rahul Baghla1; Lakshmanan Deenadayalan1; Jack Steed2; 1SICIEx, Redwood City, CA; 2SCIEx, Bangalore, India

ThP 720
CESI-MS QTRAP Quantification of the Astrocyte Glio-Transmitter Dipeptide-Binding-Inhibitor and its Bioactive Fragment Octadecaneuropeptide in Small-Volume Rat Brain Tissue Samples; Madhu Babu Paisula1; Khaggwar Bheemanevalapally1; George Mattheolabakis1; Karen P. Brisik1; 1University of Louisiana Monroe, Monroe, LA

ThP 721
Improved Quantitative Analysis of Amino Acids from Dried Blood/Plasma Spot (DPS) with Imprinted Internal Standards by SRM-FIA; Wengian Li1; Donald Chace2; 1University of Florida, GAINESVILLE, FL; 2Capitainer, Stockholm, Sweden

ThP 722
Enhanced production of surfactin using cassava wastewater and hydrophobic inducers: a prospect on new homologues; Vanessa Kristine De Oliveira Schmidt1; Paulo Alexandre Durant Moraes1; Lidiane Maria Andrade2; Maria Anita Mendes2; Débora De Oliveira1; Cristiano José Andrade1; 1Department of Chemical Engineering and Food Engineering, Federal University of Santa Catarina (UFSC), Florianópolis, Brazil; 2Dempster MS Lab, Chemical Engineering Department of Polytechnic School of University of São Paulo (USP), São Paulo, Brazil

ThP 723
Using a compact benchtop Time of Flight Mass Spectrometer(TOF) for rapid accurate mass information in a walk-up environment; Chris Henry1; Ashley Sage2; Scott Campbell2; 1Waters Corporation, Wilmilso, United Kingdom; 2SpectralWorks Limited, Runcorn, United Kingdom

ThP 724
Confirmation of Statin and Fibrate use from Small-Volume Archived Plasma Samples by Rapid LC-MS/MS Detection; Jennifer Kusovschi1; Michael Gardner1; Susan Kuklenyik1; Anna Ivanova1; John R Barr1; 1Center for Disease Control and Prevention, Atlanta, GA

ThP 725
LC/MS/MS Quantiﬁcation of Benzenesulfonic Acid in Rat Plasma; Rachel Sun1; Billie Patton1; Antonio Conzo2; Gabriele Garretta2; Melarosa Fede2; Ines C. D’Antonio1; 1Mass Spectrometry Laboratory, Henderson, NV; 2Chemates Consulting SP, Via Ribes,5, Italy

ThP 726
Three critical parameters in reducing peak suppression when performing analysis in complex matrices using LDTD-MS/MS; Jonathan Rochon1; Serge Auger1; Eshwar Jaadeero2; 1Phytonix Technologies Inc., Quebec, CA; 2FBI, Quantico, VA

ThP 727
A Rapid LC-MS/MS Screening Method for Simultaneously Detecting Ten Antiretroviral Drugs; Amanda P Schauer1; Craig Sykes2; Mackenzie Cottrell1; Angela DM Kashuba1; 1University of North Carolina at Chapel Hill, Chapel Hill, NC

ThP 728
Strategies To Minimize Epimerization During Extraction of Carnbonyl Chiral Compound in Human Plasma; Moo-Young Kim1; Garfield Simon2; Katty Wain1; Penelope Crowner1; Haihong Shi2; Olga Kavetska3; 1PDD, Middleton, WI; 2Pfizer Inc., San Diego, CA; 3Pfizer Inc., Groton, CT

ThP 729
Microfluidic Capillary Electrophoresis-Mass Spectrometry Method Development for Quantiﬁcation of Spermidine in Whole Blood; Jericha Mill1; Thomas Hauser1; Lingjun Li2; 1University of Wisconsin-Madison, Department of Chemistry, Madison, WI; 2University of Wisconsin School of Medicine and Public Health, Department of Pathology and Laboratory Medicine, Madison, WI

ThP 730
Analysis of DNPH-derivatized Aldehydes and Ketones using Agilent IQ Single Quadrapole LC MS; Sue D’Antonio1; Nikolai C. Lau1; Greg Thompson2; 1Agilent Technologies, Cedar Creek, TX; 2Agilent Technologies, Wilmington, Delaware

ThP 731
A new and innovative quality test for potency and contamination in cannabis flowers, concentrates and oils by LC-MS/MS; Claudia C Beck1; Matthew R McIntyre2; Erling Beck2; Dennis G Hooper2; 1Realtime Laboratories, Carrollton, TX; 2The University of Texas at Dallas, Richardson, Texas

ThP 732
Improvement upon a multi-residue method for Nitrosamine analysis in Losartan drug product using an enhanced LC/MS/MS system; Lee Bertram1; Linfeng Wu2; Shan-An Chari1; Winnie Huang1; 1Agilent Technologies, Santa Clara, CA; 2Agilent Technologies, Taipei, Taiwan; 3Agilent Technologies, Inc, Guangdong, China
LC-MS/MS Method for Quantification of Three Intracellular Antiretroviral Metabolites: Lamivudine Triphosphate, Carbovir Triphosphate, and Tenofovir Diphosphate in Human Whole Blood; Craig Sykes; Winstone Nyandiko; Amanda P. Schauer; Mackenzie L. Cottrell; Ashley Chory; Josephine Aluoch; Vlad Novitsky; Joel Hague; Festus Sang; Celestine Ashimosi; Eslyne Jepkemboi; Millicent Orido; Edwin Sang; Allison Delong; Rachel Vreeman; Rami Kantor; Angela DM Kashuba; 1 UNC Chapel Hill, Chapel Hill, NC; 2 Moi University College of Health Sciences, Eldoret, Kenya; 3 Academic Model Providing Access to Healthcare (AMPATH), Eldoret, Kenya; 4 Icahn School of Medicine at Mount Sinai, New York, NY; 5 Brown University Alpert Medical School, Providence, RI; 6 Brown University School of Public Health, Providence, RI

An Easy Derivatization To Block The Oxidation In The Quantitation of Catechol Compounds; Aman Parashar; Xuguang Yan; Moo-Young Kim; 1 PPD, Middleton, WI
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Computational Mass Spectrometry

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University of California, San Diego
David Fenyo
New York University School of Medicine
Olga Vitek
Northeastern University

October 13 - 16, 2023
Asilomar Conference Center • Pacific Grove, CA

34TH Sanibel Conference on Mass Spectrometry

Mass Spectrometry for Complex Mixtures in Energy and the Environment

Organizers
Janne Janis
University of Eastern Finland
Amy McKenna
Nat’l High Magnetic Field Laboratory

January 21 - 24, 2024
Hilton St. Petersburg Bayfront
St. Petersburg, Florida
34th FALL WORKSHOP ON MASS SPECTROMETRY

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November 6 - 7, 2023
Omni Royal Orleans, New Orleans, LA

ORGANIZERS

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Jace W. Jones, University of Maryland
JUNE 2 - 6, 2024
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