Welcome to the 66th ASMS Conference on Mass Spectrometry and Allied Topics. Conference program activities and exhibit booths are in the San Diego Convention Center. Corporate Member hospitality suites are located in the Hilton San Diego Bayfront.

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

Registration, Sails Pavilion upper level, is open 2:00 - 5:00 pm on Saturday, 10:00 am - 8:00 pm on Sunday, and 7:30 am - 4:45 pm Monday - Thursday.

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

4:00 - 4:45 pm, Sunday, Ballroom 20A upper level
Plan Your Strategy: What to See and Do at ASMS

TUTORIALS

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

Hall D ground level

5:00 - 5:45 pm
Strategies for Quantitative Proteomics

M. Arthur Moseley
Duke University School of Medicine

5:45 - 6:30 pm
Mass Spectrometry and the Environment

Susan D. Richardson
University of South Carolina

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

Ballroom 20A upper level

5:00 - 5:45 pm
Mass Spectrometry and Nuclear Forensics

Gregory Eiden
Pacific Northwest National Laboratory

5:45 - 6:30 pm
From the Laboratory to the Stars

Jack Beauchamp
California Institute of Technology

PLENARY SESSIONS

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

Hall D ground level

Welcome

Richard A. Yost
University of Florida
ASMS Vice President for Programs

Smart Trials: Moving from a Site-centric to Patient-centric Clinical Trials

Lisa Shipley
Pharmacokinetics, Pharmacodynamics & Drug Metabolism, Merck

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

Poster/Exhibit Hall ground level. Conference name badge is required.

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

Hall D ground level

Award for a Distinguished Contribution in Mass Spectrometry

Gert von Helden, *Fritz-Haber Institut der Max Planck-Gesellschaft*

Martin Jarrold, *Indiana University*

David Clemmer, *Indiana University*

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

Hall D ground level

Biemann Medal

Benjamin A. Garcia
University of Pennsylvania Perelman School of Medicine

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

Hall D ground level

The Fight Against Doping: From Strychnine to Turinabol

Larry Bowers
LD Bowers, LLC

Thursday Closing Event at the USS Midway, 6:30-9:00 pm, $30/person

Tickets must be purchased in advance by Monday 12 noon. Join us for an incredible evening aboard the USS Midway, a retired aircraft carrier turned museum. In addition to a buffet dinner on the flight deck there will be docents to share the Midway's history & exhibits, plus a variety of flight simulation games.

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

Ground Level
Session A (MOA, TOA, WOA, ThOA).....Hall D

Upper Level
Session B (MOB, TOB, WOB, ThOB) ..... Ballroom 20A
Session C (MOC, TOC, WOC, ThOC) ..... Ballroom 20BC
Session D (MOD, TOD, WOD, ThOD) .....Ballroom 20D
Session E (MOE, TOE, WOE, ThOE) ..... Ballroom 6A
Session F (MOF, TOF, WOF, ThOF)..... Ballroom 6B
Session G (MOG, TOG, WOG, ThOG) .....Ballroom 6CF
Session H (MOH, TOH, WOH, ThOH) ..... Ballroom 6DE

Oral Presentations are projected from ASMS computers using the 16:9 aspect ratio. There will be a PC and a Mac laptop available for speakers. Speakers are required to use the ASMS computers for their presentations.

Speakers must load presentations at least one day prior to their talks. The Speaker Ready Room is located in Room 11B, upper level. The room is open with a technician according to this schedule:

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

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

Sunday Welcome Reception....7:45 pm - 9:00 pm
Monday - Wednesday .....7:00 am - 8:00 pm
Thursday .....7:00 am - 2:30 pm

Poster Set-Up is 7:00 - 8:00 am on the day scheduled. **Refer to the poster numbers in this final program for board assignments.** A counter for poster supplies is near the main entrance to the Hall.

History Posters are on display all week in Sails Pavilion upper level.

Poster Sessions are 10:30 am - 2:30 pm, Monday through Thursday in the Poster/Exhibit Hall ground level.

Poster Authors must be present at posters on scheduled days at the scheduled presentation times. The following is NEW for 2018 and allows for a one-hour non-overlapping lunch break. All presenters are now scheduled for 3 hours (authors welcome to attend the full four hours).

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

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

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

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

Posters should be removed between 7:00 - 8:00 pm on Monday, Tuesday and Wednesday. Thursday posters should be removed between 2:30 - 3:00 pm.

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

Workshops are 5:45 - 7:00 pm on Monday, Tuesday, and Wednesday. Light refreshments are provided in the Sails Pavilion upper level.

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

Special Program for Undergraduate Students

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

Free Wifi Access and Internet Stations are available throughout the convention center.

Conference Proceedings will be published online. Upload of PDF for all posters and talks are due by June 11. Submission to the proceedings does not constitute publication and does not jeopardize the rights of authors to publish contents of their submissions. **Speaker slides will be printed to PDF and used as proceedings submission for speakers who fail to submit on their own.**

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

Corporate Hospitality Suites are open 8:00 – 11:00 pm, Monday through Wednesday. Suites are located in the **Hilton San Diego Bayfront.**

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

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

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

Gender Neutral Restroom is available on the ground level, Lobby A (directly across from the Lobby A Starbucks).

Mother’s Room is located inside the Women’s Restroom on the ground level, Lobby E (near the Lobby E Starbucks).

Visit *JASMS* booth number 215 and become a 'Face of Mass Spectrometry' – Get your own headshot photo for free!
JASMS launched a new monthly feature, 'Faces of Mass Spectrometry', in March 2018. Are you still using your high school graduation photo? Come to the JASMS booth and in a few minutes you will have a professional head shot. The finished photo will be emailed to you for your personal use.

Two Important Opportunities in the Poster/Exhibit Hall

1. **INFORMATICS HUB**
   Sign up with experts to discuss your specific questions. Check the wiki for schedule of programs and experts (https://github.com/CompMS/Overview/wiki/ASMS-2018).
2. **FUNDING AGENCY "OFFICE HOURS"**
   Consult with heads from the major U.S. funding agencies.

Conference Regulations

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

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

No smoking is permitted in the convention center.

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

No photography or recording is allowed in oral sessions or in the Poster/Exhibit Hall.

Parents. Planned conference sessions and hospitality suites may not be appropriate for children. Please respect the interests of your colleagues by allowing them to attend activities without disruption and without concern for the safety of children. Strollers, child backpack carriers or similar devices for child transport are prohibited in the Poster/Exhibit Hall and hospitality suites.

Material presented or displayed at the ASMS Conference, including but not limited to orals, posters, workshops, exhibit booths and hospitality suites, is the intellectual property of the presenter and may not be recorded, photographed, quoted, disseminated or transmitted by summary in any form without express written authority of the author.

The placement of advertising in the meeting area is prohibited. There are poster boards and tables in the Poster/Exhibit Hall for approved announcements.

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

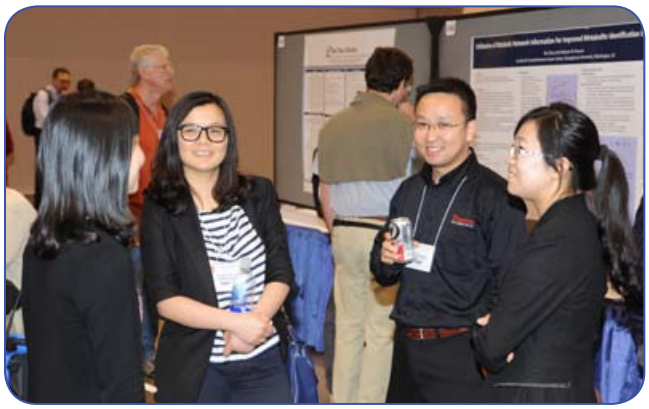
Designated publisher tables in the conference registration area are for the display of books and journals and must be reserved in advance.

There are tables in the registration area for authors who wish to display their books. Authors may use a table to promote their books, sign copies, and speak with members. Table space must be reserved at conference registration.

No organized activities (even off-site) other than those approved by ASMS are allowed during the conference week (5:00 pm on Sunday through 6:00 pm on Thursday).

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

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



Hotel	Telephone
1. Hard Rock Hotel San Diego	(619) 702-3000
2. Hilton San Diego Bayfront	(619) 564-3333
3. Hilton San Diego Gaslamp Quarter	(619) 231-4040
4. Hotel Palomar San Diego	(619) 515-3000
5. Hotel Solamar	(619) 819-9500
6. Manchester Grand Hyatt San Diego	(619) 232-1234
7. Residence Inn Bayfront	(619) 831-0225

Hotel	Telephone
8. San Diego Marriott Gaslamp Quarter	(619) 696-0234
9. Sheraton San Diego Hotel & Marina	(619) 291-2900
10. Springhill Suites Bayfront	(619) 831-0224
11. Westgate Hotel	(619) 238-1818
12. Westin San Diego Gaslamp Quarter	(619) 239-2200
13. Wyndham San Diego Bayside	(619) 232-3861

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Congratulations

to these members who were elected to the ASMS Board

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Jennifer Watson
Adrienne Kerr, Lola Priest, Miquela Sena,
Nikko Sisneros, Brent Watson

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Bioinformatics for MS	Isabel Bludau Samuel Payne
Biotherapeutics	Charles Cheng Andrew W. Dawdy
Clinical Chemistry	Tim Garrett
Data Independent Acquisition	Ben Collins Hannes Röst
Drug Metabolism & Pharmacokinetics	Mark Cancilla Jonathan Josephs
Energy, Petroleum & Biofuels	Marianny Y. Combariza David Stranz
Environmental Applications	Achille Cappiello Imma Ferrer, Andrew Ottens
Exposomics	H. M. Skip Kingston Jarrod Grossman
Flavor, Fragrance and Foodstuff	Melanie Downs Sara Kern
Forensics & Homeland Security	Kenyon Evans-Nguyen Chris Mulligan
FTMS	Melinda McFarland Matthew B. Renfrow
Fundamentals	Christian Bleiholder Victor Ryzhov
H/D Exchange, Covalent Labeling & Cross Linking	Lan Huang Kasper D. Rand
Imaging MS	Reid X. Groseclose Martina Marchetti-Deschmann
Ion Mobility MS	Brian Clowers Valerie Gabelica
Ion Trap MS	Glen Jackson Wei Xu
LC/MS Related Topics	Eric Soderblom Will Thompson
Lipids & Lipodomics	Eva Duchoslav Todd Mitchell
Metabolomics	John A. Bowden Gary Patti
Metal Ion Coordination Chemistry	Eric Dodds Nicolas Polfer
Oligonucleaotides & Nucleic Acids	Samuel Wainhaus Laixin Wang
Pharmaceuticals	Andrew W. Dawdy John Valliere-Douglass
Photoionization MS	Sven Ehlert Eleanor Riches
Polymeric Materials	Christina Mastromatteo Stephen Rumbelow
Regulated Bioanalysis	Fabio Garofolo Jian Wang
Top-Down Proteomics	Paul Martin Thomas Nicholas Young
Undergraduate Research in MS	Christine Hughey James Pesavento
Young Mass Spectrometrists	Veronica Anania Doug Phanstiel

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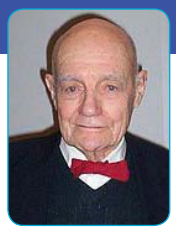
Education	John McLean, Chair Matt Crowe Travis Falconer Megan Gessel Laura Sanchez
History	P. Jane Gale, Chair Miriam ElNaggar David Sparkman Ken Tomer Al Yergey Michael Grayson, *ex-officio*
Nominating	Scott McLuckey, Chair Kristina Håkansson Hee-Yong Kim Roy Martin Nick Polfer
Publications	Amanda B. Hummon, Chair Valerie Gabelica Jody C. May Peter Nemes Olga Ovchinnikova Joseph Loo, *ex officio*
Sanibel Conference	Melinda McFarland Victor Ryzhov Shi Stone Ying Ge (ASMS Board Rep.)

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

2018 Recipients: Gert Von Helden, Martin F. Jarrold, and David E. Clemmer

Award Lecture: 4:45 pm, Monday, Hall D ground level



The ASMS Award for Distinguished Contribution in Mass Spectrometry has been renamed to honor the memory of John B. Fenn who shared the 2002 Nobel Prize for the development of electrospray Ionization. John joined ASMS in 1986 and remained an active member until his passing in 2010.

Dr. von Helden

Dr. Jarrold

Dr. Clemmer

Dr. Gert von Helden, Dr. Martin F. Jarrold, and **Dr. David E. Clemmer** are the recipients of the 2018 John B. Fenn ASMS Award for a Distinguished Contribution in Mass Spectrometry for their pioneering contributions to the development of ion mobility spectrometry (IMS).

Dr. von Helden made a major development in IMS when he applied it to the self-assembly of carbon in plasmas, and showed that carbon structurally evolved from linear chains to rings to fullerenes. Of critical importance, he used quantum chemical approximation methods to obtain model structures, adapted the little-known projection approximation method to obtain collision cross sections, and got excellent agreement with his experimentally measured cross sections. Soon after Dr. Jarrold applied similar IMS methods to silicon and aluminum assembly, and along with Dr. von Helden, showed that fullerenes are formed from activation of carbon ring systems, not C2 addition to graphitic fragments as Smalley had proposed. Dr. Jarrold went on to develop the first high-resolution instrument and, importantly, a more accurate method (the trajectory method) for obtaining collision cross-sections from complex structures such as biomolecules. While these fundamental developments were taking place, Dr. Clemmer realized that these new IMS methods could be utilized for analytical applications, and developed a new "nested" IMS-MS technology, which used ion trapping methods to dramatically increase signal-to-noise ratio and post-IMS dissociation to obtain fragmentation patterns of isomers (or conformers) in a single experiment. These ideas were later incorporated into highly successful commercial instruments, which have made advanced IMS methods available to thousands of labs around the world.

Dr. Gert von Helden is Group Leader at the Department of Molecular Physics, Fritz-Haber Institut der Max Planck-Gesellschaft, Berlin, Germany and professor at the Radboud University, Nijmegen, the Netherlands.

Dr. Martin F. Jarrold is Professor and Robert & Marjorie Mann Chair, Department of Chemistry, Indiana University.

Dr. David E. Clemmer is Distinguished Professor, Department of Chemistry, Indiana University.

RON A. HITES AWARD FOR AN OUTSTANDING RESEARCH PUBLICATION IN JASMS

Award Presentation: ASMS Meeting, 4:45 pm, Wednesday, Ballroom 20A upper level

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

The 2018 Award recognizes **Peter B. Armentrout**, University of Utah and co-authors for their paper **How Hot are Your Ions Really? A Threshold Collision-Induced Dissociation Study of Substituted Benzylpyridinium "Thermometer" Ions**; John E. Carpenter, Christopher P. McNary, April Furi, Andrew F. Sweeney, P. B. Armentrout; *Department of Chemistry, University of Utah, Salt Lake City, UT*; *JASMS* Vol. 28, Sept 2017, pp. 1876-1888, DOI 10.1007/s13361-017-1693-0.

BIEMANN MEDAL
2018 Recipient: Benjamin A. Garcia
Award Lecture: 4:45 pm, Tuesday, Hall D ground level

Dr. Benjamin A. Garcia is the recipient of the 2018 Biemann Medal for contributions to elucidation of the "histone code", the set of posttranslational modifications (PTMs) to histone proteins that are thought to regulate gene expression. The Garcia lab has developed a number of experimental and computational methods to detect novel histone PTMs, quantify their relative abundances, monitor *in vivo* histone PTM dynamics, and characterize distinct histone PTMs on specific genome locations.

Dr. Garcia has pioneered high-throughput "bottom-up" proteomic methods for detection of histone PTMs and quantitative comparison of multiple cellular states, and "middle down" proteomic approaches that facilitate computation of specific combinatorial histone proteoforms. These methods have made unique impact in chromatin biology and epigenetics research, and have been fully embraced by a growing number of research groups from all over the world.

Dr. Garcia is the Presidential Professor of Biochemistry and Biophysics at the University of Pennsylvania Perelman School of Medicine.

2018 RESEARCH AWARDS
Award Presentations: 4:45 pm, Tuesday, Hall D ground level

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

Sponsored by
Thermo Fisher Scientific

Michael T. Marty
University of Arizona

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James S. Prell
Oregon State University

2018 POSTDOCTORAL CAREER DEVELOPMENT AWARDS

Award Presentations: ASMS Meeting, 4:45 pm, Wednesday, Ballroom 20A upper level

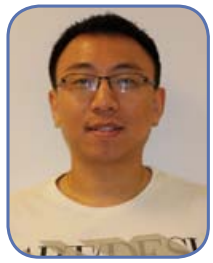
Up to five awards in the amount of $10,000 each are intended to promote the professional career development of postdoctoral fellows in the field of mass spectrometry. Activities funded by these awards include conference and workshop attendance, travel to other mass spectrometry laboratories, purchase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

Martha Chacón-Patiño
National High Magnetic Field Laboratory
Florida State University

Mac Gilliland
University of North Carolina at Chapel Hill

Alan Jarmusch
University of California, San Diego

Shen Zhang
Lunenfeld-Tanenbaum Research Institute at Mount Sinai Hospital
University of Toronto



Yanlong Zhu
University of Wisconsin-Madison

2018 STUDENT AWARDS

Award Presentations: ASMS Meeting, 4:45 pm, Wednesday, Ballroom 20A upper level

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

Graduate Student Awards

Rodell Barrientos, University of North Carolina, Greensboro

Isabell Bludau, ETH Zürich

Wenxuan Cai, University of Wisconsin-Madison

Maria Emilia Dueñas, Iowa State University

Lidong He, Florida State University

Camille Lombard-Banek, University of Maryland

Damon May, University of Washington

Logan Plath, Carnegie Mellon University

Mei Sun, University of Oklahoma

Kenneth Swanson, University of North Carolina,Chapel Hill

Undergraduate Student Awards

Amanda Bubas, Duquesne University

Devon Colby, University of Oklahoma

Liam Dugan, Allegheny College

Christopher Gongar, University of Florida

Connor Graca, Duquesne University

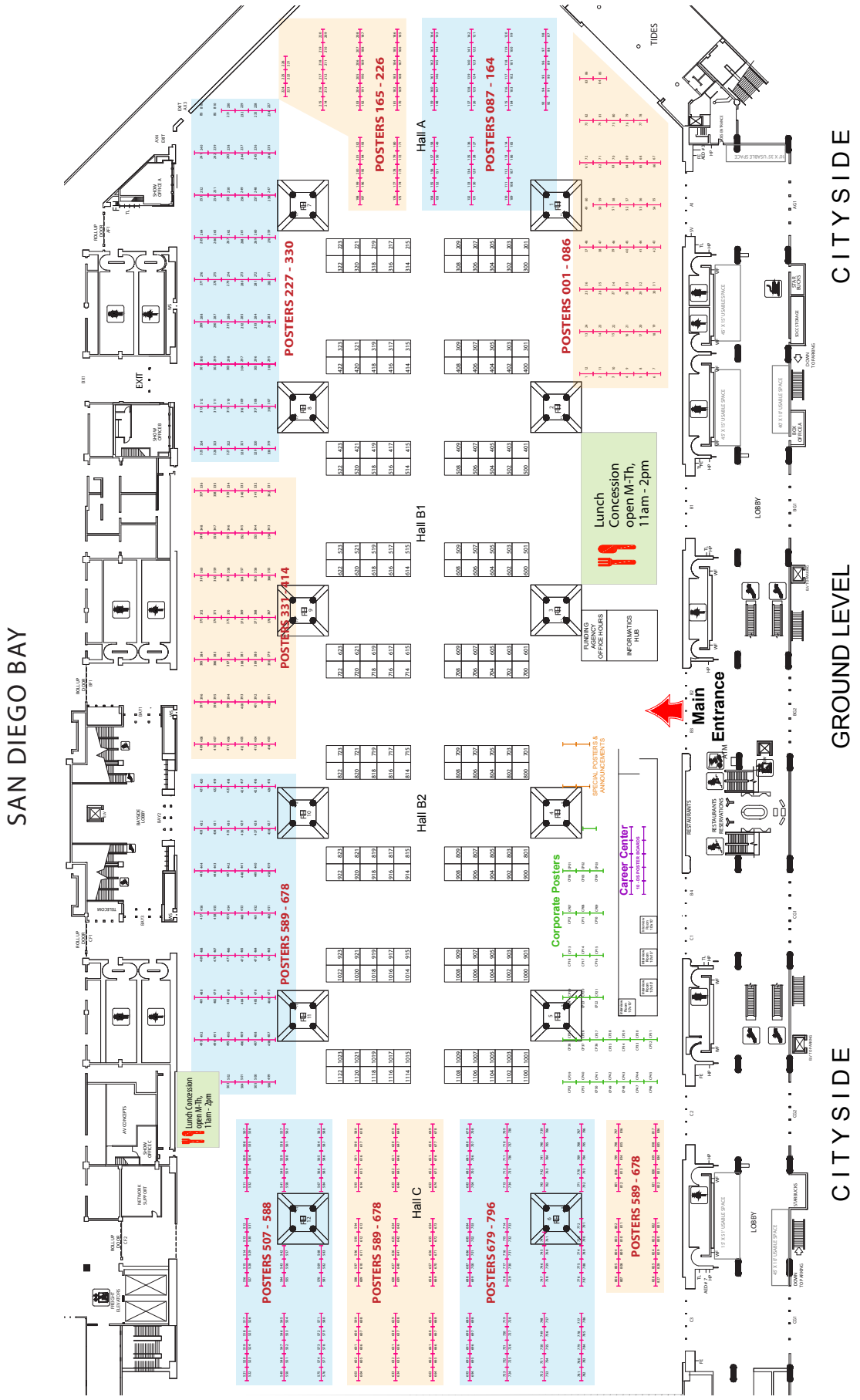
Petra Paizs, Imperial College London

Sanjit (Sunny) Uppal, University of Washington

Nikit Venishetty, Baylor College of Medicine, Rice University

Jada Walker, Saint Mary's College of California

Anne Worth, University of North Carolina, Chapel Hill


SAN DIEGO BAY
GROUND LEVEL
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CITYSIDE
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Hall B1
Hall B2
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POSTERS 679 - 796
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Lunch Concession open M-Th, 11am - 2pm
Main Entrance
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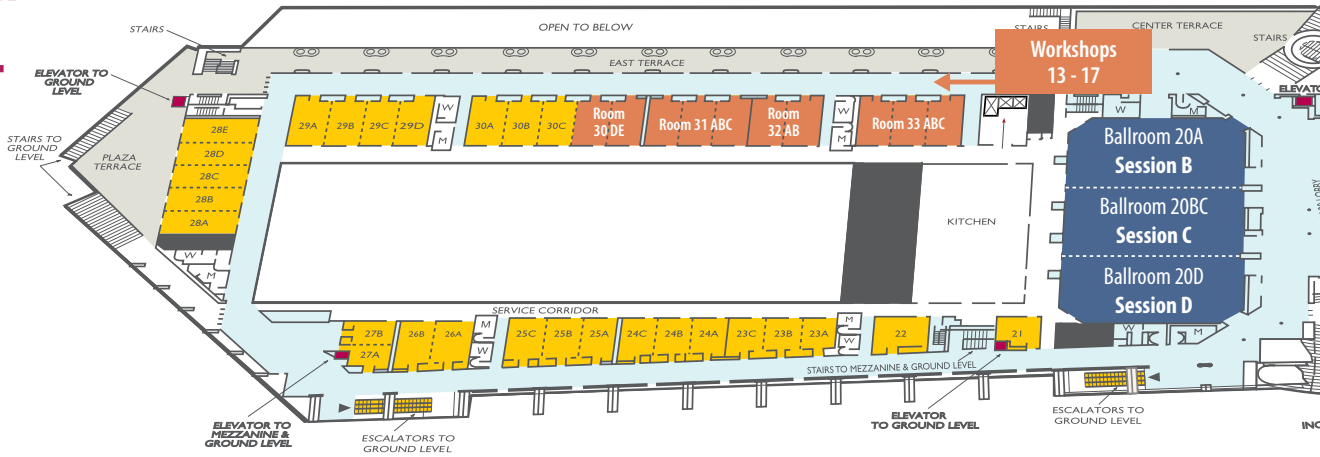
Corporate Posters
SPECIAL POSTERS & ANNOUNCEMENTS
FUNDING AGENCY OFFICE HOURS
INFORMATICS HUB
RESTAURANTS
RESERVATIONS
LOBBY
LOBBY
TIDES
EXIT
SHOW OFFICE
SHOW OFFICE A
NETWORK SUPPORT
AV CONCEPTS
STARBUCKS

BUILDING OVERVIEW

SAN DIEGO BAY

UPPER LEVEL



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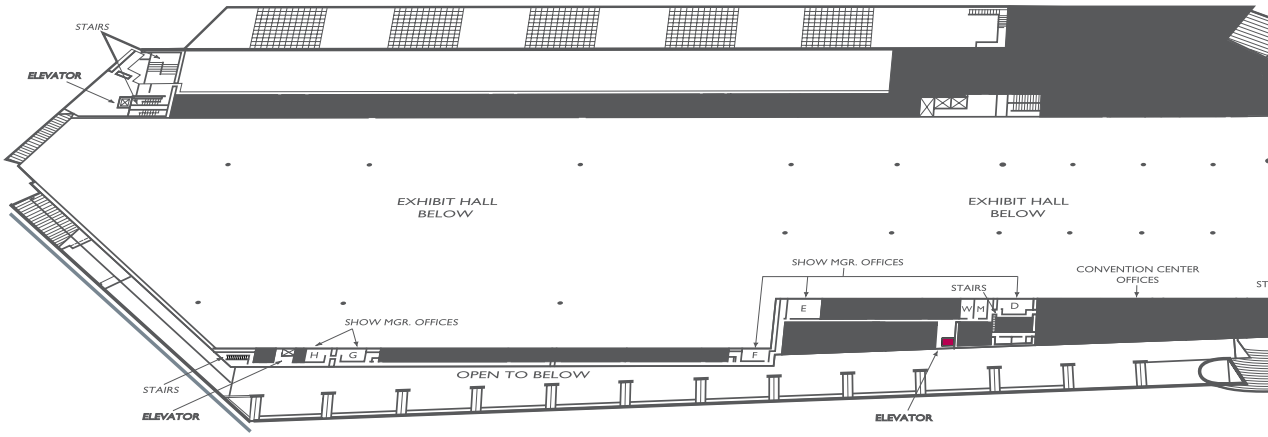

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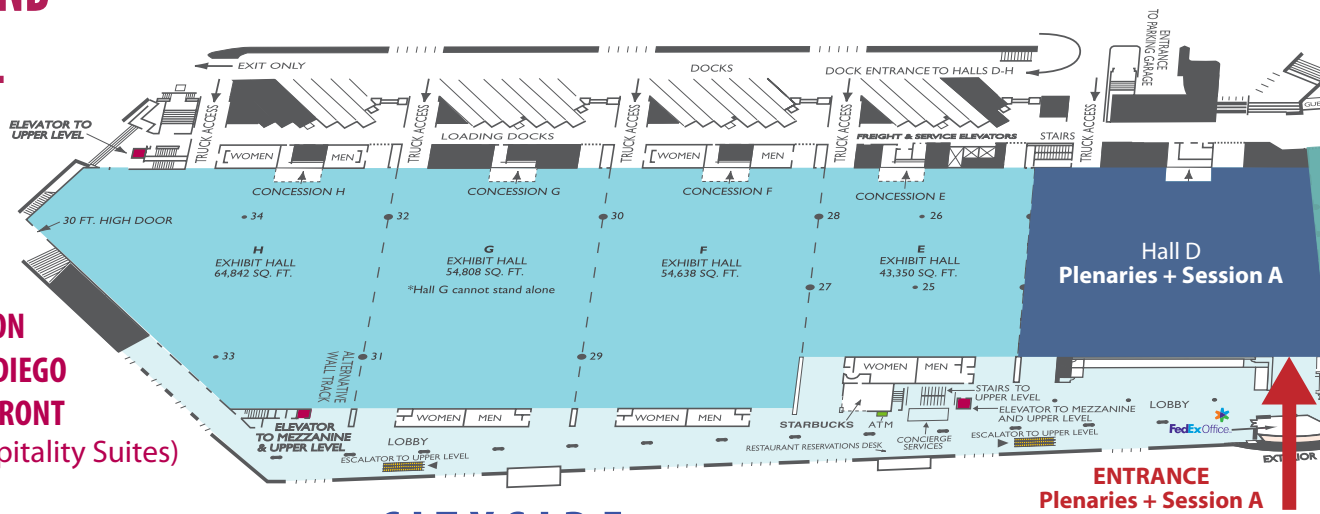


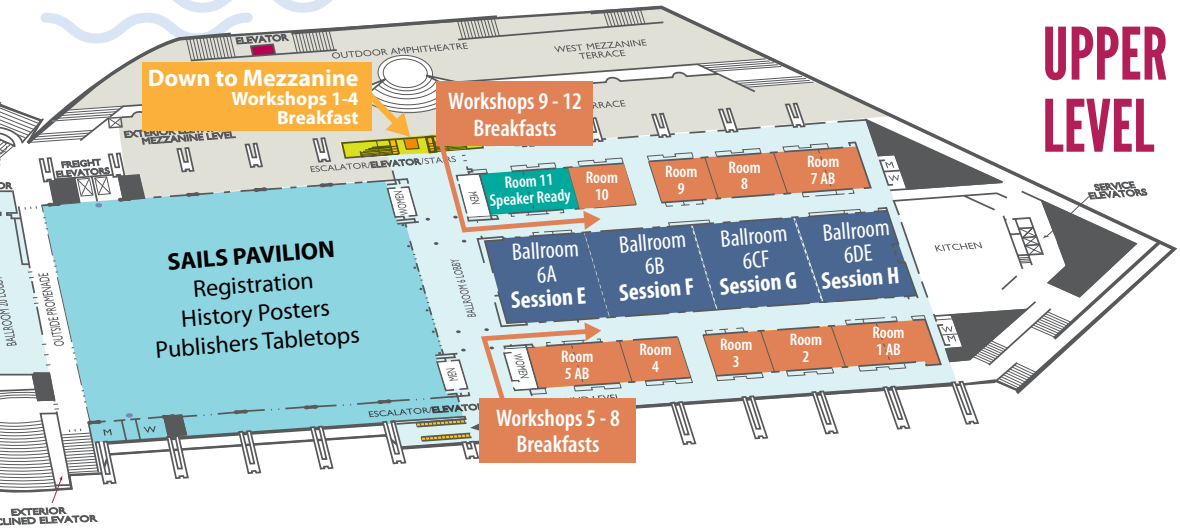
TO HILTON SAN DIEGO BAYFRONT (Hospitality Suites)

CITYSIDE

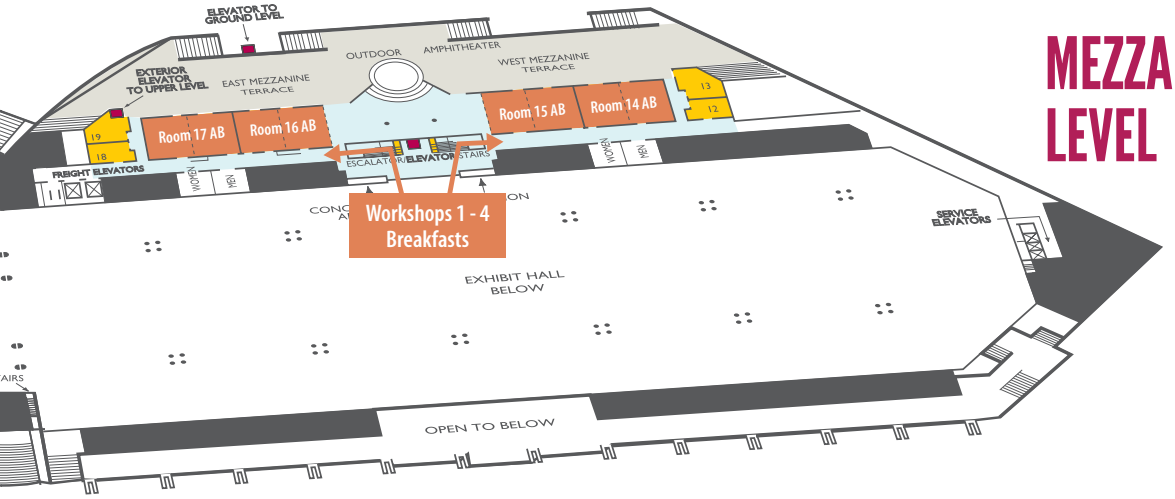
SAN DIEGO convention center CORPORATION

SAN DIEGO BAY

UPPER LEVEL



MEZZANINE LEVEL



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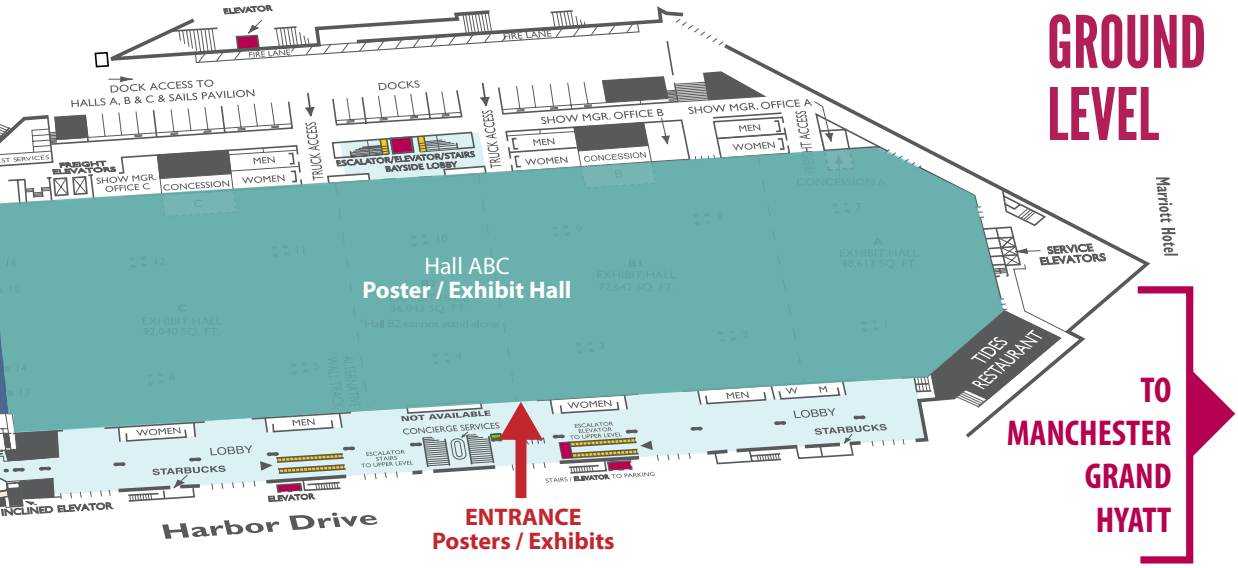

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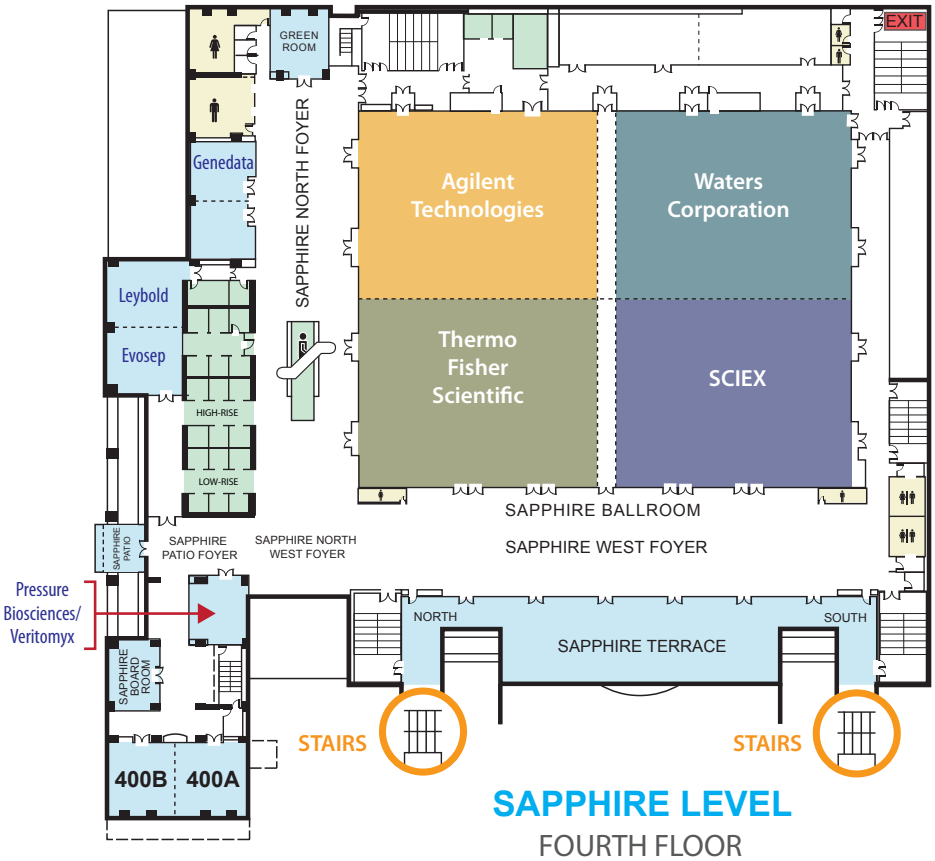


= Function Space
= Elevators & Escalators
= Restrooms
= Stairs

HOSPITALITY SUITES 2018 - BACK TO BASICS

Many years ago when the hospitality suite concept was introduced at the conference (these used to be actual guest sleeping rooms!), the intention was to provide a relaxed atmosphere where attendees could interact with industry. To provide a setting for meaningful conversations regarding the latest technology in products and services, and attendees could enjoy some refreshments.

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

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

MEDIA EVENTS (PRESS CONFERENCES)

The following media events are scheduled **Monday, June 4** in the Hilton San Diego Bayfront. All press are invited to attend these events.

8:00 - 9:00 am	Bruker Daltonics	Indigo CG
9:30 - 10:30 am	Shimadzu Scientific Instruments	Indigo ABEF
11:00 am - 12:00 pm	SCIEX	Sapphire CDGH
1:30 - 2:30 pm	Agilent	Sapphire IJMN
3:00 - 4:00 pm	Thermo Fisher Scientific	Sapphire ABEF
4:30 - 5:30 pm	Waters Corporation	Sapphire KLOP

BREAKFAST SEMINARS

Breakfast seminars are hosted by corporate members at either the Convention Center or Hilton San Diego Bayfront Hotel (inside hospitality suites). Pre-registration (RSVP) is required because room set-up and catering are arranged in advance. Please look for the Breakfast Seminars page on www.asms.org and in the mobile app to find online registration links.

MONDAY BREAKFASTS

CONVENTION CENTER *All breakfast seminars begin at 7:00 am*	
Advanced Chemistry Development (ACD/Labs)	Room 5B
Bruker Daltonics	Room 15AB
LECO Corporation	Room 4
Matrix Science	Room 2
Perkin Elmer	Room 16AB
SCIEX (2)	Room 8, Room 9
Shimadzu Scientific Instruments	Room 1AB
Waters Corporation	Room 17AB
HILTON SAN DIEGO BAYFRONT	
Agilent	Sapphire IJMN
Thermo Fisher Scientific	Sapphire ABEF
Waters Corporation	Sapphire KLOP

TUESDAY BREAKFASTS

CONVENTION CENTER *All breakfast seminars begin at 7:00 am*	
Biocrates	Room 10
Biognosys	Room 7AB
Biotage	Room 5B
Bruker Daltonics	Room 15AB
Evosep	Room 5A
LECO Corporation	Room 4
Matrix Science	Room 2
New Objective	Room 3
Phenomenex	Room 17AB
SCIEX (2)	Room 8, Room 9
Shimadzu Scientific Instruments	Room 1AB
VICI	Room 16AB
HILTON SAN DIEGO BAYFRONT	
Agilent	Sapphire IJMN
Thermo Fisher Scientific	Sapphire ABEF
Waters Corporation	Sapphire KLOP

WEDNESDAY BREAKFASTS

CONVENTION CENTER *All breakfast seminars begin at 7:00 am*	
Bruker Daltonics	Room 15AB
LECO Corporation	Room 4
New Objective	Room 3
SCIEX (3)	Room 8, Room 9, Room 10
Shimadzu Scientific Instruments	Room 1AB
HILTON SAN DIEGO BAYFRONT	
Agilent	Sapphire IJMN
Thermo Fisher Scientific	Sapphire ABEF
Waters Corporation	Sapphire KLOP

THURSDAY BREAKFASTS

CONVENTION CENTER *All breakfast seminars begin at 7:00 am*	
SCIEX (2)	Room 9, Room 10
Shimadzu Scientific Instruments	Room 1AB
Thermo Fisher Scientific	Room 8

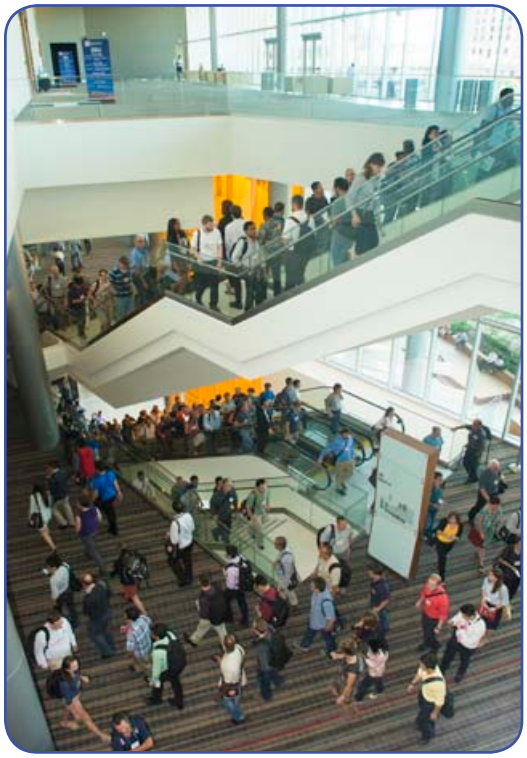
	Exhibit Booth	Corporate Poster or Publisher Tabletop	Hospitality Suite at Hilton Bayfront	Breakfast Seminar
908 Devices	509			
AcroMass Technologies, Inc.	923	Corporate Poster		
Advanced Chemistry Development (ACD/Labs)	409	Corporate Poster		Conv Ctr Rm 5B: Mon 6/4
Advanced Chromatography Technologies Ltd	314			
Advanced Energy	1004	Corporate Poster		
Advion	702			
Agilent	800	Corporate Poster	Sapphire IJMN	Hilton Bayfront Sapphire IJMN: Mon-Wed (6/4-6/6)
Alliance Pharma	619			
Altasciences Clinical Research	603			
Alternative Biomedical Solutions	419			
Analytical Sales and Services, Inc.	705	Corporate Poster		
Analytical Scientific Instruments US Inc.	918			
Anest Iwata Air Engineering	822			
Antec Scientific	614	Corporate Poster		
Apricot Designs	805	Corporate Poster		
Ardara Technologies L.P.	1020			
Ascend Diagnostics	907			
Avanti Polar Lipids, Inc.	1100			
Baran Bioscience, LLC		Corporate Poster		
BaySpec, Inc.	407			
BioChromato	804	Corporate Poster		
Biocrates Life Sciences AG	620			Conv Ctr Rm 10: Tue 6/5
Biognosys	707			Conv Ctr Rm 7AB: Tue 6/5
Bioinformatics Solutions Inc.	709	Corporate Poster		
Biopeptek Pharmaceuticals	323			
Biotage	722			Conv Ctr Rm 5B: Tue 6/5
Biotech Support Group	405			
Bruker Daltonics	715		Indigo CG	Conv Ctr Rm 15AB: Mon-Wed (6/4-6/6)
C&EN / ACS Publications		Publisher Tabletop		
Cambridge Isotope Laboratories, Inc.	608			
Cayman Chemical Company	1015	Corporate Poster		
CEM Corporation	917		Room 202AB	
Cerno Bioscience	721			
CMION	1102			
CMP Scientific Corp	904			
Compare Networks		Publisher Tabletop		
Conquer Scientific	420	Corporate Poster		
CovalX	901			
CSS Analytical Co. Inc				
CTC Analytics AG	719			
Detector Technology	1014			
Digital Proteomics	400	Corporate Poster		

	Exhibit Booth	Corporate Poster or Publisher Tabletop	Hospitality Suite at Hilton Bayfront	Breakfast Seminar
Ebara Technologies	302	Corporate Poster		
Edwards Vacuum	500			
e-MSion, Inc.	821			
Entech Instruments	300	Corporate Poster		
Eprep	505			
ETP Ion Detect	618	Corporate Poster		
Evosep	604		Room 410A	Conv Ctr Rm 5A: Tue 6/5
Extrel CMS	1104			
Fasmatech	906			
F-DGSi	423			
Genedata	703	Corporate Poster	Room 411B	
Genetic Engineering & Biotechnology News		Publisher Tabletop		
Genovis Inc	403	Corporate Poster		
GenTech Scientific, Inc.	415			
GERSTEL, Inc.	816			
GL Sciences	600			
Grenova	1006			
Hamamatsu Corporation	201			
Hamilton Company	809	Corporate Poster		
Harris Corporation	909	Corporate Poster		
HILICON AB		Corporate Poster		
HTX Technologies, LLC	817			
HVM Technology, Inc.	418			
IDEX Health & Science	504			
IMCS	807			
Imtakt USA	723			
Institute for Systems Biology	203			
Intavis, Inc	921			
Integrated Proteomics Applications	406			
International Equipment Trading Ltd.	706			
International Labmate Ltd.		Publisher Tabletop		
Intertek Pharmaceutical Services	305			
Ion Opticks Pty Ltd	717			
IonBench	815			
IONICON	1114	Corporate Poster		
Ionoptika Ltd.	303			
Ionsense Inc.	915	Corporate Poster		
IONTOF GmbH	516			
IsoSciences	920			
JASMS	215			
JEOL USA, Inc.	605			
KNAUER	1023	Corporate Poster		
Kurt J. Lesker Company	402			
LCGC	317			

	Exhibit Booth	Corporate Poster or Publisher Tabletop	Hospitality Suite at Hilton Bayfront	Breakfast Seminar
LECO Corporation	803	Corporate Poster		Conv Ctr Rm 4: Mon-Wed (6/4-6/6)
Leybold USA	606		Room 410B	
Linden CMS GmbH	1108			
MAC-MOD Analytical	316			
MasCom Technologies	416			
MassMatrix Inc.				
Masstech Mass Spectrometry Instrument Ltd.	1003			
Matrix Science	522			Conv Ctr Rm 2: Mon-Tue (6/4-6/5)
Matsusada Precision Inc.	401			
McKinley Scientific	607			
MeCour Temperature Control	922			
Mercedes Medical	1009			
Mestrelab Research	802			
Microsaic Systems plc	1005	Corporate Poster		
MilliporeSigma	304	Corporate Poster		
Moeller Medical GmbH	819			
Mott Corporation	916			
MPF Products Inc.	521			
MRM Proteomics	1122			
MS Ekspert	506			
MS Noise	808			
MSI.TOKYO, Inc.	820	Corporate Poster		
MSTM, LLC	716			
Nacalai USA	622	Corporate Poster		
National Institute of Standards and Technology (NIST)	914			
New England Biolabs	818			
New England Peptide Inc.	1002			
New Objective Inc.	609			Conv Ctr Rm 3: Tue-Wed (6/5-6/6)
Newomics Inc.	307			
Omicron	602			
Omics Informatics LLC	223			
OMNI Enclosures	615	Corporate Poster		
Omni International	623			
Optimize Technologies	900	Corporate Poster		
Peak Scientific	501	Corporate Poster	Room 204A	
PerkinElmer, Inc.	508		Indigo DH	Conv Ctr Rm 16AB: Mon 6/4
Pfeiffer Vacuum	801	Corporate Poster		
Pharmafluidics	517			
Phenomenex	1106			Conv Ctr Rm 17AB: Tues 6/5
Phoenix S&T, Inc.	704			

	Exhibit Booth	Corporate Poster or Publisher Tabletop	Hospitality Suite at Hilton Bayfront	Breakfast Seminar
PHOTONIS	714	Corporate Poster		
Phytronix Technologies	621			
PreOmics GmbH	806			
Pressure BioSciences Inc.	422	Corporate Poster	Room 402	Hilton Bayfront Room 402: Mon 6/4
Prolab Instruments GmbH	814	Corporate Poster		
Promega Corporation	1008			
Prosolia	209	Corporate Poster		
Protein Metrics Inc.	515			
Proteome Software Inc.	301			
Proton OnSite	421			
ProZyme, Inc.	1022	Corporate Poster		
PURSPEC Technologies Inc.	1001	Corporate Poster		
Rapid Novor Inc.	1018	Corporate Poster		
Resolution Labs LLC	1016			
Restek Corporation	903			
ReSyn Biosciences	1007	Corporate Poster		
Russell Publishing Ltd.		Publisher Tabletop		
Samin Science Co. Ltd.	408			
Scientific Instrument Services	908	Corporate Poster		
SCIEX	601		Sapphire CDGH	Conv Ctr Rm 8: Mon-Wed (6/4-6/6); Rm 9 - Mon-Thu (6/4-6/7); Rm 10 Wed-Thu (6/6-6/7)
Shimadzu Scientific Instruments, Inc.	701	Corporate Poster	Indigo ABEF	Conv Ctr Rm 1AB: Mon-Thu (6/4-6/7)
Shodex, Showa Denko America	309			
Sierra Analytics, Inc.	518	Corporate Poster		
Silantes GmbH	503			
Sound Analytics	507			
SP Scientific	404			
Spark Holland	1000			
SpectralWorks	720	Corporate Poster		
Spectroswiss	823			
Spellman High Voltage Electronics Corp.	718			
SPEX SamplePrep LLC	919			
SunChrom GmbH	414			
Superior Technical Ceramics	905			
Syft Technologies	514			
Takara Bio USA	315			
Teledyne SP Devices		Corporate Poster		
Teledyne SSI	523	Corporate Poster		
The Analytical Scientist		Publisher Tabletop		
Thermo Fisher Scientific	708		Sapphire ABEF	Hilton Bayfront Sapphire ABEF: Mon-Wed (6/4-6/6) Conv Ctr Rm 8: Thu 6/7
Tosoh Bioscience LLC	616			

Company	Exhibit Booth	Corporate Poster or Publisher Tabletop	Hospitality Suite at Hilton Bayfront	Breakfast Seminar
Trajan Scientific and Medical	902	Corporate Poster		
Veritomyx	308		Room 402	Hilton Bayfront Room 402: Tues-Wed (6/5-6/6)
VICI	417			Conv Ctr Rm 16AB: Tue 6/5
VRS Recruitment	617			
Waters Corporation	700	Corporate Poster	Sapphire KLOP	Hilton Bayfront Sapphire KLOP: Mon-Wed (6/4-6/6); Conv Ctr Rm 17AB: Mon 6/4
Xtreme Power	520			
YL Intruments Co., Ltd.	502			
Zef Scientific, Inc.	519			
Zhejiang Haochuang Biotech Co. Ltd.	322			



Vice President for Programs

Richard A. Yost
University of Florida

Student Assistants

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

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Jian Wang
Wei Xu
Nicolas Young

SATURDAY

9:00 AM - 4:30 PM	**SHORT COURSES**
2:00 - 5:00 PM	**REGISTRATION,** Sails Pavilion upper level

SUNDAY

9:00 AM - 4:30 PM	**SHORT COURSES**
10:00 AM - 8:00 PM	**REGISTRATION,** Sails Pavilion upper level
4:00 - 4:45 PM	**ATTENTION: FIRST-TIME GRADUATE STUDENTS AND UNDERGRADUATE STUDENTS** **Plan your Strategy: What to See and Do at ASMS,** Ballroom 20A upper level
5:00 - 6:30 PM	**TUTORIAL SESSION I**, Hall D ground level **5:00 - 5:45 pm** **Strategies for Quantitative Proteomics** **M. Arthur Moseley,** *Duke University School of Medicine*  **5:45 - 6:30 pm** **Mass Spectrometry and the Environment** **Susan D. Richardson**, *University of South Carolina*  **TUTORIAL SESSION II,** Ballroom 20A upper level **5:00 - 5:45 pm** **Mass Spectrometry and Nuclear Forensics** **Gregory Eiden,** *Pacific Northwest National Laboratory*  **5:45 - 6:30 pm** **From the Laboratory to the Stars** **Jack Beauchamp,** *California Institute of Technology* 
6:45 - 7:45 PM	**CONFERENCE OPENING,** Hall D ground level **Richard A. Yost**, *University of Florida* ASMS Vice President for Programs  **7:00 - 7:45 pm** **Smart Trials: Moving from a Site-centric to Patient-centric Clinical Trials** **Lisa Shipley** *Pharmacokinetics, Pharmacodynamics & Drug Metabolism, Merck*
7:45 - 9:00 PM	**WELCOME RECEPTION IN THE POSTER/EXHIBIT HALL** Undergraduate Student Poster Competition

MONDAY

7:00 AM	**CORPORATE BREAKFAST SEMINARS,** Convention Center and and Hilton San Diego Bayfront (page 15)
7:30 AM - 5:00 PM	**REGISTRATION,** Sails Pavilion upper level
8:30 - 10:30 AM	**ORAL SESSIONS** MOA am: Fundamentals for Everyone: Quantitation, *Hall D ground level* MOB am: Imaging: Pharmaceuticals, Metabolites, and Lipids, *Ballroom 20A upper level* MOC am: MS in the QC Lab, *Ballroom 20BC upper level* MOD am: GC/MS, GC/GC/MS, GC/MS/MS, and GC/HRMS, *Ballroom 20D upper level* MOE am: Nucleic Acids and Oligonucleotides, *Ballroom 6A upper level* MOF am: Native MS in Structural Biology, *Ballroom 6B upper level* MOG am: Informatics: Innovations, *Ballroom 6CF upper level* MOH am: Energy, Petroleum, and Biofuels: Instrumentation and Applications, *Ballroom 6DE upper level*
10:30 AM - 2:30 PM	**POSTER SESSION AND EXHIBITS,** Monday Posters, Poster/Exhibit Hall ground level **Odd-number posters present:** 10:30 - 11:30 am PLUS 12:30 – 2:30 pm **Even-number posters present:** 10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm 11:30 am - 1:00 pm: **Undergraduate students** look for reserved tables and free lunch vouchers to ***Meet the Experts***
2:30 - 4:30 PM	**ORAL SESSIONS** MOA pm: Instrumentation: Innovative Separations Approaches Coupled to MS, *Hall D ground level* MOB pm: Imaging: Biomedical Applications, *Ballroom 20A upper level* MOC pm: Drug Target Identification by MS, *Ballroom 20BC upper level* MOD pm: Top Down Protein Analysis, *Ballroom 20D upper level* MOE pm: Carbohydrates, *Ballroom 6A upper level* MOF pm: Protein-Ligand Interactions, *Ballroom 6B upper level* MOG pm: Informatics: Determination of Elemental Composition, *Ballroom 6CF upper level* MOH pm: Fundamentals: Photoionization and Photodissociation, *Ballroom* 6DE *upper level*
4:45 - 5:30 PM	**AWARD LECTURE**, **John B. Fenn Award for a Distinguished Contribution in Mass Spectrometry** **Gert von Helden** *Fritz-Haber Institut der Max Planck-Gesellschaft* **Martin F. Jarrold** *Indiana University* **David E. Clemmer** *Indiana University* 
5:45 - 7:00 PM	**WORKSHOPS** There are light refreshments in Sails Pavilion upper level 5:30 - 5:45 pm. 01. Frontiers in Ion Spectroscopy (Fundamentals Interest Group), *Room 14 AB mezzanine level* 02. Networking for Scientists: Celebrating Women Mass Spectrometrists, *Room 15 AB mezzanine level* 03. Ion Mobility Spectrometers: How to Build Your Own (Ion Mobility MS Interest Group), *Room 16 AB mezzanine level* 04. HDX, Covalent Labeling & Cross-Linking: Best Practices, Control Experiments and Data Harmonization (HDX Covalent Labeling & Cross Linking Interest Group), *Room 17 AB mezzanine level* 05. Advances in Polymer Mass Spectrometry (Polymeric Materials Interest Group), *Room 5B upper level* 06. Life After A Bachelor's Degree: A Q&A Panel for Undergraduates Interested in Graduate School and Industry Careers (Undergraduate Research in MS Interest Group), *Room 5A upper level* 07. Beyond Collisional Dissociation: Improving Metabolite Identification by Alternative Gas-Phase Techniques (DMPK Interest Group), *Room 4 upper level* 08a. Art and Cultural Heritage: Mass Spec Applications, *Room 3 upper level* 08b. Biotherapeutics Interest Group Workshop: Hot Topics, *Room 2 upper level* 09. Energy, Petroleum, and Biofuels MS: Methods for Increasing Compositional Space Coverage (Energy Petroleum & Biofuels Interest Group), *Room 10 upper level* 10. Mass Spectrometry in the Developing World: Supporting Education and Research, *Room 9 upper level* 11. MS Software: Excavating Nuggets of Information from the Massive Mound of Data, *Room 8 upper level* 12. Data Independent Acquisition: Expanding the Scope of DIA Strategies for Quantitative Mass Spectrometry (Data Independent Acquisition Interest Group), *Room 7 AB upper level* 13. Ion Traps: What Do They Hold for the Future? (Ion Trap MS), *Room 33 ABC upper level* 14. LC-MS Jeopardy: I'll Take Increasing Throughput for $200 (LCMS & Related Topics Interest Group), *Room 32 AB upper level* 15. A Career in Mass Spec: Options and Where to Start? (Young Mass Spectrometrists Interest Group), *Room 31 ABC upper level* 16. Tackling The Big Data: How-to Analyze and Share Proteomics Data Responsibly (Analytical Lab Managers Interest Group), Room 30 DE upper level
7:00 - 8:00 PM	**DINNER BREAK**
AFTER 8:00 PM	**CORPORATE HOSPITALITY SUITES,** Hilton San Diego Bayfront

TUESDAY

7:00 AM	**Corporate Breakfast Seminars,** Convention Center and Hilton San Diego Bayfront (page 15)
7:30 AM - 5:00 PM	**Registration,** Sails Pavilion upper level
8:30 - 10:30 AM	**Oral Sessions** TOA am: Fundamentals for Everyone: Peptides and Proteins (In Memory of Jack Throck Watson), *Hall D ground level* TOB am: Ion Mobility: New Developments & Applications, *Ballroom 20A upper level* TOC am: Applications of Stable Isotope Labeling in MS, *Ballroom 20BC upper level* TOD am: Metabolomics: New Technologies and Applications, *Ballroom 20D upper level* TOE am: Innovations and Applications in Forensics, *Ballroom 6A upper level* TOF am: Plant "omics", *Ballroom 6B upper level* TOG am: MS in the Field and the Clinic, *Ballroom 6CF upper level* TOH am: Synthetic Polymers, *Ballroom 6DE upper level*
10:30 AM - 2:30 PM	**Poster Session and Exhibits,** Tuesday Posters, Poster/Exhibit Hall ground level **Odd-number posters present:** 10:30 - 11:30 am PLUS 12:30 – 2:30 pm **Even-number posters present:** 10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm
2:30 - 4:30 PM	**Oral Sessions** TOA pm: Instrumentation: Ambient Ionization: Instrumentation & Applications, *Hall D ground level* TOB pm: Ion Mobility: Small Molecules and Clinical, *Ballroom 20A upper level* TOC pm: Analytical Challenges of Microdosing and Microsampling Studies, *Ballroom 20BC upper level* TOD pm: Metabolomics: Untargeted Profiling, *Ballroom 20D upper level* TOE pm: Environmental: Emerging Contaminants, *Ballroom 6A upper level* TOF pm: Innovations in Hydrogen-Deuterium Exchange MS, *Ballroom 6B upper level* TOG pm: Qualitative and Quantitative Analysis of Post-translational Modifications, *Ballroom 6CF upper level* TOH pm: Fundamentals: Ion-Ion and Ion-Neutral Interactions, *Ballroom 6DE upper level*
4:45 - 5:30 PM	**Award Lecture,** Hall D ground level **Biemann Medal**  **Benjamin A. Garcia** *University of Pennsylvania* *Perelman School of Medicine*
5:45 - 7:00 PM	**Workshops** There are light refreshments in Sails Pavilion upper level 5:30 - 5:45 pm. 01. Deconvolution of FT-MS Spectra: How it Works and What's Available (FTMS Interest Group), *Room 14 AB mezzanine level* 02. Reporting of Multi-Analyte Assays in Clinical Analyses (Clinical Chemistry Interest Group), *Room 15 AB mezzanine level* 03. Quantitative Glycomics and Glycoproteomics: Needs of Standards or Methods?, *Room 16 AB mezzanine level* 04. Current Trends in High Spatial Resolution 2D and 3D Mass Spectrometry Analysis, *Room 17 AB mezzanine level* 05. Galaxy for MS Software Dissemination: How to Easily Publish Your Tools, *Room 5B upper level* 06. ASMS Diversity and Outreach Workshop, *Room 5A upper level* 07. Debunking the Myth of Stress: A Career Development Workshop, *Room 4 upper level* 08. Exposomics Tools (Exposomics Interest Group), *Room 3 upper level* 09. The Roles of Metal in Ion Chemistry and Structure: In Honor of the Late Robert C. Dunbar (Metal Ion Coordination Chemistry Interest Group), *Room 10 upper level* 10. Environmental MS: New Trends in Sampling and Separations (Environmental Applications Interest Group), R*oom 9 upper level* 11. MassIVE Big Data: Revealing, Sharing and Reusing Discoveries of Deep Proteome Diversity in Repository-Scale Mass Spectrometry Data, *Room 8 upper level* 12. Bioanalysis of Intact Biotherapeutics by Hybrid LBA/LCMS: Challenges & Solutions (Regulated Bioanalysis Interest Group), *Room 7 AB upper level* 13. Forensic ID: Qualitative Identification in Forensic Mass Spectrometry (Forensics & Homeland Security Interest Group), *Room 33 ABC upper level* 14. Computational Biology and Biology for Metabolomics: Bridging the Gap Matchmaking Session , *Room 32 AB upper level* 15. Lipidomics: Current Trends in Mass Spectrometry Data Collection (Lipids & Lipodomics), *Room 31 ABC upper level* 16. FAIMS/DIMS/DMS: Basics and Applications, *Room 30 DE upper level*
7:00 - 8:00 PM	**Dinner Break**
After 8:00 PM	**Corporate Hospitality Suites,** Hilton San Diego Bayfront

WEDNESDAY

7:00 AM	**Corporate Breakfast Seminars,** Convention Center and Hilton San Diego Bayfront (page 15)
7:30 AM - 5:00 PM	**Registration,** Sails Pavilion upper level
8:30 - 10:30 AM	**Oral Sessions** WOA am: Instrumentation: Mass Analyzer Innovations, *Hall D ground level* WOB am: Ion Mobility: Structure, *Ballroom 20A upper level* WOC am: Quantitative Analysis in Drug Discovery and Development, *Ballroom 20BC upper level* WOD am: MS in Clinical Analysis, *Ballroom 20D upper level* WOE am: Exposomics, *Ballroom 6A upper level* WOF am: Macromolecular Complexes, *Ballroom 6B upper level* WOG am: Informatics: Peptide and Protein Identification, Proteomics, *Ballroom 6CF upper level* WOH am: Fundamentals: Ion Spectroscopy (In Memory of Rob Dunbar), *Ballroom 6DE upper level*
10:30 AM - 2:30 PM	**Poster Session and Exhibits,** Wednesday Posters, Poster/Exhibit Hall ground level **Odd-number posters present:** 10:30 - 11:30 am PLUS 12:30 – 2:30 pm **Even-number posters present:** 10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm
2:30 - 4:30 PM	**Oral Sessions** WOA pm: Instrumentation: Innovations in FT-based Mass Analyzers, *Hall D ground level* WOB pm: Microorganisms and the Microbiome, *Ballroom 20A upper level* WOC pm: MS in Extractable and Leachable Analysis, *Ballroom 20BC upper level* WOD pm: Quantitative Proteomics in Systems Biology, *Ballroom 20D upper level* WOE pm: Environmental: Innovative Approaches and Instrumentation, *Ballroom 6A upper level* WOF pm: Covalent Labeling and Chemical Crosslinking, *Ballroom 6B upper level* WOG pm: Informatics: Metabolomics, *Ballroom 6CF upper level* WOH pm: Fundamentals: Ion Activation and Dissociation, *Ballroom 6DE upper level*
4:45 - 5:30 PM	**ASMS Meeting,** Ballroom 20A upper level: Awards, board reports, wine, beer, soft drinks - and more!
5:45 - 7:00 PM	**Workshops** There are light refreshments in Sails Pavilion upper level 5:30 - 5:45 pm. 01. How New Methods are Enabling the Characterization of Isomeric Glycans, *Room 14 AB mezzanine level* 02. Using R for Mass Spectrometry Data Analysis and Workflows, *Room 15 AB mezzanine level* 03. Multi-MS-Omics Data Integration (Bioinformatics MS Interest Group), *Room 16 AB mezzanine level* 04. Metabolomics: Best Practices for Standardization and Data Exchange (Metabolomics Interest Group), *Room 17 AB mezzanine level* 05. The NIH and NSF Review and Funding Process, *Room 5B upper level* 06. Photoionization as a Powerful Analytical Tool in Mass Spectrometry: Back to the Roots (Photoionization MS Interest Group), *Room 5A upper level* 07. Trans-Proteomic Pipeline: Current Applications and Future Directions, *Room 4 upper level* 09. Food Safety & Security: HRMS Applications (Flavor, Fragrance & Foodstuff Interest Group), *Room 10 upper level* 10. Applications of Solid Phase Microextraction in Mass Spectrometry, *Room 9 upper level* 11. Improving Scientific Writing Skills, *Room 8 upper level* 12. Career and Collaboration Opportunities in China, *Room 7 AB upper level* 13. ADC Research and Development: The Role of Mass Spectrometry in ADC Biotherapeutic Development (Pharmaceuticals Interest Group), *Room 33 ABC upper level* 14. Imaging Mass Spectrometry Data Analysis and Interpretation: Are You Getting the Most out of Your Data? (Imaging MS Interest Group), *Room 32 AB upper level* 15. Top Down Proteomics: Strategies for Analysis (Top-Down Proteomics Interest Group), *Room 31 ABC upper level* 16. Implicit Bias, *Room 30 DE upper level*
7:00 - 8:00 PM	**Dinner Break**
After 8:00 PM	**Corporate Hospitality Suites,** Hilton San Diego Bayfront

THURSDAY

7:00 AM	**Corporate Breakfast Seminars,** Convention Center (page 15)
7:30 AM - 5:00 PM	**Registration,** Sails Pavilion upper level
8:30 - 10:30 AM	**Oral Sessions** ThOA am: Instrumentation: Ion Detection, *Hall D ground level* ThOB am: Imaging: Instrumentation & Method Development, *Ballroom 20A upper level* ThOC am: Food Safety & Chemistry: Innovations, *Ballroom 20BC upper level* ThOD am: Biomarkers: Qualitative Analysis, *Ballroom 20D upper level* ThOE am: Lipidomics: Lipids and Profiling, *Ballroom 6A upper level* ThOF am: Glycopeptides and Glycoproteins, *Ballroom 6B upper level* ThOG am: Informatics: Data-Independent Acquisition: Innovative Methods and Applications, *Ballroom 6CF upper level* ThOH am: Membrane Protein MS, *Ballroom 6DE upper level*
10:30 AM - 2:30 PM	**Poster Session and Exhibits,** Thursday Posters, Poster/Exhibit Hall ground level **Odd-number posters present:** 10:30 - 11:30 am PLUS 12:30 – 2:30 pm **Even-number posters present:** 10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm
2:30 - 4:30 PM	**Oral Sessions** ThOA pm: Instrumentation: New Developments in Ionization and Sampling, *Hall D ground level* ThOB pm: Imaging: Computational Methods and Analysis, *Ballroom 20A upper level* ThOC pm: Food Safety & Chemistry: Foodomics, Allergens, Bacteria, Foods, *Ballroom 20BC upper level* ThOD pm: Therapeutic Proteins, Antibodies, and Antibody/Drug Conjugates, *Ballroom 20D upper level* ThOE pm: Lipidomics: New MS Technologies and Applications, *Ballroom 6A upper level* ThOF pm: Biomarkers: Quantitative Analysis, *Ballroom 6B upper level* ThOG pm: Informatics: Multiomics Integration and Applications, *Ballroom 6CF upper level* ThOH pm: Fundamentals: Computational Methods in Ion Mobility and MS, *Ballroom 6DE upper level*
4:45 - 5:30 PM	**Plenary Lecture,** Hall D ground level  **The Fight Against Doping: From Strychnine to Turinabol** **Larry Bowers** *LD Bowers, LLC*
6:30 - 9:00 PM	**Closing Event** **USS Midway Museum.** *Tickets must be purchased in advance by Monday 12 pm (noon).* Join us for an incredible evening aboard the USS Midway, a retired aircraft carrier turned museum. In addition to a buffet dinner on the flight deck there will be docents to share the Midway's history & exhibits, plus a variety of flight simulation games. 

SUNDAY EVENING, 4:00 - 9:00 PM

4:00-4:45 pm Sunday
Attention First-time Graduate Students and Undergrads
Plan your Strategy: What to See and Do at ASMS
Megan Gessel
(University of Puget Sound)
Ballroom 20A upper level

5:00-6:30 pm Sunday
TUTORIAL SESSION I
Richard A. Yost (University of Florida)
Hall D ground level

5:00-5:45 pm
Strategies for Quantitative Proteomics
M. Arthur Moseley
Duke University School of Medicine

5:45-6:30 pm
Mass Spectrometry and the Environment
Susan D. Richardson
University of South Carolina

5:00-6:30 pm Sunday
TUTORIAL SESSION II
John A. McLean (Vanderbilt University)
Ballroom 20A upper level

5:00-5:45 pm
Mass Spectrometry and Nuclear Forensics
Gregory Eiden
Pacific Northwest National Laboratory

5:45- 6:30 pm
From the Laboratory to the Stars
Jack Beauchamp
California Institute of Technology

6:45- 7:45 pm Sunday
CONFERENCE OPENING
Richard A. Yost (University of Florida)
Hall D ground level

Welcome, Richard A. Yost, *University of Florida*
ASMS Vice President for Programs

6:00-7:45 pm
Smart Trials: Moving from a Site-centric to Patient-centric Clinical Trials
Lisa Shipley
Pharmacokinetics, Pharmacodynamics & Drug Metabolism, Merck

7:45 – 9:00 pm SUNDAY
WELCOME RECEPTION
Poster/Exhibit Hall ground level
Conference name badge is required.

MONDAY MORNING ORAL SESSIONS

7:00 am Monday
CORPORATE BREAKFAST SEMINARS
CONVENTION CENTER AND
HILTON SAN DIEGO BAYFRONT
See page 15 for detailed schedule.
Reservation or RSVP required.

8:30-10:30 am Monday
FUNDAMENTALS FOR EVERYONE: QUANTITATION
Session Chair: Bob Bethem (Consultant)
Hall D ground level

MOA am 08:30 **Instrument Detection Limit (IDL) as a Measurement of Intrinsic MS Sensitivity**; Patrick M. Batoon[1]; Haopeng Wang[1]; Behrooz Zekavat[1]; Laura L. Pollum[1]; Shane E. Tichy[1]; *[1]Agilent Technologies, Inc., Santa Clara, CA*

MOA am 08:50 **Semiquantitative ESI/MS Analysis of Metabolites in Biological Matrices Made Feasible via Prediction of Ionization Efficiencies**; Piia Liigand[1]; Jaanus Liigand[2]; Filip Cuyckens[3]; Rob J. Vreeken[3, 4]; Anneli Kruve[2, 5]; *[1], Tartu, Estonia; [2]University of Tartu, Institute of Chemistry, Tartu, Estonia; [3]Discovery Sciences, Janssen Research and Development, Beerse, Belgium; [4]Maastricht Multimodal Molecular Imaging (M4I) Institute, Division of Imaging Mass Spectrometr, Maastricht, Netherlands; [5]Free University of Berlin, Institute of Chemistry and Biochemistry, Berlin, Germany*

MOA am 09:10 **Selecting a Structural Analog as an Internal Standard in Quantitative LC-MS/MS**; Kathryn Smith[1]; Stephen Merrigan[2]; Kamisha Johnson-Davis[2]; *[1]ARUP, Salt Lake City, UT; [2]ARUP Institute for Clinical and Experimental Pathology, Salt Lake City, UT*

MOA am 09:30 **GC-MS Method Development for 62 Emerging Disinfection By-Products to Evaluate Granular Activated Carbon in Full-Scale Plants and at Home**; Amy A Cuthbertson[1]; Susana Y. Kimura[1, 2]; Hannah K. Liberatore[1]; Detlef R.U. Knappe[3]; Benjamin Stanford[4, 5]; R. Scott Summers[6]; Eric Dickenson[7]; Clark Maness[3]; Riley E. Mulhern[6]; Caitlin Glover[7]; Meric Selbes[4]; Susan D. Richardson[1]; Vincent Esposito[1, 8]; Ashley Perkins[1, 9]; *[1]University of South Carolina, Columbia, SC; [2]University of Calgary, Calgary, AB, Canada; [3]North Carolina State University, Raleigh, NC; [4]Hazen and Sawyer, Raleigh, NC; [5]American Water, Voorhees, NJ; [6]University of Colorado, Boulder, CO; [7]Southern Nevada Water Authority, Henderson, NV; [8]University of Pennsylvania, Philadelphia, PA; [9]Clemson University, Clemson, SC*

MOA am 09:50 **Analogue to Digital Mass Spectrometry Quantification in the 21st Century;** Skip Kingston[1]; Scott Faber[2]; Logan Miller[1]; James Henderson[1]; Jeremiah Jamrom[1]; Weier Hao[1]; Lauren Stubbert[1]; John Kern[1]; Matt Pamuku[3]; *[1]Duquesne University, Pittsburgh, PA; [2]The Children's Institute of Pittsburgh, Pittsburgh, PA; [3]Applied Isotope Technologies, Pittsburge, PA*

MOA am 10:10 **Acoustic-OPP-MS: The Next Generation BioAnalytical Platform for Drug Discovery with Ultra-High Throughput**; Hui Zhang[1]; Chang Liu[2]; Jianhua Liu[1]; Wenyi Hua[1]; Tom Covey[2]; Luke Ghislain[3]; Sammy Datwani[3]; Timothy Foley[1]; John Janiszewski[1]; Matt Troutman[1]; Don Arnold[4]; *[1]Pfizer Inc., Groton, CT; [2]SCIEX, Concord, ON, Canada; [3]Labcyte, San Jose, CA; [4]SCIEX, Redwood City, CA*

8:30-10:30 am Monday
IMAGING: PHARMACEUTICALS, METABOLITES, AND LIPIDS
Session Chair: Sheerin K. Shahidi-Latham (Genentech, Inc.)
Ballroom 20A upper level

MOB am 08:30 **Mass-Tag Based Imaging Mass Spectrometry Approach to Investigate the Biodistribution of a Therapeutic Oligonucleotide**; Reid Groseclose[1]; Stephen Castellino[2]; *[1]GlaxoSmithKline, King Of Prussia, PA; [2]GlaxoSmithKline, King of Prussia, PA*

MOB am 08:50 **Elucidating the Effect of Ciprofloxacin Treatment for Salmonella Enterica Infection in an *in vivo* Mouse Model**; Nicole Strittmatter[1]; Gregory Hamm[1]; Richard Goodwin[1]; Panchali Kanvatirth[2]; Pietro Mastroeni[2]; *[1]AstraZeneca, UK, Cambridge, UK; [2]Cambridge University, Cambridge, UK*

MOB am 09:10 **Visualizing the Role of Cholesterol Metabolism in Statin-Mediated Protection Against Bacterial Infection**; Alison J Scott[1]; Anne Bruinen[2]; Shane R Ellis[2]; Ron M.A. Heeren[2]; Robert K. Ernst[1]; *[1]Department of Microbial Pathogenesis, School of Dentistry, University of Maryland, Baltimore, MD; [2]Maastricht MultiModal Molecular Imaging (M4I) insitute, Division of Imaging Mass Spectrometry (IMS), Maastricht, Netherlands*

MOB am 09:30 **Tracing the Metabolism of L-Dopa in Experimental Parkinson's Disease Brains by MALDI-MSI**; Elva Fridjonsdottir[1]; Mohammadreza Shariatgorji[1]; Anna Nilsson[1]; Theodosia Vallianatou[1]; Xiaoqun Zhang[2]; Per Svenningsson[2]; Erwan Bezard[3]; Per E. Andren[1]; *[1]Uppsala University, Uppsala, Sweden; [2]Karolinska Institutet, Stockholm, Sweden; [3]Université de Bordeaux, Bordeaux, France*

MOB am 09:50 **Quantitative Mass Spectrometry Imaging of Prostaglandins as Silver Ion Adducts with Nanospray Desorption Electrospray Ionization**; Kyle D Duncan[1]; Ru Fang[1]; Jia Yuan[2]; Rosalie K. Chu[3]; Sudhansu K. Dey[2]; Kristin E. Burnum-Johnson[3]; Ingela Lanekoff[1]; *[1]Department of Chemistry - BMC, Uppsala University, Uppsala, Sweden; [2]Devision of Reproductive Sciences, Cincinnati Children's Hospital Medical Center, Cincinnati, OH; [3]Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA*

MOB am 10:10 **Visualizing the Lipidome at Cellular Resolution Using a Modified MALDI FT-ICR MS Capable of 5 µm Imaging**; Jeffrey M Spraggins[1, 2]; Boone M. Prentice[1]; Daniel Ryan[1]; William J. Perry[1]; Marissa Jones[1]; Raf Van de Plas[2, 3]; Richard M. Caprioli[1, 2]; *[1]Vanderbilt University, Nashville, TN; [2]Vanderbilt Mass Spectrometry Research Center and Department of Biochemistry, Vanderbilt University School of Medicine, Nashville, TN; [3]Delft University of Technology, Delft, Netherlands*

8:30-10:30 am Monday
MS IN THE QC LAB
Session Chair: Jason Rouse (Pfizer, Inc.)
Ballroom 20BC upper level

MOC am 08:30 **Improving Critical Quality Attribute Coverage and MAM Throughput By Leveraging a Multi-Enzyme Multi-Attribute Method**; Richard Rogers[1]; Michael Rosenblatt[2]; Nancy S Nightlinger[1]; Marjeta Urh[2]; Yuko Ogata[1]; Chris Hosfield[2]; *[1]Just Biotherapeutics, Seattle, WA; [2]Promega Corporation, Madison, WI*

MOC am 08:50 **Unattended Just-In-Time Antibody Digestion and Analysis on a Regular LC/MS System Without Additional Equipment**; Jason L. Richardson[1]; Zhongqi Zhang[1]; *[1]Amgen, Thousand Oaks, CA*

MOC am 09:10 **Mass Spectrometry-Based Characterization of a Non-Originator NISTmAb**; John Schiel[1]; Katharina Yandrofski[1]; John Giddens[1]; Trina Mouchahoir[1]; Lila Kashi[1]; Zvi Kelman[1]; *[1]NIST, Rockville, MD*

MOC am 09:30 **Development and Assessment of the Multi-Attribute Method (MAM): New Peak Detection and Orthogonal Method Comparisons**; Xiaoshi Wang[1]; Phillip Angart[1]; Brandon Kim[1]; Ramesh Venna[1]; David Naoki Powers[1]; Ilan Geerlof-Vidavsky[2]; Hongping Ye[2]; David Keire[2]; Sarah Rogstad[1]; *[1]FDA, Silver Spring, MD; [2]FDA Division of Pharmaceutical Analysis, St Louis, MO*

MOC am 09:50 **Streamlining the Identification and Monitoring of Product and Process Attributes in Biopharmaceutical Development and QC with MAM-based Workflows**; Robert Birdsall[1]; Ximo Zhang[1]; Weibin Chen[1]; Ying Qing Yu[1]; Brooke Koshel[1]; *[1]Waters Corporation, Milford, MA*

MOC am 10:10 **ID Testing by HRMS of Large-Molecule Biological Reagents for GMP Manufacturing**; Philip Anderson[1]; Laura Hayter[1]; *[1]Avista Pharma Solutions, Longmont, CO*

8:30-10:30 am Monday
GC/MS, GC/GC/MS, GC/MS/MS, AND GC/HRMS
Session Chair: Irwin J. Kurland (Albert Einstein College of Medicine)
Ballroom 20D upper level

MOD am 08:30 **Structural Annotation and Identification of Metabolites by Mass Spectrometry-Based Cheminformatics**; Oliver Fiehn[1]; Hiroshi Tsugawa[2]; Ivana Blazenovic[1]; Megan Showalter[1]; Gert Wohlgemuth[1]; Sajjan Mehta[1]; Zijuan Lai[1]; Masanori Arita[3]; *[1]UC Davis, Davis, CA; [2]RIKEN CSRS, Yokohama, Japan; [3]National Institute of Genetics, Mishima, Japan*

MOD am 08:50 **Improving and Extending a High-Quality and Comprehensive Reference Electron Ionization (EI) Mass Spectral Library**; Weihua Ji[1]; Yufang Zheng[1]; Gary Mallard[1]; Dmitrii V. Tchekhovskoi[1]; Yuri A. Mirokhin[1]; Oleg V. Toropov[1]; Tytus Mak[1]; William E. Wallace[1]; Stephen E. Stein[1]; *[1]NIST, Gaithersburg, MD*

MOD am 09:10 **A Gas Chromatography – Mass Spectrometry Workflow for the Accurate Quantification of Traces of 13C-Enriched Metabolites in Human Plasma**; Lisa Krämer[1]; Christian Jäger[2]; Jean-Pierre Trezzi[2]; Doris M. Jacobs[3]; Karsten Hiller[1, 4]; *[1]Department of Biochemistry and Bioinformatics, BRICS, Technische Universität Braunschweig, Braunschweig, Germany; [2]Luxembourg Centre for Systems Biomedicine, Belvaux, Luxembourg; [3]Unilever R&D, Vlaardingen, Netherlands; [4]Helmholtz Centre for Infection Research, Braunschweig, Germany*

MOD am 09:30 **Quadrupole GC/MS Fragment Analysis for Improving Compound Identification**; Don Kuehl[1]; Yongdong Wang[1]; *[1]Cerno Bioscience, Norwalk, CT*

MOD am 09:50 **GC-APCI-MS Platform for Profiling Plant and Gut Microbial Metabolites**; Johana S Revel[1, 2, 3]; Laurent Deluc[4]; Gombart F Adrian[2]; Jan F Stevens[2, 3]; Claudia S Maier[1, 2, 3]; *[1]Department of Chemistry, Oregon State University, Corvallis, OR; [2]Linus Pauling Institute, Oregon State University, Corvallis, OR; [3]Mass Spectrometry Center, Oregon State University, Corvallis, OR; [4]Department of Horticulture, Oregon State University, Corvallis, OR*

MOD am 10:10 **The DBP Exposome: Development of a New Method to Simultaneously Quantify Priority Disinfection By-Products and Comprehensively Identify Unknowns**; Susana Y Kimura Hara[1]; Amy A Cuthbertson[2]; Jonathan Byer[3]; Susan D. Richardson[2]; *[1]University of Calgary, Calgary, AB; [2]University of South Carolina, Columbia, SC; [3]LECO Corporation, Saint Joseph, MI*

8:30-10:30 am Monday
NUCLEIC ACIDS AND OLIGONUCLEOTIDES
Session Chair: Daniele Fabris
(The RNA Institute, University at Albany)
Ballroom 6A upper level

MOE am 08:30 **Native Top-Down Mass Spectrometry Puts a Spotlight on RNA-Protein and RNA-Drug Complexes**; Eva-Maria Schneeberger[1]; Kathrin Breuker[1]; *[1]University of Innsbruck, Innsbruck, Austria*

MOE am 08:50 **Structure, Stability and Interactions of Cocaine-Binding Aptamers Using Native IM-MS**; Elise Daems[1]; Debbie Dewaele[1]; Karolien De Wael[1]; Frank Sobott[1, 2, 3]; *[1]University of Antwerp, Antwerp, Belgium; [2]Astbury Centre for Structural Molecular Biology, Leeds, UK; [3]School of Molecular and Cellular Biology, Leeds, UK*

MOE am 09:10 **Double Stranded Nucleic Acids *in-vacuo*: Spine Stiffening with Silver Ions - an Ion Mobility and QM Study**; Frederic Rosu[1]; Steven M. Swasey[2]; Elisabeth G. Gwinn[2]; Valérie Gabelica[3]; *[1]CNRS, INSERM & University of Bordeaux (IECB), Pessac, France; [2]UCSB, Santa Barbara, California; [3]INSERM, CNRS & University of Bordeaux (ARNA Laboratory), Pessac, France*

MOE am 09:30 **Reaction Dynamic Simulations for Fragmentation Spectra Prediction and DNA Adducts Structural Determination**; Andrea Carra[1]; Riccardo Spezia[2, 3]; Peter W. Villalta[4]; Veronica Macaluso[3]; Silvia Balbo[4]; *[1]University of Minnesota, Minneapolis, MN; [2]Sorbonne Université, Paris, France; [3]Université Evry, Paris, France; [4]Masonic Cancer Center, University of Minnesota, Minneapolis, MN*

MOE am 09:50 **DNA-Protein Cross-Links and Their Effects on DNA Replication and Transcription**; Shaofei Ji[1]; Daeyoon Park[1]; Qiyuan Han[1]; Natalia Tretyakova[1]; *[1]University of Minnesota, Twin Cities, Minneapolis, MN*

MOE am 10:10 **Investigating Metabolism and Tissue Distribution of Phosphorothioate Linked Oligonucleotides in Rats Using Untargeted LC-HRMS and Complementary MALDI-FTICR Imaging**; Andreas Brink[1]; Fernando Romero-Palomo[1]; Christophe Husser[1]; Bernd Steinhuber[1]; Rachel Neff[2]; Annamaria Braendli-Baiocco[1]; Matthias Festag[1]; Barbara Lenz[1]; Simone Schadt[1]; *[1]Pharmaceutical Sciences, Pharma Research and Early Development, Roche Innovation Center Basel, F. Hoffmann-La Roche Ltd., Basel, Switzerland; [2]Pharmaceutical Sciences, Pharma Research and Early Development, Roche Innovation Center Basel F. Hoffmann-La Roche Ltd., Basel, Switzerland*

8:30-10:30 am Monday
NATIVE MS IN STRUCTURAL BIOLOGY
Session Chair: Jeffrey C. Smith (Carleton University)
Ballroom 6B upper level

MOF am 08:30 **Native Nanospray-MS Enables the Direct Observation of the Conformational Dynamics of RNA Kissing Complexes in the HIV-1 Genome**; Botros Toro[1]; Pan T.X. Li[2]; Daniele Fabris[2]; *[1]State University of New York at Albany, Albany, NY; [2]RNA Institute, University at Albany, Albany, NY*

MOF am 08:50 **Formation, Stability and Topology of DNA Nanopores Investigated by Native MS and Ion Mobility**; Jeroen F. Van Dyck[1]; Jonathan R. Burns[2]; Albert Konijnenberg[1]; Stefan Howorka[2]; Frank Sobott[1, 3, 4]; *[1]Biomolecular & Analytical Mass Spectrometry, Chemistry Department, University of Antwerp, Antwerp, Belgium; [2]Institute of Structural and Molecular Biology, Department of Chemistry, University College London, London, United Kingdom; [3]Astbury Centre for Structural Molecular Biology, Leeds, UK; [4]School of Molecular and Cellular Biology, Leeds, UK*

MOF am 09:10 **Mass Spectrometric Analysis of Disease Triggering Amyloids: Combining ESI-IMS and LILBID-MS**; Tobias Lieblein[1]; Rene Zangl[1]; Janosch Martin[1]; Nina Morgner[1]; *[1]Physical Chemistry, Goethe-University Frankfurt, Frankfurt, Germany*

MOF am 09:30 **Multi-Stage Native UVPD-MS to Characterize Single Amino Acid Variants of Human Mitochondrial BCAT2**; M Rachel Mehaffey[1]; Carol L Nilsson[2]; Jennifer S Brodbelt[1]; *[1]The University of Texas at Austin, Austin, TX; [2]Lund University, Lund, Sweden*

MOF am 09:50 **Determining Mass and Stoichiometry of MegaDa Particles by Native MS on the Q-Exactive Ultra-High Mass Range (QE-UHMR)**; Tobias Wörner[1]; Arjan Barendregt[1]; Albert J.R. Heck[1]; *[1]Utrecht University, Utrecht, Netherlands*

MOF am 10:10 **Is Native Mass Spectrometry Really Native? Comparisons of Protein Structures in Ammonium Acetate and in Common Biochemical Buffers**; Zijie Xia[1]; Joseph DeGrandchamp[1]; Evan R Williams[1]; *[1]UC Berkeley, Berkeley, CA*

8:30-10:30 am Monday
INFORMATICS: INNOVATIONS
Session Chair: Rob Smith (University of Montana)
Ballroom 6CF upper level

MOG am 08:30 **Accurate Assessment of Peptide Differential Expression Using a Bayesian Inference Approach**; Linh VH Nguyen[1]; Shelley A Deeke[1];

Daniel Figeys[1]; Mathieu Lavallée-Adam[1]; [1]*University of Ottawa, Ottawa*

MOG am 08:50 **A Combined Identification and Quantification Error Model of Label-Free Protein Quantification**; Matthew The[1]; Lukas Käll[1]; [1]*Royal Institute of Technology - KTH, Solna, Sweden*

MOG am 09:10 **An Averaging Strategy to Reduce Variance in Target-Decoy Estimates of False Discovery Rate**; William Noble[1]; Uri Keich[2]; [1]*University of Washington, Seattle, WA;* [2]*University of Sydney, Sydney, Australia*

MOG am 09:30 **Using Synthetic Peptides from the Proteometools Project to Estimate FDR in HLA-Datasets**; Mathias Wilhelm[1]; Daniel P Zolg[1]; Siegfried Gessulat[1, 2]; Tobias K Schmidt[1]; Patroklos Samaras[1]; Karsten Schnatbaum[3]; Johannes Zerweck[3]; Tobias Knaute[3]; Ulf Reimer[3]; Hans-Christian Ehrlich[2]; Stephan Aiche[2]; Pedro Navarro[4]; Bernard Delanghe[4]; Andreas Huhmer[5]; Bernhard Kuster[1, 6, 7]; [1]*Technical University of Munich, Chair of Proteomics and Bioanalytics, Freising, Germany;* [2]*SAP SE, Potsdam, Germany;* [3]*JPT Peptide Technologies GmbH, Berlin, Germany;* [4]*Thermo Fisher Scientific, Bremen, Germany;* [5]*Thermo Fisher Scientific, San Jose, CA;* [6]*Center for Integrated Protein Science (CIPSM), Munich, Germany;* [7]*Bavarian Center for Biomolecular Mass Spectrometry, Freising, Germany*

MOG am 09:50 **Orbitrap FTMS-Based Normalized (Non-Kendrick) Mass Maps of Poly-Oxy Oligomers in 3D Space**; Robert J Strife[1]; Jason M. Price[1]; [1]*Procter & Gamble, Mason, OH*

MOG am 10:10 **Combine, Visualize and Compare Proteomic Datasets with PACOM, the Proteomics Assay COMparator**; Salvador Martínez-Bartolomé[1, 2]; J. Alberto Medina-Aunon[2]; Miguel Ángel López-García[2]; Carmen González-Tejedo[2]; Gorka Prieto[3]; Rosana Navajas[2]; Emilio Salazar-Donate[2]; Carolina Fernández-Costa[1, 4]; John R. Yates III[1]; Juan Pablo Albar[2]; [1]*Department of Molecular Medicine - The Scripps Research Institute, La Jolla, CA;* [2]*Proteomics Laboratory - National Center for Biotechnology, CSIC, Madrid, Spain;* [3]*Department of Communications Engineering, University of the Basque Country (UPV/EHU), Bilbao, Spain;* [4]*Immunology, Centro de Investigaciones Biomédicas (CINBIO), Centro singular de Investigación de Galicia: Instituto de Investigación Sanitaria Galicia Sur (IIS-GS). University of Vigo, Vigo, Spain*

8:30-10:30 am Monday
ENERGY, PETROLEUM, AND BIOFUELS: INSTRUMENTATION AND APPLICATIONS
Session Chair: Carolyn Hutchinson (Willamette University)
Ballroom 6DE upper level

MOH am 08:30 **Molecular Level Insights in Heavy Gas Oil Hydrodenitrogenation by Fourier Transform Ion Cyclotron Resonance Mass Spectrometry**; Minh Tuan Nguyen[1]; Gerhard D. Pirngruber[1]; Fabien Chainet[1]; Florian Albrieux[1]; Melaz Tayakout-Fayolle[2]; Christophe Geantet[3]; [1]*IFPEN, Solaize, France;* [2]*Laboratoire d'Automatique et de Génie des Procédés, Université Claude Bernard Lyon 1, CNRS/UCBL, UMR 5007, Villeurbanne Cedex, France;* [3]*Institut de Recherches sur la Catalyse et L'environnement de Lyon, IRCELYON, UMR 5256/ CNRS-Université Lyon 1, Villeurbanne Cedex, France*

MOH am 08:50 **Aromatic Core Formation and Side Chain Losses from Series of Isomeric Model Compounds of Petroleum: Energetics and Practical Applications**; Maha Abutokaikah[1]; Joseph Frye[2]; Curtis Stump[2]; Giri Gnawali[2]; Christopher D. Spilling[2]; Benjamin J. Bythell[2]; [1]*UMSL, St Louis;* [2]*University of Missouri-St. Louis, St Louis, MO*

MOH am 09:10 **Advances in Asphaltene Petroleomics: Overcoming Limitations in Selective Ionization to Reveal the Structural Continuum of Island and Archipelago Motifs**; Martha Liliana Chacón-Patiño[1]; Steven M Rowland[1, 2]; Ryan P Rodgers[1, 2, 3]; [1]*National High Magnetic Field Laboratory, Tallahassee, FL;* [2]*Future Fuels Institute, Tallahassee, FL;* [3]*Department of Chemistry, Florida State University, Tallahassee, FL*

MOH am 09:30 **Characterization of NAFCs in Laboratory Constructed Wetlands by GCxGC/HRMS and FTMS**; Sophia A Schreckenbach[1, 2]; David T Bowman[2, 3]; Chukwuemeka Ajaero[4]; Eric J Reiner[2]; Karl J Jobst[2]; Ralph Ruffolo[2]; Kerry M Peru[4]; Dena W McMartin[5]; Gwen O'Sullivan[1]; John V Headley[4]; [1]*Mount Royal University, Calgary, ON, Canada;* [2]*Ontario Ministry of Environment and Climate Change, Toronto, ON, Canada;* [3]*University of Toronto, Toronto, ON, Canada;* [4]*Environment and Climate Change Canada, Science and Technology Branch, Saskatoon, SK, Canada;* [5]*University of Saskatchewan, Saskatoon, SK, Canada*

MOH am 09:50 **Compositional Analysis of Low and High Volatility Species within a Bio-Oil and Its Esterified Product**; Diana Catalina Palacio Lozano[1]; Claudia X. Ramírez[2]; Matthias Witt[3]; José A. Sarmiento Chaparro[4]; Enrique Mejía-Ospino[2]; Mark P. Barrow[1]; [1]*University of Warwick, coventry, UK;* [2]*Universidad Industrial de Santander, Bucaramanga, Colombia;* [3]*Bruker Daltonik GmbH, Bremen, Germany;* [4]*Ecopetrol, Piedecuesta, Colombia*

MOH am 10:10 **Detecting and Identifying Volatile Chemical Signatures of Algae Pond Crash**; Curtis Mowry[1]; Matthew W. Moorman[1]; Adam S. Pimentel[1]; Jason P. Sammon[1]; Todd W. Lane[2]; Carolyn L. Fisher[2]; Stephen M. Anthony[1]; [1]*Sandia National Laboratories, Albuquerque, NM;* [2]*Sandia National Laboratories, Livermore, CA*

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

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

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

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

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

2:30-4:30 pm Monday
INSTRUMENTATION: INNOVATIVE SEPARATIONS APPROACHES COUPLED TO MS
Session Chair: J. Scott Mellors (908 Devices, Inc.)
Hall D ground level

MOA pm 02:30 **A Novel Nanoflow LCMS Limited Sample Proteomics Approach Using Micro Pillar Array Columns (µPACTM)**; Aran Paulus[1]; Jeff op de Beeck[2]; Paul Jacobs[2]; Wim de Malsche[3]; Gert Desmet[3]; Pamela Saliba[4]; Tabbiwang N. Array[5]; Aaron Gajadhar[6]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]PharmaFluidics NV, Gent, Belgium; [3]Vrije Universiteit Brussel, Brussels, Belgium; [4]Thermo Fisher Scientific, Dreieich, Germany; [5]Thermo Fisher Scientific, Bremen, Germany; [6]Thermo Scientific, San Jose, CA*

MOA pm 02:50 **On-Line Mass Spectrometric Characterization of Intact Proteins in Highly ESI-Interfering Separation Systems**; Christian Neususs[1]; Jennifer Roemer[1]; Cristina Montealegre[1]; Kevin Jooss[1]; Steffen Kiessig[2]; Bernd Moritz[2]; *[1]Aalen University, Aalen, Germany; [2]F. Hoffmann-La Roche Ltd, Basel, Switzerland*

MOA pm 03:10 **Exploring the Limits of Resolution in Structures for Lossless Ion Manipulations (SLIM) Traveling Wave-Based Ion Mobility -MS**; Richard D. Smith[1]; Roza Wojcik[2]; Christopher D. Chouinard[2]; Gabe Nagy[2]; Sandilya Garimella[2]; Spencer A. Prost[2]; Ian K. Webb[2]; Erin S. Baker[2]; Yehia M. Ibrahim[2]; *[1]PNNL, Richland, WA; [2]Pacific Northwest National Laboratory, Richland, WA*

MOA pm 03:30 **Characterising Monoclonal Antibody Heterogeneity via Charge Variant Analysis Hyphenated to On-Line High Resolution Native Mass Spectrometry**; Florian Fuessl[1]; Anne Trappe[1]; Jonathan Bones[1]; *[1]National Institute for Bioprocessing Research and Training, Dublin, Ireland*

MOA pm 03:50 **Investigation of Protein-Protein Interaction Specificity for Computationally Designed Heterodimers Using Ion Exchange Chromatography (IEX) Coupled to Native Mass Spectrometry (MS)**; Mengxuan Jia[1]; Florian Busch[1]; Zachary VanAernum[1]; Aniruddha Sahasrabuddhe[1]; Zibo Chen[2]; Scott Boyken[2]; David Baker[2]; Vicki H. Wysocki[1]; *[1]The Ohio State University, Columbus, OH; [2]University of Washington, Seattle, WA*

MOA pm 04:10 **Enhancing Proteomic Throughput in Capillary Electrophoresis-Mass Spectrometry by Sequential Sample Injection**; Klaus Faserl[1]; Bettina Sarg[1]; Herbert Lindner[1]; *[1]Innsbruck Medical University, Innsbruck, Austria*

2:30-4:30 pm Monday
IMAGING: BIOMEDICAL APPLICATIONS
Session Chair: Shama Mirza
(University of Wisconsin - Milwaukee)
Ballroom 20A upper level

MOB pm 02:30 **Quantifying the Neuromolecular Phenotype of Murine GM1 Gangliosidosis with Mass Spectrometry Imaging and Region of Interest Analysis**; Khaja Muneeruddin[1, 2]; Bindesh Shrestha[3]; Sophia Todeasa[4, 5]; Miguel Sena-Esteves[4, 5]; Scott A Shaffer[1, 2]; *[1]Department of Biochemistry and Molecular Pharmacology, University of Massachusetts Medical School, Worcester, MA; [2]Mass Spectrometry Facility, University of Massachusetts Medical School, Worcester, MA; [3]Waters Corp, Beverly, MA; [4]Department of Neurology, University of Massachusetts Medical School, Worcester, MA; [5]Horae Gene Therapy Center, University of Massachusetts Medical School, Worcester, MA*

MOB pm 02:50 **Mapping Metabolism in Glioblastoma with MALDI MSI**; Elizabeth C Randall[1]; Sankha S Basu[1]; Begona G. C. Lopez[1]; Walid M Abdelmoula[1]; Michael S Regan[1]; Forest M White[2]; Jann N Sarkaria[3]; Nathalie Y. R. Agar[1, 4]; *[1]Brigham and Women's Hospital/ Harvard Medical Sch, Boston, MA; [2]The Koch Institute for Integrative Cancer Research at MIT, Boston, MA; [3]Mayo Clinic, Rochester, MN; [4]Dana-Farber Cancer Institute, Boston, MA*

MOB pm 03:10 **Visualizing the Distribution of Anti-Retroviral Agents in Sheep Vaginal Tissue by Imaging Mass Spectrometry**; Michelle L. Reyzer[1]; Michael D. Tuck[1]; Jennifer L. Harvey[1]; M. Lisa Manier[1]; Mark Marzinke[2]; Kathy Vincent[3]; Massoud Motamedi[3]; John A. Moss[4]; Marc M. Baum[4]; Richard M. Caprioli[1]; *[1]Vanderbilt University, Nashville, TN; [2]Johns Hopkins School of Medicine, Baltimore, MD; [3]University of Texas, Galveston, TX; [4]Oak Crest Institute of Science, Monrovia, CA*

MOB pm 03:30 **Top-Down Mass Spectrometry Imaging of Endogenous Secretory Peptides in Clinical Human FFPE Material of Many Years Old with Immunohistochemical Validation**; Peter D. Verhaert[1, 2]; Marc Ramael[3]; Ann-Christin Niehoff[4]; Marthe A. Verhaert[5]; Raf Sciot[5]; *[1]M4i Maastricht Multimodal Molecular Imaging Institute, Maastricht, Netherlands; [2]ProteoFormiX, Beerse, Belgium; [3]University of Antwerp, Antwerp, Belgium; [4]Shimadzu Europa GmbH, Duisburg, Germany; [5]University Hospital Leuven, Leuven, Belgium*

MOB pm 03:50 **How Innovative Imaging MS Approaches Shed Light on What Happens in Traumatic Brain Injury**; Amina S. Woods[1]; Luidovic Muller[1]; Jeremy Post[1]; Damon C Barbacci[2]; Carey D Balaban[3]; J. Albert Schultz[2]; Brian M Cox[4]; Shelley N Jackson[1]; *[1]NIDA-IRP, NIH, Baltimore, MD; [2]Ionwerks, Inc, Houston, TX; [3]Departments of Otolaryngology, Neurobiology, University of Pittsburgh, Pittsburgh, PA; [4]Uniformed Services University, Bethesda, MD*

MOB pm 04:10 **Development of a Dual Imaging Strategy Combining Radio- and Mass Spectrometry-Imaging to Study the Biodistribution of 14C-Graphene Oxide**; Hélène Cazier[1]; Dominique Georgin[2]; Carole Malgorn[3]; Frederic Taran[2]; Vincent Dive[3]; Christophe Junot[1]; François Fenaille[1]; Benoit Colsch[1]; *[1]Service de Pharmacologie et d'Immunoanalyse, Laboratoire d'Etude du Métabolisme des Médicaments, CEA, INRA, Université Paris Saclay, MetaboHUB, F-91191 Gif-sur-Yvette, France; [2]Service de Chimie Bioorganique et de Marquages, CEA, Université Paris Saclay, F-91191 Gif-sur-Yvette, France; [3]Service d'Ingénierie Moléculaire des Protéines, CEA, Université Paris Saclay, F-91191 Gif-sur-Yvette, France*

2:30-4:30 pm Monday
DRUG TARGET IDENTIFICATION BY MS
Session Chair: Chris Turck (Max Planck Institute)
Ballroom 20BC upper level

MOC pm 02:30 **MS-CETSA for Target Deconvolution of Phenotypic Screening Hits and Approved Drugs**; Nayana Prabhu[1]; Brenda Puspita[1]; Linguyn Dai[1]; Jerzy Dziekan[1]; Loo Chien Wang[1]; Yu Han[1]; Radoslaw M Sobota[2]; Par Nordlund[1, 2, 3]; *[1]Nanyang Technological University, Singapore, Singapore; [2]Institute of Molecular and Cell Biology, Singapore, Singapore; [3]Karolinska Institutet, Stockholm, Sweden*

MOC pm 02:50 **Aspirin Reprograms Acetylome in Mouse**; Lin Guo[1]; Jiali Qiang[1]; Yaoyang Zhang[1]; *[1]Interdisciplinary Research Center on Biology and Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai, China*

MOC pm 03:10 **Discovery and Characterization of Druggable Proteins That Regulate Human T Cell Activation**; Ekaterina V Vinogradova[1]; Daniel Lazar[1]; Yu Yamashita[1]; Michael Lazear[1]; Sifei Yin[1]; Megan Blewett[1]; John Teijaro[1]; Benjamin Cravatt[1]; *[1]The Scripps Research Institute, La Jolla, CA*

MOC pm 03:30 **Identification of a Mitochondrial ATP Synthase as a Drug Target for Aging-associated Pathologies and Dementia**; Wolfgang Fischer[1]; Joshua Goldberg[1]; Marguerite Prior[1]; Chandramouli Chiruta[1]; Daniel Daugherty[1]; Richard Dargusch[1]; Antonio Currais[1]; Pamela Maher[1]; David Schubert[1]; *[1]SALK Institute, La Jolla, CA*

MOC pm 03:50 **Bioactivity Based Molecular Networking for the Discovery of Drug Leads in Bioassay-Guided Fractionation**; Louis Felix Nothias[1, 2]; Mélissa Nothias-Esposito[2, 3]; Ricardo Silva[1]; Ivan Protsyuk[4]; Mingxun Wang[1]; Zheng Zhang[1]; Abinesh Sarvepali[1]; Pieter Leyssen[5]; David Touboul[2]; Jean Costa[3]; Julien Paolini[3]; Theodore Alexandrov[1, 4]; Marc Litaudon[2]; Pieter C. Dorrestein[1]; *[1]University of California San Diego, Skaggs School of Pharmacy and Pharmaceutical Sciences, La Jolla, CA; [2]CNRS, Gif-sur-Yvette, France; [3]University of Corsica, Corte, France; [4]EMBL, European Molecular Biology Laboratory, Heidelberg, Germany; [5]Rega Institute for Medical Research, KU Leuven, Leuven, Belgium*

MOC pm 04:10 **Fighting the Opioid Crisis Using Mobile Mass Spectrometry and DART-HRMS**; Sara Kern[1]; Travis M. Falconer[1]; Frederick Li[2]; Valerie M. Toomey[1]; Jonathan J. Litzau[1]; *[1]FDA, Cincinnati, OH; [2]IonSense, Inc., Saugus, MA*

2:30-4:30 pm Monday
TOP DOWN PROTEIN ANALYSIS
Session Chair: Si Wu (University of Oklahoma)
Ballroom 20D upper level

MOD pm 02:30 **"Complex-Down" Native MS-SID-IM-MS and Crosslinking Reveal Differences in Quaternary Structures of Homolog Protein Complexes**; Florian Busch[1]; Andrew Norris[1]; Florian Semmelmann[2]; Reinhard Sterner[2]; Vicki Wysocki[1]; *[1]The Ohio State University, Columbus, OH; [2]University of Regensburg, Regensburg, Germany*

MOD pm 02:50 **Native Top-Down Mass Spectrometry of Membrane Proteins: Challenges and Solutions**; Joseph A. Loo[1]; Huilin Li[1]; Wonhyeuk Jung[1]; Pascal Egea[1]; Michael Nshanian[1]; *[1]UCLA, Los Angeles, CA*

MOD pm 03:10 **Top-Down Quantitative Proteomics for Assessing the Maturation of Human Pluripotent Stem Cell-Derived Cardiomyocytes**; Wenxuan Cai[1]; Jianhua Zhang[1]; William de Lange[1]; Zachery Gregorich[1]; John Carter Ralphe[1]; Timothy Kamp[1]; Ying Ge[1]; *[1]University of Wisconsin, Madison, WI*

MOD pm 03:30 **False Quantitative Discovery Rate (FQDR): A Tunable Metric that Enables Quantitative Top Down Proteomics via Empirical False Discovery Estimation**; Matthew V. Holt[1]; Tao Wang[1]; Nicolas L. Young[1]; *[1]Baylor College of Medicine, Houston, TX*

MOD pm 03:50 **Extending the Mass Range of Top-Down Proteomics Applying Ion-Ion Proton Transfer Reactions on a Tribrid Mass Spectrometer**; Romain Huguet[1]; Luca Fornelli[2]; Kristina Srzentić[2]; Christopher Mullen[1]; John E. P. Syka[1]; Joshua A Silveira[1]; Helene Cardasis[1]; Stephane Houel[1]; Vlad Zabrouskov[1]; Neil Kelleher[2]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Northwestern University, Evanston, IL*

MOD pm 04:10 **Enhancing Dissociation Strategies for High-Resolution Top-Down Integral Membrane Protein Analysis**; Whitaker Cohn[1]; Piotr Ruchala[1]; Chris Gisriel[2]; Raimund Fromme[2]; Romain Huguet[3]; Christopher Mullen[3]; Vlad Zabrouskov[3]; Frederic Halgand[4]; Julian Whitelegge[1]; *[1]University of California LA, Los Angeles, CA; [2]School of Molecular Sciences, Arizona State University, Tempe, AZ; [3]ThermoFisher, San Jose, CA; [4]Université Paris Sud-CNRS, Orsay, France*

2:30-4:30 pm Monday
CARBOHYDRATES
Session Chair: Catherine E. Costello (Boston University)
Ballroom 6A upper level

MOE pm 02:30 **Competitive Universal Proxy Receptor Assay (CUPRA) for Quantitative High-Throughput Glycan Library Screening**; John S. Klassen[1, 2]; Elena N. Kitova[1, 2]; Pavel Kitov[1, 2]; Zhixiong Li[1, 2]; *[1]University of Alberta, Edmonton, AB, Canada; [2]Alberta Glycomics Centre, Edmonton, AB, Canada*

MOE pm 02:50 **Comparing Hydrogen/Deuterium Exchange – Mass Spectrometry Methods for Sampling Solvated Carbohydrate Conformations**; H. Jamie Kim[1]; O. Tara Liyanage[1]; Elyssia S. Gallagher[1]; *[1]Department of Chemistry and Biochemistry, Baylor University, Waco, Texas*

MOE pm 03:10 **Combining Cryogenic Ion Spectroscopy with Ion Mobility and Mass Spectrometry for the Identification of Glycans**; Chiara Masellis[1]; Neelam Khanal[2]; Robert P. Pellegrinelli[1]; Maximillian Doppelbauer[1]; David E. Clemmer[2]; Thomas Rizzo[1]; *[1]Ecole Polytechnique Fédérale de Lausanne, Ch-1015 Lausanne, Switzerland; [2]Department of Chemistry, Indiana University, Bloomington, IN*

MOE pm 03:30 **Negative Ion Electron Capture Dissociation (niECD) of Glycans**; Isaac Agyekum[1]; Kristina Hakansson[1]; *[1]University of Michigan, Ann Arbor, MI*

MOE pm 03:50 **Capillary Electrophoresis Analysis of Anionically Tagged N- Linked Carbohydrates by Simultaneous LIF and MS Detection**; Andras Guttman[1]; Mate Szarka[2]; Marton Szigeti[2]; *[1]Sciex, Brea, CA; [2]Horvath Csaba Laboratory of Bioseparation Sciences, Debrecen, Hungary*

MOE pm 04:10 **Negative Electron Transfer Dissociation Paired with Capillary Electrophoresis-Mass Spectrometry for the Investigation of Glycosaminoglycan Mixtures**; Morgan Stickney[1]; Patience Sanderson[1]; Franklin E. Leach III[1]; Joshua J Coon[2]; Michael S Westphall[2]; Nicholas M Riley[2]; James Xia[3]; Fuming Zhang[4]; Robert J Linhardt[4]; I. Jonathan Amster[1]; *[1]University of Georgia, Athens, GA; [2]University of Wisconsin–Madison, Madison, WI; [3]CMP Scientific, Corp., Brooklyn, NY; [4]Rensselaer Polytechnic Institute, Troy, NY*

2:30-4:30 pm Monday
PROTEIN-LIGAND INTERACTIONS
Session Chair: Ganesh S. Anand (NUS Singapore)
Ballroom 6B upper level

MOF pm 02:30 **Integrating Structural Proteomics into Lead Optimization and Chemical Probe Development: Insights to RORγ Structure and Function**; Tim Strutzenberg[1]; Patrick R. Griffin[1]; Scott J Novick[1]; Ruben Garcia-Ordonez[1]; *[1]The Scripps Research Institute, Palm Beach Gardens, FL*

MOF pm 02:50 **High Resolution Structural Footprinting for Drug Binding Site Assessment**; Janna Kiselar[1]; Liwen Wang[1]; Sichun Yang[1]; Mark R Chance[1]; *[1]Case Western Reserve Univ, Cleveland, OH*

MOF pm 03:10 **Structural Dynamic Elucidation by Hydrogen/Deuterium Exchange: Protein-Ligand Interaction Through Thermodynamically Disfavored Conformational Switchi**; Xiaojing Huang[1]; Erfei Song[1]; Gary Sweeney[1]; Derek J. Wilson[1]; *[1]York University, Toronto, ON, Canada*

MOF pm 03:30 **Using Native Top-Down nESI FTICR-MS to Characterize the Interaction of Tau Protein with Assembly Modulator CLR01**; Michael Nshanian[1]; Piriya Wongkongkathep[1]; Carter Lantz[1]; Gal Bitan[1]; Joseph A Loo[1]; *[1]UCLA, Los Angeles, CA*

MOF pm 03:50 **The Missing Link: Methods for Analysis of Proteins Bound to Long Non-Coding RNAs**; Christina R Hartigan[1]; Mathias Munschauer[1]; Monica Schenone[1]; Steven A Carr[1]; Eric S Lander[1]; *[1]Broad Institute of MIT and Harvard, Cambridge, MA*

MOF pm 04:10 **Systematic Profiling of HLA Class I Peptide Epitopes by LC-MS/MS in Mono-Allelic Cells Improves Neoantigen Binding Prediction Algorithms**; Susan Klaeger[1]; Derin B Keskin[2, 3]; Siranush Sarkizova[4]; Karl R Clauser[1]; Oliver Spiro[1]; Hasmik Keshishian[1]; Christina R Hartigan[1]; Jennifer G Abelin[1]; Nir Hacohen[1, 5]; Catherine J Wu[1, 2, 3, 4]; Steven A Carr[1]; *[1]The Broad Institute of MIT and Harvard, Cambridge, MA; [2]Department of Medical Oncology, Dana-Farber Cancer Institute, Boston, MA; [3]Department of Medicine, Brigham and Women's Hospital, Boston, MA; [4]Harvard Medical School, Boston, MA; [5]Massachusetts General Hospital, Boston, MA*

2:30-4:30 pm Monday
INFORMATICS: DETERMINATION OF ELEMENTAL COMPOSITION
Session Chair: Don Kuehl (Cerno Bioscience)
Ballroom 6CF upper level

MOG pm 02:30 **Determining Molecular Formulas for Unknown Analysis of Small Molecules Using High Resolution and Accurate Mass**; E. Michael Thurman[1]; Imma Ferrer[1]; Jerry Zweigenbaum[2]; *[1]University of Colorado, Boulder, CO; [2]Agilent Technologies, Inc., Wilmington, DE*

MOG pm 02:50 **Elemental Composition Assignment in Complex Mixtures by Accurate Mass Measurement and Resolution of Isotopic Fine Structure**; Christopher L. Hendrickson[1, 2]; Greg T. Blakney[1]; Yuri E. Corilo[1]; Alan G Marshall[1, 2]; Ryan P. Rodgers[1, 2]; Donald F Smith[1]; Chad R. Weisbrod[1]; *[1]National High Magnetic Field Laboratory, Tallahassee, FL; [2]Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL*

MOG pm 03:10 **Improved Spectral Accuracy Analysis to Identify the Correct Elemental-Composition Candidate from Orbitrap Accurate Mass Data at 240,000 Resolution**; Robert J Strife; *Procter & Gamble, Mason, OH*

MOG pm 03:30 **Determination of Elemental Composition by Fitting Isotopic Distributions**; Magnus Palmblad; *Leiden University, Leiden, Netherlands*

MOG pm 03:50 **The Whole Is Easier Than the Parts: Improving Molecular Formula Identification Using Gibbs Sampling on Fragmentation Trees**; Marcus Ludwig[1]; Kai Dührkop[1]; Louis-Félix Nothias[2]; Pieter C. Dorrestein[2, 3]; Sebastian Böcker[1]; *[1]Friedrich-Schiller-University Jena, Jena, Germany; [2]Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA; [3]Collaborative Mass Spectrometry Innovation Center, Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA*

MOG pm 04:10 **Probe Adduct Formation to Aid Mass Spectrum Interpretation and Formula Determination by Modulating Ionization Solvent Composition**; Hanghui Liu; *Senomyx Inc., San Diego, CA*

2:30-4:30 pm Monday
FUNDAMENTALS: PHOTOIONIZATION AND PHOTODISSOCIATION
Session Chair: Alexandre Giuliani (Synchrotron Soleil)
Ballroom 6DE upper level

MOH pm 02:30 **Structure and Dynamics of Gas-Phase Biomolecules Studied by Mass Spectrometry at Advanced Light Sources**; Sadia Bari; *Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany*

MOH pm 02:50 **N-substituted Auxiliaries for Aerobic Oxidative Dehydrogenation of Tetrahydroisoquinoline: A Theory Guided Rational Photo-Catalytic Design/Screening**; Savithra Jayaraj[1]; Abraham Kwame Badu-Tawiah[1]; *[1]The Ohio State University, Columbus, OH*

MOH pm 03:10 **Ultraviolet Photodissociation Allows Accurate Residue-Specific Analysis of the H/D Exchange of Peptides**; Ulrik H. Mistarz[1]; Bruno Bellina[2]; Pernille F. Jensen[1]; Jeffery M. Brown[3]; Perdita E. Barran[2]; Kasper D. Rand[1]; *[1]Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark; [2]University of Manchester, Manchester, UK; [3]Waters Corporation, Wilmslow, UK*

MOH pm 03:30 **Characterization of Heavily Modified Histone Tails by 193 nm Ultraviolet Photodissociation**; Sylvester M Greer[1]; Simone Sidoli[2]; Mariel Coradin[2]; Benjamin A Garcia[3]; Jennifer Brodbelt[4]; *[1]University of Texas at Austin, Austin, TX; [2]University of Pennsylvania, Philadelphia, PA; [3]University of Pennsylvania School of Medicine, Philadelphia, PA; [4]The University of Texas, Austin, TX*

MOH pm 03:50 **New Developments and Applications of 2D UV-MS Fingerprinting of Cold Biological Ions**; Vladimir Kopysov[1]; Erik Saparbayev[1]; Oleg V. Boyarkine[1]; *[1]EPFL, Lausanne, Switzerland*

MOH pm 04:10 **Ultraviolet Photodissociation of ESI and MALDI Generated Protein Ions on a Q-Exactive Mass Spectrometer**; Marialaura Dilillo[1]; Erik L. de Graaf[1]; Avinash Yadav[1, 2]; Mikhail Belov[3]; Liam A. McDonnell[1, 4, 5]; *[1]Fondazione Pisana per la Scienza - ONLUS, Pisa, Italy; [2]Scuola Normale Superiore, Pisa, Italy; [3]Spectroglyph, LLC, Kennewick, WA; [4]Center for Proteomics and Metabolomics, Leiden University Medical Center, Leiden, Netherlands; [5]Department of Pathology, Leiden University Medical Center, Leiden, Netherlands*

4:45-5:30 PM MONDAY
AWARD LECTURE
Vicki H. Wysocki (The Ohio State University)
Hall D ground level

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

Gert von Helden
Fritz-Haber Institut der Max Planck-Gesellschaft

Martin F. Jarrold
Indiana University

David E. Clemmer
Indiana University

There are light refreshments in Sails Pavilion upper level 5:30 - 5:45 pm.

01. Frontiers in Ion Spectroscopy (Fundamentals Interest Group)
Presiding: Victor Ryzhov, Christian Bleiholder
Room 14 AB

Ion spectroscopy is an important area of fundamental mass spectrometry and is gaining popularity as a tool for determining ion structure. It encompasses multiple ion excitation regimes (IR, UV) and can be used as a stand-alone tool or in conjunction with separation techniques like ion mobility or chromatography. The purpose of the workshop is to give an overview of "action" spectroscopy to a broader audience and to discuss recent advances in the field. The workshop will focus on four different areas: (1) ion IR spectroscopy of cold ions and reactive intermediates, (2) specifics of ion UV spectroscopy, (3) coupling ion spectroscopy to ion mobility, and (4) coupling ion spectroscopy to liquid chromatography. The format of the workshop is that of a discussion, moderated by experts (or their group members) in the respective areas: Jos Oomens (principles and instrumentation of action IRMPD spectroscopy), Etienne Garand (spectroscopy of cold ions), Frank Turecek (UV-PD spectroscopy), Tom Rizzo (ion spectroscopy/ion mobility) and Nick Polfer (LC/ion spectroscopy). The workshop is expected to stimulate researchers to expand their current arsenal of MS-based spectroscopic techniques and to help them in identifying and overcoming challenges in modern ion spectroscopy.

02. Networking for Scientists: Celebrating Women Mass Spectrometrists
Presiding: Erin Baker
Room 15 AB

We would like to start a new workshop series focusing on networking for scientists, while also highlighting different groups of people within ASMS. This year we would like to highlight women mass spectrometrists who have excelled in diverse careers ranging from academia to industry. We plan to have a short keynote speech to kickoff off this workshop. Following this, we will set up areas around the room for people to meet successful women from different MS career areas. We plan to ask ~15 women to be available for the one-on-one interactions during this workshop with the ultimate goal of enabling more networking and interactions with the ASMS members. We also feel this will give anyone who would like to attend, the chance to meet these women and ask them specific questions about their career paths in a social and nonthreatening environment.

03. Ion Mobility Spectrometers: How to Build Your Own (Ion Mobility MS Interest Group)
Presiding: Brian Clowers, Valérie Gabelica, Jakub Ujma
Room 16 AB

Despite the availability of commercial ion mobility enabled platforms, many researchers want to develop custom IMS systems, for example to enhance experimental flexibility, or to develop new operational modes and hyphenated experiments. Moreover, construction and use of the "DIY" instrumentation provides an invaluable opportunity for in-depth training within academic groups. In an effort to provide the community with a historical and practical perspective on the design, construction, and operation of modern IMS instrumentation a series of lessons learned will serve as the basis for discussion towards realizing functional IMS instrumentation across a range of IM technologies (e.g. drift tube, DMS, TIMS, T-Wave). In addition, systems that operate well above and below ambient conditions will be discussed. Researchers new to the field must realize that successful designs often emerge after many failed attempts. In a workshop spirit, we will invite participants to share tips, potential pitfalls and lessons learned through from failed attempts. The lessons shared are aimed at stimulating new instrumental innovations that enhance separation capacity, open the new avenues for structural characterization, and strengthen the underlying interpretations of mobility theory. During the discussion, we hope to facilitate interaction between the well-established DIYers and new researchers in the instrument development field.

04. HDX, Covalent Labeling & Cross-Linking: Best Practices, Control Experiments and Data Harmonization (HDX Covalent Labeling & Cross Linking Interest Group)
Presiding: Lan Huang, Kasper Rand
Room 17 AB

Recent technological innovations have significantly facilitated the developments and applications of HDX, covalent labeling and cross-linking approaches in protein structural analysis. A substantial amount of data in these research areas has been reported and the field continues to grow rapidly. In order to allow robust data evaluation and result comparison among experiments and across laboratories, data acquisition, analysis and interpretation need to be standardized. This workshop will provide a forum to discuss best practices and control experiments required for the field. A panel of experts will present current status on data harmonization in each area. In addition, questions formulated by experts will be sent out to the interest group before the meeting, which will be discussed and debated during the workshop among participants.

05. Advances in Polymer Mass Spectrometry (Polymeric Materials Interest Group)
Presiding: Christina Mastromatteo, Stephen Rumbelow
Room 5B

This year's meeting will follow the format used last year, which proved to be very popular with the attendees. It will consist of three distinct sections; a workshop, student posters and an open forum.

To start with, Chrys Wesdemiotis (University of Akron) will give a short presentation highlighting the work by his team in the use of mass spectrometry and tandem mass spectrometry, ranging from fundamental investigations to their applications in characterizing and analysing macromolecules (both synthetic polymers and biopolymers).

This will be followed by a series of short presentations (3-5 min each) by any poster presenters, in the Polymers Section, on their forthcoming poster presentations. This will provide each presenter an opportunity to promote their work externally to a professional scientific audience in their specialized field.

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

06. Life After A Bachelor's Degree: A Q&A Panel for Undergraduates Interested in Graduate School and Industry Careers (Undergraduate Research in MS Interest Group)
Presiding: Chrisi Hughey, Jim Pesavento
Room 5A

This panel discussion, aimed at undergraduate students and their mentors, will focus on helping undergraduate students leverage their undergraduate research experiences into successful scientific careers. Panelists will discuss their experiences applying to graduate school and transitioning to a graduate school research environment, as well as working in industrial labs. Students interested in attending are encouraged to post their questions on the ASMS interest group forum prior to the workshop (https://goo.gl/hNGYPg).

07. Beyond Collisional Dissociation: Improving Metabolite Identification by Alternative Gas-Phase Techniques (DMPK Interest Group)
Presiding: Mark Cancilla, Jonathan Josephs
Room 4

Structural elucidation of small molecule drug metabolites is often successfully accomplished by gas-phase fragmentation via collision-induced dissociation (CID). Yet in multiple instances the site of bioactivation may not be fully resolved due to lack of informative fragments. The remaining ambiguous metabolite would then be represented by a Markush structure or with brackets placed around

There are light refreshments in Sails Pavilion upper level 5:30 - 5:45 pm.

a particular portion of the molecule indicating the potential site or sites of bioactivation. The ability to easily obtain more conclusive structural information of unknown metabolites by mass spectrometry-based methods continues to remain as a gap in the field.

The goal of this workshop is to discuss the benefits and drawbacks of alternative gas-phase techniques that may provide additional structural information of unknown metabolites in real-world settings. Example discussions will revolve around the utility of alternative dissociation techniques that produce greater or different fragmentation pathways compared to CID, such as Electron Induced Dissociation (EID) and Ultraviolet Photon Dissociation (UVPD). Furthermore the current topics of gas-phase ion-molecule reactions and the utility of ion mobility will also be explored for their ability to facilitate the identification of unknown drug metabolites. Topics will focus on real world samples and their effectiveness on a chromatographic time scale.

08a. Art and Cultural Heritage: Mass Spec Applications
Presiding: Mehdi Moini
Room 3

The purpose of this workshop is to bring together scientists, conservators, and curators interested in mass spectrometry (MS) applications to art and cultural heritage objects, as well as natural history specimens. This will be an interactive workshop in which various subjects relevant to the application of MS to museums' specimens will be discussed in a casual, dialog format. A preliminary list of topics include: 1) Analysis of proteinaceous and organic specimens such as silk and wool textiles, leather and animal guts objects, bone and tissues, ink, paper, paint, coatings, binders, and wood. 2) Analysis of the fundamental factors that cause degradation of museums' objects; identification of their deterioration markers, using degradation markers as clocks for dating objects, and studying environmental factors that affect deterioration. 3) Application of MS to paleo-organic matter such as fossilomics, amino acid racemization, and ancient DNA. 4) To be determined.

08b. Biotherapeutics Interest Group Workshop: Hot Topics
Presiding: Charles Chang, Andrew Dawdy
Room 2

This workshop will be a forum to discuss hot topics in the analysis of biotherapeutics by mass spectrometry. Mass spectrometry is now used for protein characterization from discovery through product development. Discussion may include a variety of topics, ranging from protein modifications, higher order structure characterization, protein batch comparability and biosimilarity, and biotherapeutic lot release testing.

Recent development of noval separation in conjunction with mass spectrometry, including ion exchange, size exclusion, CE-MS, etc. will be one of the focus of this year's discussion.

Characterization of non-mAb biotherapeutic modalities (gene therapies, CAR-T, fusion protein, bispecifics, nanoparticles) will also be discussed in this forum.

09. Energy, Petroleum, and Biofuels MS: Methods for Increasing Compositional Space Coverage (Energy Petroleum & Biofuels Interest Group)
Presiding: Marianny Combariza, David Stranz
Room 10

New instrumental data acquisition and sampling techniques are improving the compositional space coverage for complex petroleum, DOM/NOM, and biofuels samples. These include ultrahigh resolution FT-ICR-MS cells, segmented data acquisition and spectral stitching, and hyphenated methods such as LC/MS and GC x GC/MS, and ion mobility / MS. Each of these has its advantages, disadvantages, complementarity to the others. The acquired data presents new challenges for data handling and processing. In this workshop, practitioners from several of these areas will each present the development and applicability of their methods, and will participate in a panel discussion with the audience to compare the pros and cons.

10. Mass Spectrometry in the Developing World: Supporting Education and Research
Presiding: Kym Faull
Room 9

This will be a follow-up to the original workshop on the same topic presented at the 2017 Indianapolis ASMS meeting. The point will be to report on progress and interest during the preceding 12 months. Invitations will be extended to representatives from Research Organization for Research Opportunities (RORO, Giles Edwards, Technical Director) and Seeding Labs (Nina Dudnik, Founder & CEO), and perhaps other organizations, to make brief presentations. The point is that students in developing nations learn about mass spectrometry from text books. They rarely if ever get to actually see one, and never get to use them. In the Developed World old but working instruments that are replaced with new versions could be made available to Universities and research organizations in developing countries to be used for research and teaching purposes. This would entail shipping, installation, training and maintenance which would all require funding and support. Some aspects of maintenance and training could probably be handled remotely via email, Skype, etc. The big questions is: Is this feasible? It would be a noble aspiration for ASMS to embrace. It would improve our relations with the developing world and perhaps provide an example for other organizations (e.g. the NMR Society, etc) to follow. The Presider will begin with a brief description of his personal experiences that stimulated him to organize this workshop. These were memorable experiences that forged enduring friendships. All those interested are invited to join in a friendly and constructive discussion on this topic.

11. MS Software: Excavating Nuggets of Information from the Massive Mound of Data
Presiding: David Kilgour, Magnus Palmblad
Room 8

This workshop is aimed at the many ASMS members who write their own software to control mass spectrometers or process mass spectrometry data - and those who might want to.
Mass spectrometers are highly complex systems that can shine the light of knowledge onto important problems in many areas. Advances in mass spectrometry instrumentation have led to startling improvements in performance. But, these new amazing powers of mass spectrometry would be unusable if it wasn't for the software that is available to control the instruments and make sense of the data.

The software available for commercial mass spectrometers is remarkable. But, as the quantity and diversity of data that can be recorded and the density of information in that data grows ever larger, in ever more complex mass spectrometry experiments, there is a continuous drive for new algorithms and bespoke software to process that data and find the right information. Consequently, there are many researchers who develop their own mass spectrometry software, and many more who might want to either collaborate with someone who can help develop a software solution to their problem or learn how to start writing their own software.

So, as a community, what do we do? What problems are we trying to solve? Have they been addressed before? What languages and platforms are we using and why? What file formats are easier or harder to work with, and which do we like the best? How can we make what we do most useful to others?

12. Data Independent Acquisition: Expanding the Scope of DIA Strategies for Quantitative Mass Spectrometry (Data Independent Acquisition Interest Group)
Presiding: Ben Collins, Hannes Röst
Room 7 AB

In quantitative proteomics, the fundamental aim is to accurately identify and quantify analytes across various conditions. Data independent acquisition (DIA) has recently emerged as a promising method to accurately quantify analytes in complex samples, allowing consistent detection and quantification of thousands of proteins across large

There are light refreshments in Sails Pavilion upper level 5:30 - 5:45 pm.

sample cohorts. Utilizing MS2-based quantification (as in SRM/PRM) in high throughput (as in DDA) has led to impressive results with highly consistent and accurate quantitative data matrices suitable for systems biology, systems medicine and personalized medicine applications. However, most current methods focus on accurate protein quantification using a label-free approach. However, the DIA approach can readily be applied to other MS-based questions and can be beneficial if high-quality fragment ion data is essential for correct analyte characterization. This workshop will discuss the challenges and opportunities of expanding the scope of DIA analysis beyond protein abundance measurements. How can DIA improve identification and quantification of modified peptides? Which unique advantages can be leveraged from DIA data when analyzing protein phosphorylation or other PTMs? How can DIA methods be used to analyze protein isoforms quantitatively? How do DIA methods contribute in protein complex elucidation? What specific challenges await when expanding the scope of DIA beyond unmodified peptides (PTMs, SAV, lipids, small molecules). How can we control the quantification error under these circumstances? This workshop will focus on existing and emerging approaches in applying DIA beyond protein abundance measurements and discuss some unique challenges, and opportunities, of translating the recently developed DIA approaches (such as targeted extraction) to these fields.

The workshop will focus on introducing the most recent concepts addressing these aspects and develop ideas to ensure the reporting of high-quality quantification matrices.

13. Ion Traps: What Do They Hold for the Future?
(Ion Trap MS Interest Group)
Presiding: Glen Jackson, Wei Xu
Room 33 ABC

Ion traps form a diverse category of mass spectrometers that occupy a major segment of the mass spectrometry market; they are invaluable tools for concentrating, isolating, storing and manipulating ions. This year's workshop will highlight several young ion trap mass spectrometrists, from senior graduate students to assistant professors, who are pushing the boundaries of ion trap capabilities. The workshop will also feature a unique historical perspective from a legendary ion trapper and opportunities for dialogue on current and future challenges.

14. LC-MS Jeopardy: I'll Take Increasing Throughput for $200
(LCMS & Related Topics Interest Group)
Presiding: Erik Soderblom, Will Thompson
Room 32 AB

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

15. Young Mass Spectrometrists:
A Career in Mass Spec: Options and Where to start?
Presiding: Veronica Anania, Doug Phanstiel
Room 31 ABC

This workshop is intended to serve as a resource for young scientists interested in pursuing a career in the field of mass spectrometry. Come prepared for an interactive panel discussion on professional development with panelists from academia, government, and industry (domestic and foreign, biotech and pharma). Topics will be centered around fundamental training, internships, career options, and career planning and management.

16. Tackling The Big Data: How-to Analyze and Share Proteomics Data Responsibly
(Analytical Lab Managers Interest Group)
Presiding: Emily Chen, David Quilici
Room 30 DE

Modern quantitative proteomic experiments are producing massive amounts of data and most of the analytical laboratories are now tasked with the handling of these data. These large datasets need to be properly analyzed and presented in a manner that is comprehensible and suitable for publication. These data also need to be made available to other researchers after publishing, but it is extremely challenging because there is not yet a community standard. The 2018 ASMS Analytical Lab Managers Workshop will be dedicated to sharing insights into proteomic data management in an effort to assist lab managers in their quest to efficiently and appropriately manage large proteomic datasets. Three areas of data management will be covered: Statistical analysis/presentation, bioinformatics analysis of data generated from different laboratories, and data repository. The format will be a 15 minute overview by invited speakers on each topic followed by 10 minutes of Q&A.

AFTER 8:00 PM
CORPORATE HOSPITALITY SUITES
HILTON SAN DIEGO BAYFRONT

TUESDAY MORNING ORAL SESSIONS

7:00 am Tuesday
CORPORATE BREAKFAST SEMINARS
CONVENTION CENTER AND
HILTON SAN DIEGO BAYFRONT
See page 15 for detailed schedule.
Reservation or RSVP required.

8:30-10:30 am Tuesday
FUNDAMENTALS FOR EVERYONE: PEPTIDES AND PROTEINS
(IN MEMORY OF JACK THROCK WATSON)
Session Chair: John T. Stults (Genentech, Inc.)
Hall D ground level

TOA am 08:30 **A Novel Ion Mobility – Mass Spectrometry Based Hydrophobicity Scale for Amino Acids**; Waldemar Hoffmann[1]; Michael T Bowers[2]; Gert von Helden[3]; Kevin Pagel[1]; *[1]Free University of Berlin, Institute of Chemistry and Biochemistry, Berlin, Germany; [2]University of California, Santa Barbara, Santa Barbara, CA; [3]Fritz Haber Institute of the Max Planck Society, Molecular Physics, Berlin, Germany*

TOA am 08:50 **Quantification of Serum High Mobility Group Box-1 by Liquid Chromatography-Mass Spectrometry: Implications for a Prototypic Danger Molecule's Role in Disease**; Liwei Weng[1]; Lil Guo[1]; Clementina Mesaros[1]; Ian A. Alexander Blair[2]; *[1]University of Pennsylvania School of Medicine, Philadelphia, PA; [2]Univ. of Penn/SOM/ Pharmacol, Philadelphia, PA*

TOA am 09:10 **A Novel Method to Identify Functional Post-Translational Modification Sites Across the Proteome**; Ian R Smith[1]; Ricard A Rodriguez-Mias[1]; Miguel Martin-Perez[1]; Ariadna Llovet[1]; Kyle N Hess[1];

Judit Villén[1]; [1]*University of Washington Genome Sciences, Seattle, WA*

TOA am 09:30 **Predicting Agents That "Supercharge"**; Rachel O. Loo[1]; Reid O'Brien Johnson[1]; Michael Nshanian[1]; Joseph A Loo[1]; [1]*UCLA, Los Angeles, CA*

TOA am 09:50 **Ion-Ion Reaction Facilitated Mass Spectrometry Method for Early-Stage Aggregation Detection**; Nan Wang[1]; Scott A McLuckey[1]; Alice L Pilo[2]; Alexey A Makarov[2]; Hao Luo[2]; Weijuan Tang[2]; [1]*Purdue University, West Lafayette, IN;* [2]*Merck Research Laboratories, Rahway, NJ*

TOA am 10:10 **Intact Protein Analysis: Moving Beyond Molecular Weight Determination**; Caroline J. DeHart[1]; Luca Fornelli[1]; Kristina Srzentic[1]; Luis F Schachner[2]; Ashley N. Ives[2]; Ryan Fellers[1]; Philip D. Compton[1]; Steven M. Patrie[2]; Paul M. Thomas[1]; Neil Kelleher[1, 2]; [1]*Proteomics Center of Excellence, Northwestern University, Evanston, IL;* [2]*Northwestern University, Evanston, IL*

8:30-10:30 am Tuesday
ION MOBILITY: NEW DEVELOPMENTS & APPLICATIONS
Session Chair: David E. Clemmer (Indiana University)
Ballroom 20A upper level

TOB am 08:30 **A Multi-Function Cyclic Ion Mobility – Mass Spectrometry System**; Jakub Ujma[1]; Sandra Richardson[1]; Kevin Giles[1]; [1]*Waters Corporation, Wilmslow, UK*

TOB am 08:50 **High-Definition Differential IMS with Orbitrap Mass Spectrometry for IMS/MS Analyses with High 2-D Resolution**; Matthew A. Baird[1]; Eugene Moskovets[2]; Victor Laiko[2]; Alexandre Shvartsburg[1]; [1]*Wichita State University, Wichita, KS;* [2]*MassTech, Inc., Columbia, MD*

TOB am 09:10 **Pushing the Mobility Sensitivity, Resolution and Range with New Electrode Geometries in Trapped Ion Mobility Spectrometry**; Alyssa Garabedian[1]; Juan Camilo Molano-Arevalo[1]; Kevin Jeanne Dit Fouque[1]; Mark E Ridgeway[2]; Melvin A Park[2]; Francisco Fernandez Lima[1]; [1]*Florida International University, Miami, FL;* [2]*Bruker Daltonics Inc., Billerica, MA*

TOB am 09:30 **On-Line Nanolc-Ion Mobility-Electron Capture Dissociation Tandem MS Analysis of Peptide Mixtures and Glycoprotein Digests on an IM-QTOF Mass Spectrometer**; James A. Hill[1, 2]; Valery G. Voinov[3]; Rebecca S. Glaskin[1]; Christian F Heckendorf[1]; Joseph S. Beckman[3]; Mark E McComb[1]; Catherine E Costello[1]; [1]*Boston University School of Medicine, Boston, MA;* [2]*James A. Hill Instrument Services, Inc., Arlington, MA;* [3]*e-MSion, Inc., Corvallis, OR*

TOB am 09:50 **CIUSuite 2: Next-Generation Software for the Analysis of Gas-Phase Protein Unfolding Data**; Daniel A. Polasky[1]; Sugyan M. Dixit[1]; Sarah M. Fantin[1]; Ruwan T. Kurulugama[2]; Brandon T. Ruotolo[1]; [1]*University of Michigan, Ann Arbor, MI;* [2]*Agilent Technologies, Inc., Santa Clara, CA*

TOB am 10:10 **Ion Mobility MS (IM-MS) Investigation of Naturally-Occurring Chirality-Driven Oligomerization and Recognition of Amyloid Beta Peptide**; Gongyu Li[1]; Lingjun Li[2]; [1]*University of Wisconsin-Madison, Madison, WI;* [2]*University of Wisconsin-Madison, Madison, WI*

8:30-10:30 am Tuesday
APPLICATIONS OF STABLE ISOTOPE LABELING IN MS
Session Chair: Stanley M. Stevens, Jr. (Albany College of Pharmacy and Health Sciences)
Ballroom 20BC upper level

TOC am 08:30 **EASI-Tag Enables Accurate Multiplexed and Interference-Free MS2-Based Proteome Quantification**; Sebastian Virreira Winter[1]; Florian Meier[1]; Christoph Wichmann[1]; Jürgen Cox[1]; Matthias Mann[1]; Felix Meissner[1]; [1]*Max Planck Institute of Biochemistry, Martinsried, Germany*

TOC am 08:50 **Mapping the Incorporation of 13C-Labeled Monosaccharides into the Mouse Cell Surface Metaglycome by LC-MS/MS Analysis**; Mariana Barboza[1]; Maurice Wong[1]; Johnathan Luke[2]; Zhi Cheng[2]; Gege Xu[1]; Melanie Gareau[1]; Helen Raybould[1]; Carlito B. Lebrilla[1]; [1]*University of California Davis, Davis, CA;* [2]*University of California Davis, Davis, CA*

TOC am 09:10 **Determining the Chromatin Compaction State of All Histone Modifications Using Stable Isotope Labeling and State-Of-The-Art MS Histone Analysis**; Simone Sidoli[1]; Natarajan V. Bhanu[1]; Peder J. Lund[1]; Mariel Coradin[1]; Benjamin A. Garcia[1]; [1]*University of Pennsylvania, Philadelphia, PA*

TOC am 09:30 **Multi-Isotope Tracing Analysis in Both *in vitro* and *in vivo* Models Identifies *de novo* Acetate Production from Glucose Metabolism**; Xiaojing Liu[1]; Daniel Cooper[2]; Juan Liu[1]; Jason W. Locasale[1]; [1]*Department of Pharmacology and Cancer Biology, Duke University School of Medicine, Durham, NC;* [2]*Department of Radiation Oncology, Duke University Medical Center, Durham, NC*

TOC am 09:50 **Label-Assisted Untargeted Metabolomics Reveals Hepatocyte-Macrophage Ketone Shuttle that Protects Against Tissue Fibrosis**; Patrycja Puchalska[1, 2]; Shannon E Martin[3]; Xiaojing Huang[4]; Xianlin Han[5]; Gary J Patti[4]; Peter A Crawford[1, 2]; [1]*Division of Molecular Medicine, Department of Medicine, University of Minnesota, Minneapolis, MN;* [2]*Center for Metabolic Origins of Disease, Sanford Burnham Prebys Medical Discovery Institute, Orlando, FL;* [3]*Pathobiology Graduate Program, Brown University, Providence, RI;* [4]*Department of Chemistry, Washington University, St Louis, MO;* [5]*Barshop Institute for Longevity and Aging Studies, San Antonio, TX*

TOC am 10:10 **Deuterium Labeling in Humans Followed by PRM on the Orbitrap Lumos Provides First View of Classical Cardiovascular Disease-Associated Protein Kinetics**; Sasha Singh[1]; Allison B Andraski[2]; Hideyuki Higashi[1]; Lang Ho Lee[1]; Frank M Sacks[2]; Masanori Aikawa[1]; [1]*Brigham and Women's Hospital/ Harvard Medical School, Boston, MA;* [2]*Harvard School of Public Health, Boston, MA*

8:30-10:30 am Tuesday
METABOLOMICS: NEW TECHNOLOGIES AND APPLICATIONS
Session Chair: Gary J. Patti (Washington University)
Ballroom 20D upper level

TOD am 08:30 **Rapid Analysis of NCI60 Panel Metabolic and Lipid Profiles with an Automatic Well Plate Reader Using Laser Assisted REIMS**; Julia Balog[1, 2]; Richard Schaffer[1]; Daniel Simon[1]; Nora Kucsma[3]; Anna Lovrics[3]; Gergely Szakacs[3, 4]; Steven D Pringle[5]; Zoltan Takats[2]; [1]*Waters Research Center, Budapest, Hungary;* [2]*Imperial College London, London, UK;* [3]*MTA TTK, Budapest, Hungary;* [4]*Medical University of Vienna, Vienna, Austria;* [5]*Waters Corporation, Wilmslow, UK*

TOD am 08:50 **Merging Metabolomics and Lipidomics in One Analytical Run by Parallel HILIC/RP-HRMS**; Michaela Schwaiger[1]; Gerrit Hermann[1, 2]; Harald Schoeny[1, 3, 4]; Yasin El Abiead[1]; Evelyn Rampler[1, 3, 4]; Gunda Koellensperger[1, 3, 4]; [1]*University of Vienna,*

Vienna, Austria; [2]ISOtopic Solutions, Vienna, Austria; [3]Vienna Metabolomics Center (VIME), University of Vienna, Vienna, Austria; [4]Chemistry Meets Microbiology, Vienna, Austria

TOD am 09:10 **Comprehensive Lipid C=C Location Isomer Analysis for Biomarker Discovery and Disease Differentiation**; Wenpeng Zhang[1, 2]; Donghui Zhang[3]; Qinhua Chen[4]; Zheng Ouyang[2, 3]; Yu Xia[1, 5]; *[1]Department of Chemistry, Tsinghua University, Beijing, China; [2]Weldon School of Biomedical Engineering, Purdue University, West Lafayette, IN; [3]State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instruments, Tsinghua University, Beijing, China; [4]Affiliated Dongfeng Hospital, Hubei University of Medicine, Shiyan, China; [5]Department of Chemistry, Purdue University, West Lafayette, IN*

TOD am 09:30 **Developing Advanced and Integrated Technologies to Address the Grand Challenges of Metabolomics Including Metabolite Identification and Depth of Coverage**; Lloyd W. Sumner[1]; Feng Qiu[2]; Dennis Fine[3]; Daniel Wherritt[4]; Zhentian Lei[2]; Anil Bhatia[2]; Mark Schroeder[2]; Sven Meyer[5]; Aiko Barsch[5]; *[1]The University of Missouri at Columbia, Columbia, MO; [2]University of Missouri, Columbia, MO; [3]Samuel Roberts Noble Foundation, Ardmore, OK; [4]University of Texas at San Antonio, San Antonio, TX; [5]Bruker Daltonik GmbH, Bremen, Germany*

TOD am 09:50 **Rapid Clinical Sample Screening with Minimum Sample Preparation Using Chip-Based Capillary Electrophoresis and High Resolution Tandem Mass Spectrometry**; J. Will Thompson[1]; J. Scott Mellors[2]; Sarah Rains[1]; Matthew Foster[1]; Thomas Burke[1]; Elizabeth Petzold[1]; Christopher Woods[1]; M. Arthur Moseley[1]; *[1]Duke University School of Medicine, Durham, NC; [2]908 Devices Inc., Boston, MA*

TOD am 10:10 **Enhanced Sensitivity of Metabolite Detection for Single-Cell Metabolomics by Field Amplified Sample Stacking Capillary Electrophoresis Electrospray Ionization-Mass Spectrometry**; Hsiao-Wei Liao[1]; Stanislav S. Rubakhin[1]; Marina C. Philip[1]; Amit Patel[1]; Jonathan V. Sweedler[1]; *[1]University of Illinois at Urbana-Champaign, Urbana, IL*

8:30-10:30 am Tuesday
INNOVATIONS AND APPLICATIONS IN FORENSICS
Session Chair: Mitch Wells (FLIR Detection, Inc.)
Ballroom 6A upper level

TOE am 08:30 **Systematic Drug Surveillance by Multisegment Injection-Capillary Electrophoresis-Mass Spectrometry: A High Throughput Method for Comprehensive Screening of Drugs of Abuse**; Philip Britz-McKibbin[1]; Alicia DiBattista[1, 2]; Zachary Kroezen[1]; Sabrina Macklai[1]; Dianne Rampersaud[2]; Howard Lee[2]; Marcus Kim[3]; *[1]McMaster University, Hamilton, ON, Canada; [2]Seroclinix Corporation, Mississauga, ON, Canada; [3]Agilent Technologies Inc., Mississauga, ON, Canada*

TOE am 08:50 **Screening Illicit Drugs in Oral Fluids Using Paper Spray Mass Spectrometry Cartridge with Integrated Solid Phase Extraction**; Veronica Carvalho[1, 2]; Nicholas E. Manicke[3]; Boniek G Vaz[2]; *[1]IUPUI, Indianapolis, IN; [2]Universidade Federal de Goiás, Goiânia, Brazil; [3]IUPUI Department of Chemistry & Chemical Biology, Indianapolis, IN*

TOE am 09:10 **Detection of Exogenous Substances in Latent Fingermarks by Silver-Assisted LDI Imaging MS**; Nidia Lauzon[1]; Pierre Chaurand[1]; *[1]University of Montreal, Montreal, QC, Canada*

TOE am 09:30 **DART-HRMS/Kendrick Mass Defect Analysis Applied to the Sourcing of Plastic Bonded Explosives**; Gabriel Gaiffe[1, 2]; Richard B. Cole[1]; Nolwenn Floch[3]; Maxime Cyril Bridoux[2]; *[1]Sorbonne Universités UPMC Paris, Paris, France; [2]CEA, Bruyères-Le Châtel, France; [3]Laboratoire Central de la Préfecture de Police de Paris, Paris, France*

TOE am 09:50 **Proteomic Variation along the Length of Scalp Hair for Protein-Based Human Identification**; Fanny Chu[1, 2]; Katelyn E. Mason[1]; Deon S. Anex[1]; A. Daniel Jones[2]; Bradley Hart[1]; *[1]Lawrence Livermore National Laboratory, Livermore, CA; [2]Michigan State University, East Lansing, MI*

TOE am 10:10 **Identification of Carrion Sources from the Stable Isotope Analysis of Larvae, Pupae, and Adult Calliphora Vicina Blow Flies**; Mayara P. V. Matos[1]; Rachel M. Mohr[1]; Glen P. Jackson[1]; *[1]West Virginia University, Morgantown, WV*

8:30-10:30 am Tuesday
PLANT "OMICS"
Session Chair: Dil Ramanathan (Kean University)
Ballroom 6B upper level

TOF am 08:30 **Determining Terpene Profiles of Cannabis Strains Using GC and GCxGC with High Performance TOFMS**; Lorne Fell[1]; David E Alonso[1]; Julie Kowalski[2]; Joseph E Binkley[1]; *[1]LECO Corporation, Saint Joseph, MI; [2]Trace Analytics, Spokane, WA*

TOF am 08:50 **Investigation of Polyphenol Diversity among Wild Lentil (Lens spp.) Species Using Both Untargeted and Targeted Metabolomics**; Randy W Purves[1]; Fatma Elessawy[1]; Roger Munro[2]; Haixia Zhang[1]; Hamid Khazaei[1]; Bryn O Shurmer[2]; Albert Vandenberg[1]; *[1]University of Saskatchewan, Saskatoon, SK, Canada; [2]Canadian Food Inspection Agency, Saskatoon, SK, Canada*

TOF am 09:10 **Deep Metabolite Identification of Xenobiotic Metabolites in Plants**; Dorde Tadic[1]; Josep Maria Bayona[1]; Michal Gramblicka[2]; Juraj Lutisan[2]; Robert Mistrik[2]; *[1]CID - CSIC, Barcelona, Spain; [2]HighChem, Bratislava, Slovakia*

TOF am 09:30 **Mass Spectrometric Imaging of Labile Cyanogenic Glycosides in Plants**; Berin A Boughton[1]; Frederik B Schmidt[2, 3, 4]; Edita Ritmejeryte[5, 6]; Mike Bayly[6]; Rebecca E Miller[5]; Kirsten Jørgensen[2, 3, 4]; Birger L Møller[2, 3, 4]; *[1]Metabolomics Australia, University of Melbourne, Parkville, Australia; [2]Plant Biochemistry Laboratory, Department of Plant and Environmental Sciences, University of Copenhagen, Copenhagen, Denmark; [3]VILLUM Research Center "Plant Plasticity", Copenhagen, Denmark; [4]Center for Synthetic Biology "bioSYNergy", Copenhagen, Denmark; [5]School of Ecosystem and Forest Sciences, The University of Melbourne, Richmond, Australia; [6]School of BioSciences, University of Melbourne, Melbourne, Australia*

TOF am 09:50 **3D Molecular Cartography of the Greening Disease**; Alexander Aksenov[1]; Caroline Roper[2]; Greg McCollum[3]; Alexey V. Melnik[4]; Pieter C. Dorrestein[1]; *[1]UCSD, La Jolla, CA; [2]University of California, Riverside, CA; [3]United States Department of Food and Agriculture, Agricultural Research Service, Fort Pierce, FL; [4]UCSD, San Diego, CA*

TOF am 10:10 **Detection and Quantification of Commercially Processed Soy Ingredients in a Cookie Matrix Using PRM**; Shimin Chen[1]; Charles Yang[2]; Melanie Downs[1]; *[1]Food Allergy Research and Resource Program, Department of Food Science and Technology, University of Nebraska-Lincoln, Lincoln, NE; [2]Thermo Fisher Scientific, San Jose, CA*

8:30-10:30 am Tuesday
MS IN THE FIELD AND THE CLINIC
Session Chair: Alan Rockwood (Rockwood Scientific Consulting)
Ballroom 6CF upper level

TOG am 08:30 **Proteomic Genotyping, Now at Your Fingertips**; Christopher M. Shuford[1]; Meghan N. Bradley[1]; Michael Levandoski[1]; Russell P. Grant[1]; *[1]Laboratory Corporation of America, Burlington, NC*

TOG am 08:50 **Mass Spectrometry Guides Western Blot Screening for Presence of Metastases in Lymph Nodes from Breast Cancer Patients**; Cornelia Koy[1]; Claudia Roewer[1]; Christian George[2]; Toralf Reimer[2]; Bernd Stengel[3]; Anngret Radtke[3]; Bernd Gerber[2]; Michael O. Glocker[1]; *[1]Proteome Center Rostock, Rostock, Germany; [2]Department of Obstetrics and Gynecology, University of Rostock, Rostock, Germany; [3]Partnership of Specialists of Pathology, Rostock, Germany*

TOG am 09:10 **Rapid Detection of 2-Hydroxyglutarate in Tumor Frozen Sections by MALDI-TOF Mass Spectrometry**; Rémi Longuespée[1]; Annika Wefers[2]; David Reuss[2, 3]; Mark Kriegsmann[1]; Andreas von Deimling[2, 3]; Stefan Pusch[2, 3]; *[1]University of Heidelberg, Institute of Pathology, Heidelberg, Germany; [2]University of Heidelberg, Institute of Pathology, Department Neuropathology, Heidelberg, Germany; [3]Clinical Cooperation Unit Neuropathology, German Cancer Research Center (DKFZ), Heidelberg, Germany*

TOG am 09:30 **Comparison of High- and Low-Resolution MS Data for Direct Tissue Profiling on a way from Laboratory to Clinic**; Igor Popov[1, 2]; Evgeny Zhvansky[1, 2]; Anatoly Sorokin[1, 3]; Stanislav Pekov[1, 2]; Vasily Eliferov[1]; Alexander Vorobyev[1]; Vsevolod Shurkhay[1, 4]; Alexander Potapov[4]; Eugene (Evgeny) Nikolaev[5]; *[1]Moscow Institute of Physics and Technology, Moscow, Russia; [2]Institute for Energy Problems of Chemical Physics of RAS, Moscow, Russia; [3]Institute of Cell Biophysics RAS, Pushchino, Russia; [4]N. N. Burdenko Scientific Research Neurosurgery Institute, Moscow, Russia; [5]Skolkovo Institute of Science and Technology, Moscow, Russia*

TOG am 09:50 **Integrating Inborn Errors of Metabolism and Hemoglobin Variant Clinical Research into a Single HRAM Mass Spectrometer Workflow**; Xiaolei Xie; *ThermoFisher Scientific, San Jose, CA*

TOG am 10:10 **Free Fraction Analysis for Therapeutic Drug Monitoring of Antiepileptic Drugs**; Emily Barrey[1]; Candace Price[1]; Craig Aurand[1]; *[1]Millipore Sigma, Bellefonte, PA*

8:30-10:30 am Tuesday
SYNTHETIC POLYMERS
Session Chair: Christina J. Mastromatteo (Lubrizol Advanced Materials Inc)
Ballroom 6DE upper level

TOH am 08:30 **Rapid Analysis Techniques for Deconstructing Isocyanate-Based Formulations**; Anthony Paul Gies[1]; William H. Heath[1]; Praveenkumar Boopalachandran[1]; Nathan J. Rau[1]; *[1]Dow Chemical Company, Freeport, TX*

TOH am 08:50 **Optimizing the Structure of Sequence-Controlled Synthetic Polymers for *de novo* MS/MS Sequencing of Long Coded Chains**; Laurence Charles[1]; Jean-Arthur Amalian[2]; Abdelaziz Al Ouahabi[3]; Jean-François Lutz[4]; *[1]Aix-Marseille University, Marseille Cedex 20, France; [2]Aix-Marseille University, Marseille, France; [3]Institut Charles Sadron, Strasbourg, France; [4]Institut Charles Sadron, Strasbourg, France*

TOH am 09:10 **Characterization of Multi–Functionalized, High Molecular Weight PEG Compounds Using Two Dimensional Chromatography Coupled to Charge Reduction – Mass Spectrometry**; Samuel H Yang[1]; Bifan Chen[2]; Jenny Wang[3]; Kelly Zhang[3]; *[1]Genentech, South San Francisco; [2]University of Wisconsin–Madison, Madison, WI; [3]Genentech, SSF*

TOH am 09:30 **Fractions, Flames and Fullerenes, Circles and Segments: New Enhancements to Kendrick Mass Defect Analysis for Polymers, PAH's and Carbon Clusters**; Robert B Cody[1]; Thierry Nicolas Jean Fouquet[2]; Hiroaki Sato[2]; *[1]JEOL USA, Inc., Peabody, MA; [2]AIST, Tsukuba, Japan*

TOH am 09:50 **Nanoscale Co-Localization Analysis of Polymer Blends via Massive Cluster Secondary Ion Mass Spectrometry**; Jesse Manuel Sandoval[1]; Dillon Reed Adams[1]; Jared Price[2]; Michael J. Eller[1]; Noel C Giebink[2]; Peter Trefonas[3]; Emile A. Schweikert[1]; *[1]Texas A&M University, College Station, TX; [2]Penn State University, University Park, PA; [3]Dow Electronic Materials, Marlborough, MA*

TOH am 10:10 **Determining Covalently Crosslinked Polymer Connectivities by ASAP-MS**; Kevin J. Endres[1]; Rodger A. Dilla[1]; Matthew L. Becker[1]; Chrys Wesdemiotis[1]; *[1]University of Akron, Akron, OH*

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

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

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

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

TUESDAY AFTERNOON ORAL SESSIONS

2:30-4:30 pm Tuesday
INSTRUMENTATION: AMBIENT IONIZATION: INSTRUMENTATION & APPLICATIONS
Session Chair: Andre Venter (Western Michigan University)
Hall D ground level

TOA pm 02:30 **Development of Laparoscopic MasSpec Pen for Real-Time Diagnosis in Minimally Invasive Surgery**; Jialing Zhang[1]; Noah Giese[1]; Nitesh Katta[2]; Kevin Choy[2]; Kevin Jian Yee[1]; Marta Sans[1]; Clara Feider[1]; Thomas Milner[2]; Livia S. Eberlin[1]; *[1]Department of Chemistry, The University of Texas at Austin, Austin, TX; [2]Department of Biomedical Engineering, The University of Texas at Austin, Austin, TX*

TOA pm 02:50 **Subcellular Analysis of Neuropeptides in Single Identified Neurons by Mass Spectrometry**; Linwen Zhang[1]; Nikkita Khattar[1]; Ildiko Kemenes[2]; Gyorgy Kemenes[2]; Zita Zrinyi[3]; Zsolt Pirger[3]; Akos

Vertes[1]; *[1]The George Washington University, Washington, DC; [2]University of Sussex, Brighton, UK; [3]Balaton Limnological Institute, Tihany, Hungary*

TOA pm 03:10 **Photoinduced Thermal Desorption Coupled with Atmospheric Pressure Chemical Ionization Mass Spectrometry for Multimodal Imaging**; Matthias Lorenz[1, 2]; R. Cannon S. Buechley[2]; Elisabeth T. Gallmeier[2]; Mario Viani[3]; Aleksander Labuda[3]; Stephen Jesse[2]; Eloy R. Wouters[4]; Alexander Makarov[5]; Roger Proksch[3]; Olga S. Ovchinnikova[2]; *[1]University of Tennessee, Knoxville, TN; [2]Oak Ridge National Laboratory, Oak Ridge, TN; [3]Oxford Instruments, Santa Barbara, CA; [4]Thermo Fisher Scientific, San Jose, CA; [5]Thermo Fisher Scientific, Bremen, Germany*

TOA pm 03:30 **Structured Conductive Probes for Ambient Ionization in Mass Spectrometry**; Dragan Vuckovic[1]; Jose Moran-Mirabal[2]; *[1]VBM Science Ltd., Dundas, Ontario, Canada; [2]McMaster University, Hamilton, Ontario, Canada*

TOA pm 03:50 **LADI of the Wood: Imaging of Small-Molecule Spatial Distributions in Endangered Wood Species by a Novel Ambient Ionization Imaging Technique**; Kristen L. Fowble[1]; Edgard Espinoza[2]; Robert B. Cody[3]; Rabi A. Musah[1]; *[1]University at Albany-SUNY, Albany, NY; [2]US Fish and Wildlife Service- National Forensics Laboratory, Ashland, OR; [3]JEOL USA, Inc., Peabody, MA*

TOA pm 04:10 **Spring-Electrode Configuration Greatly Enhances Ionization Efficiency of Nonpolar Compounds in a DBD Plasma**; Mario Francesco Mirabelli[1]; Anna Katarina Huba[1]; Renato Zenobi[1]; *[1]ETH Zürich, Zurich, Switzerland*

2:30-4:30 pm Tuesday
ION MOBILITY: SMALL MOLECULES AND CLINICAL
Session Chair: Michael T. Costanzo (Breathtec Biomedical, Inc.)
Ballroom 20A upper level

TOB pm 02:30 **Metabolite Selectivity and Separation Performance of a Differential Mobility Spectrometry-Mass Spectrometry Platform**; Stefanie Wernisch[1]; Subramaniam Pennathur[1]; *[1]University of Michigan, Ann Arbor, MI*

TOB pm 02:50 **Differential Ion Mobility Separation and Infrared Identification of Isomers of Amino Acids**; Francis Berthias[1]; Fathi Moussa[1]; Philippe Maitre[2]; *[1]Université Paris-Sud, Orsay, France; [2]Université Paris Sud, Orsay, France*

TOB pm 03:10 **High-Resolution Enantiomeric Separations on a SLIM IM-MS Platform**; Gabe Nagy[1]; Christopher D. Chouinard[1]; Isaac K. Attah[1]; Ian K. Webb[1]; Yehia M. Ibrahim[1]; Erin S. Baker[1]; Richard D. Smith[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

TOB pm 03:30 **How Far Can We Go with Drift Tube IM-MS in Metabolomics? Fundamental Ion Trapping Behavior and Multiplexing in Non-Targeted Analysis**; Tim Causon[1]; Ruwan T. Kurulugama[2]; Hung Le Si[1]; John Fjeldsted[2]; Stephan Hann[1]; *[1]Division of Analytical Chemistry, Department of Chemistry, University of Natural Resources and Life Sciences (BOKU), Vienna, Austria; [2]Agilent Technologies, Santa Clara, CA*

TOB pm 03:50 **Predicting Breast Cancer by Paper Spray Ion Mobility Spectrometry Mass Spectrometry and Machine Learning**; Ying-Chen Huang[1]; Hua-Yi Hsieh[1]; Chih-Lin Chen[1]; Hsin-Hsiang Chung[1]; Yae-lin Sheu[2]; Bo-Rong Chen[3]; Ming-Yang Wang[3]; Cheng-Chih Hsu[1]; *[1]Department of Chemistry, National Taiwan University, Taipei, Taiwan; [2]Industrial Technology Research Institute, Hsinchu, Taiwan; [3]Department of Surgery, National Taiwan University Hospital, Taipei, Taiwan*

TOB pm 04:10 **Enhancing Analyte Separation in Metabolomics Using Comprehensive Liquid Chromatography Modifier Assisted Differential Mobility Spectrometry/Mass Spectrometry**; David Ruskic[1]; Gerard Hopfgartner[1]; *[1]Life Sciences Mass Spectrometry, University of Geneva, Geneva, Switzerland*

2:30-4:30 pm Tuesday
ANALYTICAL CHALLENGES OF MICRODOSING AND MICROSAMPLING STUDIES
Session Chair: Qin C. Ji (Bristol-Myers Squibb Co.)
Ballroom 20BC upper level

TOC pm 02:30 **High-Resolution Spatially-Resolved Proteome Mapping through Seamless Integration of Laser-Capture Microdissection with Nanodroplet Sample Preparation and Ultrasensitive NanoLC-MS**; Ying Zhu[1]; Maowei Dou[1]; Paul D. Piehowski[1]; Yiran Liang[1]; Fangjun Wang[2]; Rosalie K. Chu[1]; William B. Chrisler[1]; Rui Zhao[1]; Ronald J. Moore[1]; Richard D. Smith[1]; Weijun Qian[1]; Ryan Kelly[1]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]Dalian Institute of Chemical Physics, The Chinese Academy of Sciences, Dalian, China*

TOC pm 02:50 **Proteomic Analysis of Single Cell Clusters Using Laser Capture Microdissection**; Simon Davis[1]; Connor Scott[1]; Benedikt M Kessler[1]; Olaf Ansorge[1]; Roman Fischer[1]; *[1]University of Oxford, UK, Oxford, UK*

TOC pm 03:10 **Towards Rapid Quantitation of Lipids From Single Cells and Tissue Microdissections Using Laser Microdissection-Liquid Vortex Capture/ Electrospray Ionization-Mass Spectrometry (LMD-LVC/ESI-MS)**; John F. Cahill[1]; Vilmos Kertesz[1]; Tiffany Porta[2]; J.C. Yves Leblanc[3]; Ron M.A. Heeren[2]; Gary J. Van Berkel[1]; *[1]Oak Ridge National Laboratory, Oak Ridge, TN; [2]M4I Institute, Maastricht, Netherlands; [3]SCIEX, Concord, ON, Canada*

TOC pm 03:30 **Development of Chemical Isotope Labeling Nanoflow LC-MS for Metabolomic Profiling of Exosomes**; Xian Luo[1]; Mingrui An[2]; Kyle C. Cuneo[2]; David M. Lubman[2]; Liang Li[1]; *[1]University of Alberta, Edmonton, AB; [2]University of Michigan Medical Center, Ann Arbor, MI*

TOC pm 03:50 **Spatially-Resolved Tissue Micro-Sampling Coupled to Sensitive Nano-LC-MS to Determine the Heterogeneous Distribution of mAb and Targets in Tissues**; Bo An[1]; Ming Zhang[1]; Jun Qu[1]; *[1]SUNY at Buffalo, Buffalo, NY*

TOC pm 04:10 **Evaluating Zepto-Liter Volumes: A Label-Free Method of Determining Ligand Loading on Asymmetrical Nanoparticles**; Michael J. Eller[1]; Kavita Chandra[2]; Teri W. Odom[2]; Emile A. Schweikert[1]; *[1]Texas A&M University, College Station, TX; [2]Northwestern University, Evanston, IL*

2:30-4:30 pm Tuesday
METABOLOMICS: UNTARGETED PROFILING
Session Chair: Jessica Prenni (Colorado State University)
Ballroom 20D upper level

TOD pm 02:30 **Metabolomics Sample Preparation Without a Concentration/Evaporation Step – Effects on Throughput and Metabolome Coverage and Integrity**; Tony Karlsborn[1]; Magesh Muthu[1]; Barbara Witek[1]; Anders Nordstrom[2]; *[1]Umeå University,*

Umeå, Sweden; [2]Umea University, Umeå, Sweden

TOD pm 02:50 **Hierarchical Cluster Analysis of Technical Replicates to Identify Interferents in Untargeted Mass Spectrometry Metabolomics**; Lindsay K Caesar[1]; Olav M Kvalheim[2]; Nadja B Cech[1]; *[1]Department of Chemistry and Biochemistry, The University of North Carolina at Greensboro, Greensboro, NC; [2]Department of Chemistry, University of Bergen, Bergen, Norway*

TOD pm 03:10 **GC- and LC-MS Metabolomics Data Processing, Correction and Analysis**; Hayley Abbiss[1]; Scott J Campbell[2]; Joel P.A. Gummer[1, 3]; John H Moncur[2]; Robert D Trengove[1, 3]; *[1]Separation Science and Metabolomics Laboratory, Murdoch University, Perth, Australia; [2]SpectralWorks Ltd., Runcorn, UK; [3]Metabolomics Australia, Murdoch University Node, Perth, Australia*

TOD pm 03:30 **COSMA: A Novel Methodology for High-Throughput Chemical Classification of Unidentified Compounds in Metabolomics via Adaptive MS/MS Spectral Motif Based Searching**; Tytus D Mak[1]; Stephen E. Stein[1]; *[1]National Institute of Standards and Technology, Gaithersburg, MD*

TOD pm 03:50 **Using Relative Response Factors and EMBL-MCF Library for Quantitative Untargeted Metabolomics**; Prasad Phapale[1]; Andrew Palmer[1]; Ivan Protsyuk[1]; Theodore Alexandrov[1, 2]; *[1]EMBL, European Molecular Biology Laboratory, Heidelberg, Germany; [2]Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California, San Diego, La Jolla, CA*

TOD pm 04:10 **The Global FoodOmics Project: A Darwinian-Style Molecular and Microbial Inventory of Foods and Beverages**; Julia M. Gauglitz[1]; Morgan W. Panitchpakdi[1]; Francesca Di Ottavio[2]; Christine M. Aceves[1]; Elizabeth A. Brown[3]; Nicole C. Sikora[1]; Greg Humphrey[4]; Lindsay DeRight Goldasich[4]; Tara Schwartz[4]; MacKenzie Bryant[4]; Rachel J. Dutton[3]; Rob Knight[4]; Pieter C. Dorrestein[1]; *[1]University of California San Diego, Skaggs School of Pharmacy and Pharmaceutical Sciences, La Jolla, CA; [2]University of Teramo, Teramo, Italy; [3]University of California San Diego, Division of Biological Sciences, La Jolla, CA; [4]University of California San Diego, Department of Pediatrics, La Jolla, CA*

2:30-4:30 pm Tuesday
ENVIRONMENTAL: EMERGING CONTAMINANTS
Session Chair: Eunha Hoh (San Diego State University)
Ballroom 6A upper level

TOE pm 02:30 **High-Resolution Mass Spectrometry of Skin Mucus for Monitoring Physiological Impacts and Biotransformation Products in Fish Exposed to Wastewater Effluent**; Jonathan Mosley[1]; Drew Ekman[1]; Jenna Cavallin[2]; Dan Villeneuve[2]; Gerald Ankley[2]; Tim Collette[1]; *[1]US EPA, Athens, GA; [2]US EPA, Duluth, MN*

TOE pm 02:50 **Retrospective Suspect and Non-Target Screening of Emerging Pollutants and Transformation Products in Wastewater Effluent Using UHPLC-QTOF-MS/MS**; Hailemariam A Assress[1]; Hlengilizwe Nyoni[1]; Bhekie B Mamba[1]; Titius AM Msagati[1]; *[1]University of South Africa(UNISA), Johannesburg, South Africa*

TOE pm 03:10 **Using Mass Spectrometry to Vet Cyanotoxin Concentrations by Enzyme-Linked Immunosorbent Assay (ELISA)**; Judy Westrick[1]; Johnna Birbeck[2]; Jason Huntley[3]; Alison Margaret Thees[3]; Mark Citriglia[4]; David Szlag[5]; *[1]Wayne State University, Detroit, MI; [2]Wayne State University, Detroit , MI; [3]University of Toledo, Toledo, OH; [4]Northeast Ohio Regional Sewer District, Cuyahoga Heights, OH; [5]Oakland University, Rochester, MI*

TOE pm 03:30 **Organic Pollutants in the Snow of Russian Arctic Islands: 2016-2017 Expeditions**; Dmitrii Mazur[1]; Dmitrii Kosyakov[2]; Aleksandr Kozhevnikov[2]; Tomas Latkin[2]; Yulia Andreeva[2]; Viatcheslav Artaev[3]; Albert T Lebedev[1]; *[1]Moscow State University, Moscow, Russia; [2]Lomonosov Northern (Arctic) Federal University, Centre of Collective Usage "Arctica", Arkhangelsk, Russia; [3]LECO Corporation, Saint Joseph, Michigan*

TOE pm 03:50 **Energy Extraction and Utilization Impacts on Drinking Water Disinfection By-Product Formation and Toxicity**; Hannah Liberatore[1]; Michael J. Plewa[2]; Elizabeth D. Wagner[2]; Joshua M. Allen[1]; Danielle C. Westerman[1]; Jeanne M. VanBriesen[3]; David B. Burnett[4]; Leslie H. Cizmas[4]; Susan D. Richardson[1]; *[1]University of South Carolina, Columbia, SC; [2]University of Illinois at Urbana-Champaign, Urbana, Illinois; [3]Carnegie Mellon University, Pittsburgh, PA; [4]Texas A&M University, College Station, TX*

TOE pm 04:10 **Targeted Analysis of Oxygen Transformation Products Derived from Weathered Oil by FT-ICR MS**; Amy M. McKenna[1]; Huan Chen[1]; Sydney F. Niles[1, 2]; Logan C. Krajewski[1, 2]; Martha L. Chacón-Patiño[1]; Cameron C. Davis[1]; Ryan P. Rodgers[1, 2]; *[1]Natl High Magnetic Field Laboratory, Tallahassee, FL; [2]Florida State University, Tallahassee, FL*

2:30-4:30 pm Tuesday
INNOVATIONS IN HYDROGEN-DEUTERIUM EXCHANGE MS
Session Chair: Elyssia S. Gallagher (Baylor University)
Ballroom 6B upper level

TOF pm 02:30 **Chasing Tails: Cathepsin-L Paves the Way for the Analysis of Histones by HDX-MS**; Malvina Papanastasiou[1]; Besnik Bajrami[1]; Shawn Egri[1]; Samuel A Myers[1]; Stephen E Johnston[1]; Steven A Carr[1]; Jacob D Jaffe[1]; *[1]Broad Institute of MIT and Harvard, Cambridge, MA*

TOF pm 02:50 **Evaluation of Cross-Path Reactive Chromatography as a Platform for Dilution-Free H/D Exchange with MS Detection (HDX MS)**; Miaowei Xu[1]; Jake W. Pawlowski[1]; Igor A Kaltashov[2]; *[1]University of Massachusetts-Amherst, Amherst, MA; [2]Univ. of Massachusetts/Chemistry Dept., Amherst, MA*

TOF pm 03:10 **Isotopic Fine Structure from HDX-Derived Isotopologues Baseline Resolved by Ultrahigh Resolution 21 T FT-ICR Mass Spectrometry**; Peilu Liu[1]; Lissa C Anderson[2]; Greg T. Blakney[2]; Donald F Smith[2]; Chad R. Weisbrod[2]; Christopher L Hendrickson[2]; Alan G Marshall[1, 2]; *[1]Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL; [2]Ion Cyclotron Resonance Program, National High Magnetic Field Laboratory, Tallahassee, FL*

TOF pm 03:30 **Backbone Amide Hydrogen Exchange Rates Determined by Electron Transfer Dissociation Data**; Yoshitomo Hamuro[1]; Sook Yen E[2]; *[1]SGS, West Chester, PA; [2]Regeneron, Tarrytown, NY*

TOF pm 03:50 **Thiol-ene Microfluidic Chip for Sub-Second Timescale HDX-MS Analysis of Proteins**; Rasmus R. Svejdal[1]; Eleanor R. Dickinson[1]; Drago Sticker[1]; Jörg P. Kutter[1]; Kasper D. Rand[2]; *[1]University of Copenhagen, Copenhagen, Denmark; [2]University of Copenhagen, Copenhagen, Denmark*

TOF pm 04:10 **Continuous-Flow Hydrogen-Deuterium Exchange to Study Quadruplex Nucleic Acids Structures, Stability, and Interactions**; Eric Largy[1]; Valérie Gabelica[1]; *[1]Université de Bordeaux, Pessac, France*

2:30-4:30 pm Tuesday
QUALITATIVE AND QUANTITATIVE ANALYSIS OF POST-TRANSLATIONAL MODIFICATIONS
Session Chair: Michael A. Freitas (Ohio State University)
Ballroom 6CF upper level

TOG pm 02:30 **The Dynamic CBP/p300-Regulated Acetylome**; Brian Weinert[1]; Takeo Narita[1]; Shankha Satpathy[2]; Bala Srinivasan[3]; Bogi K. Hansen[1]; Beth E. Zucconi[4]; William Hamilton[1]; Christian Schölz[5]; Edward A. Kesicki[6]; Albert Lai[7]; Kenneth D. Bromberg[7]; Joshua Brickman[1]; Philip A. Cole[4]; Chunaram Choudhary[1]; *[1]University of Copenhagen, Copenhagen, Denmark; [2]Massachusetts Institute of Technology, Cambridge, MA; [3]Max Planck Institute for Biology of Ageing, Cologne, Germany; [4]Johns Hopkins School of Medicine, Baltimore, MD; [5]Max-von-Pettenkofer Institute, Munich, Germany; [6]Acylin Therapeutics, Seattle, WA; [7]Abbvie Inc., North Chicago, IL*

TOG pm 02:50 **Quantitative Top Down Proteomic Determination of Proteoform-Level Substrate Specificity of the Acetyltransferase P300 and Underlying Mechanisms of Specificity**; Nikit Venishetty[1, 2]; Tao Wang[1]; Matthew V. Holt[1]; Nicolas L. Young[1]; *[1]Baylor College of Medicine, Houston, TX; [2]Rice University, Houston, TX*

TOG pm 03:10 **Top-Down Analysis of KRAS Proteoforms Reveals Correlations Between KRAS Genetic State and PTM Patterns in the Context of Colorectal Cancer.**; Luca Fornelli[1]; Caroline J. DeHart[1]; Ioanna Ntai[2]; Josiah E. Hutton[1]; Peter F. Doubleday[1]; Richard LeDuc[1]; Ryan Fellers[1]; Wenan Qiang[1]; Emily S. Boja[3]; Gordon R. Whiteley[4]; Henry Rodriguez[3]; Neil L. Kelleher[1]; *[1]Northwestern University, Evanston, IL; [2]Thermo Scientific, San Jose, CA; [3]National Cancer Institute, Bethesda, MD; [4]Frederick National Laboratory for Cancer Research, Frederick, MD*

TOG pm 03:30 **Co-Existing Modifications on Histone Proteins are Reliable Biomarkers of the Cell Cycle State**; Congcong Lu[1]; Simone Sidoli[1]; Mariel Coradin[1]; Kevin Janssen[1]; Benjamin A. Garcia[1]; *[1]University of Pennsylvania School of Medicine, Philadelphia, PA*

TOG pm 03:50 **Time Resolved Quantitative Phospho-Tyrosine Analysis Reveals Bruton's Tyrosine Kinase Mediated Signaling Downstream of the Mutated Granulocyte-Colony Stimulating Factor Receptors**; Pankaj Dwivedi[1]; David E Muench[2]; H L Grimes[2]; Kenneth D Greis[1]; *[1]University of Cincinnati, Cincinnati, OH; [2]Cincinnati Children's Hospital Medical Center, Cincinnati, OH*

TOG pm 04:10 **ModDecode: Decoding Hundreds of Post Translational Modifications from Unrestrictive Database Search**; Seungjin Na[1]; Nuno Bandeira[2]; *[1]University of California, San Diego, La Jolla, CA; [2]University of California San Diego, La Jolla, CA*

2:30-4:30 pm Tuesday
FUNDAMENTALS: ION-ION AND ION-NEUTRAL INTERACTIONS
Session Chair: Prentice M. Boone (Vanderbilt University)
Ballroom 6DE upper level

TOH pm 02:30 **Reducing Congestion in Ultraviolet Photodissociation Spectra of Large Protein Ions Using Proton Transfer Reactions**; James Sanders[1]; Dustin D. Holden[2]; Jennifer S Brodbelt[1]; *[1]University of Texas at Austin, Department of Chemistry, Austin, TX; [2]Thermo Fisher Scientific, San Jose, CA*

TOH pm 02:50 **Diamonds and Dice: Insights into the Contrasting Chemistries of Adamantyl and Cubyl Radicals Using a Distonic Ion Approach**; Berwyck Poad[1]; David Marshall[1]; David Harman[2]; Craig M Williams[3]; Stephen J Blanksby[1]; *[1]Queensland University of Technology, Brisbane, Australia; [2]Western Sydney University, Sydney, Australia; [3]University of Queensland, Brisbane, Australia*

TOH pm 03:10 **Deducing Association Energies from Shifts in Arrival Time Distributions: Impacts of Selective Gas-Phase Ion-Vapor Clustering**; Pearl Kwantwi-Barima[1]; Christopher J Hogan Jr[2]; Brian H. Clowers[1]; *[1]Department of Chemistry, Washington State University, Pullman, WA; [2]Department of Mechanical Engineering, University of Minnesota, Minneapolis, MN*

TOH pm 03:30 **Diazirine Photo-Stapler and UVPD in Unraveling the Noncovalent Bonding Within DNA/Peptide "Illogical" Fragments**; Yang Liu[1]; Frantisek Turecek[1]; *[1]University of Washington, Seattle, WA*

TOH pm 03:50 **Kinetic Reactivity Study of Novel Carbon-Based Distonic Carbene Ions in Gas Phase by Using Linear Quadrupole Ion Trap Mass Spectrometry**; Erlu Feng[1]; Thinh Hoang[1]; Zaikuan Joshua Yu[1]; Jacob Milton[1]; Hilkka I. Kenttämaa[1]; *[1]Purdue University, West Lafayette, IN*

TOH pm 04:10 **Gas-Phase Ion/Ion Reactions Employing Tris-Phenanthroline Alkaline Earth Metal Complexes for the Detailed Structural Characterization of Fatty Acids**; Caitlin E Randolph[1]; David J Foreman[1]; Scott A McLuckey[1]; Stephen J Blanksby[2]; *[1]Purdue University, West Lafayette, IN; [2]Central Analytical Research Facility, Queensland University of Technology, Brisbane, Australia*

4:45-5:30 pm Tuesday
AWARD LECTURE
Vicki H. Wysocki (The Ohio State University)
Hall D ground level

Presentation of the Research Awards

- Award sponsored by Thermo Scientific by Iain Mylchreest to Michael T. Marty (University of Arizona).
- Award sponsored by Waters Corporation by Lance Nicolaysen to James S. Prell (University of Oregon).

Biemann Medal

Benjamin A. Garcia
University of Pennsylvania Perelman School of Medicine

There are light refreshments in Sails Pavilion upper level 5:30 - 5:45 pm.

01. Deconvolution of FT-MS Spectra: How it Works and What's Available (FTMS Interest Group)
Presiding: Melinda McFarland, Matthew Renfrow
Room 14 AB

Mass spectrometry has been called on to deal with increasingly complex samples, ranging from complex mixtures of intact proteins to non-targeted screening for contaminants. The result is a heightened need for software for accurate determination of masses from overlapping or poorly resolved charge state species. This year's FT-MS workshop will focus on methods for spectral deconvolution. A general overview of mass spectral deconvolution methods will be given. Other topics of discussion will include commonly available software, treatment of resolved and unresolved data, spectra with diverse isotopic peak widths, dealing with elution profiles in LC-MS data, and the problem of maximum entropy's deconvolution artifacts. Experts from both academia and industry will be available to help answer questions. The goal is to give users new to the field starting points for performing spectral deconvolution.

02. Reporting of Multi-Analyte Assays in Clinical Analyses (Clinical Chemistry Interest Group)
Presiding: Don Chace, Timothy Garrett
Room 15 AB

Metabolomics is emerging as a tool for clinical diagnostics and thus the reporting of multiple analytes associated with a disease is more common than in only newborn screening. However, reporting of results from multi-analyte assays can lead to confusion and the potential for misinterpretation may increase with the number of metabolites in a given assay. While algorithms can be used to identify changes and develop predictive models based on patterns of expression, describing the results of these model driven approaches can often be difficult. How can a clinical lab report results from complex metabolic panels in a clear and concise manner enabling improved clinical care? This workshop will examine current issues in multi-analyte metabolic assays both quantitative and non-quantitative and drive a discussion of practices that can lead to a more clear understanding of metabolism for clinical care.

03. Quantitative Glycomics and Glycoproteomics: Needs of Standards or Methods?
Presiding: Yehia Mechref
Room 16 AB

The demand for quantitative glycomics and glycoproteomics strategies, enabling sensitive monitoring of changes in the abundance glycans and glycoproteins is pressing because of the correlations between protein glycosylation and many biological processes and diseases. Currently, several analytical techniques are employed to address such demands, including capillary electrophoresis, liquid chromatography and mass spectrometry. Additionally, the availability of reliable glycan and glycoprotein standards is prompted by the demand for the reliable quantitative glycomics and glycoproteomics strategies. This workshop describes and discusses the different analytical methods and approaches routinely employed to achieve reliable quantitative MS-based glycomics and glycoproteomics, including the analysis of native, labeled and isotopically labeled glycans and glycoproteins. The workshop will also discuss the needs for reliable glycan/glycoprotein standards. The workshop will also discuss the combined needs and demands for reliable methods and standards.

04. Current Trends in High Spatial Resolution 2D and 3D Mass Spectrometry Analysis
Presiding: Christopher R. Anderton, Francisco Fernandez-Lima, Gregory Fisher
Room 17 AB

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

In this second workshop, we will provide an overview of the state of the art in high-spatial resolution 2D and 3D MS analysis from experts in the field and will continue the discussion towards the integration of new strategies into the sample preparation, analysis, and data processing workflows.

A preliminary list of topics will include:

i. 2D and 3D high spatial resolution MS analysis (tutorial)
ii. Efficacy and accuracy of ion imaging;
iii. Matrix effects and ion suppression;
iv. Quantitation strategies;
v. What information can actually be garnered from ion images;
vi. Technological Applications in Material, Biological and Forensic Sciences;
vii. 3D MS analysis and depth profiling;

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

05. Galaxy for MS Software Dissemination: How to Easily Publish Your Tools
Presiding: Tim Griffin, Pratik Jagtap, James Johnson
Room 5B

The free and open Galaxy bioinformatics platform has emerged as a valuable workflow engine for mass spectrometry (MS)-based informatics. Galaxy enables integration of disparate software tools to build sophisticated workflows for the analysis of biological MS data generated from proteomics and even metabolomics studies. An active and collaborative community of researchers, including the Galaxy for proteomics (Galaxy-P) team, continues to extend Galaxy for these applications, including those which integrate MS data with genomic information for multi-omic approaches.

For biological MS software developers, Galaxy provides a valuable resource to disseminate their tools to a wider-community of potential users. Once tools are implemented (wrapped) in Galaxy, they can be made available in the Tool Shed, which enables any Galaxy user to import software into their own instance and use these for their informatics needs.

Despite the upside, many software developers lack experience in wrapping tools in Galaxy. This workshop will provide participants a forum to discuss the process of implementing tools in Galaxy. Topics discussed will include software architecture that is most compatible with Galaxy implementation, as well as resources available, such as the Galaxy Training Network (GTN), for providing training and help to developers interested in tool wrapping in Galaxy. We will also provide an opportunity for hands-on training in the use of command-line utilities for streamlined publishing of software tools in Galaxy, wrapping an example MS-based software tool and depositing it in the Tool Shed. Participants are encouraged to bring a laptop to participate in this hands-on demonstration.

06. ASMS Diversity and Outreach Workshop
Presiding: Benjamin Garcia, Renã Robinson
Room 5A

The ASMS Diversity and Outreach workshop will feature an invited speaker, Dr. Alison Gammie, who is currently the Director of the

There are light refreshments in Sails Pavilion upper level 5:30 - 5:45 pm.

NIGMS's Division of Training, Workforce Development, and Diversity. In her role at the NIH, she supports the Institute's research training, career development and diversity-building activities through a number of programs at the undergraduate, graduate, postdoctoral and faculty levels. Her talk will center on the need for diversity in science, and ways that scientists at all levels can become involved to begin making a difference. Additionally, we also plan to devote time at this workshop to update the attendees on current ASMS Diversity and Outreach activities, and also solicit ideas for future initiatives.

07. Debunking the Myth of Stress: A Career Development Workshop
Presiding: Lucinda Hittle, Mike Lee
Room 4

Feeling stressed out? Anxious? Wondering how to take control of your own happiness? This is the workshop for you! Using the ActivInsightTM approach from Andrew Bernstein's The Myth of Stress, this workshop will take participants through an organized stress reduction exercise, then break out into small group discussions facilitated by veteran scientists across diverse sectors including industry, government and non-profit agencies, and academia. The goals of this workshop will be to foster relationships across the society that span the boundaries of geography, age, level of experience, and academic training as well as enabling networking and small group discussions. No experience required, but imagination and an open mind are pre-requisites!

08. Exposomics Tools
(Exposomics Interest Group)
Presiding: Jerod Grossman, H. M. 'Skip' Kingston
Room 3

The primary goal of the Exposomics workshop is to stimulate thoughts and encourage participation to discuss needs and directions of this field.

This year, the exposomics workshop will have two viewpoints:

1. Software/informatic needs present/future directions.
2. Targeted measurement studies accumulating as evidence of significant influence of exposure and effect on wellness.

Small molecule-omics fields are inherently "big data" fields and thus require statistics and informatics expertise to reach conclusions efficiently and accurately. Exposomics is a multi-disciplinary field and often researchers don't have a completely multi-disciplinary background, therefore many researchers are without the tools or the background to handle and process data in this way. This workshop is designed to give researchers a look into how others in the field are overcoming this barrier and what approaches they are using, as well as to connect exposomic researchers with statistic and chemoinformatic experts in the field. Dr. Jarod Grossman will provide an overview from the tools and mass spectrometry (MS) perspective.

Examples and discussions will include exposomics update on targeted data and inclusion of MS in many related fields contributing to the growth of exposomics. Targeted data in exposomics is an important piece of the overall picture that helps reveal the significance of exposure and validate the influence of environmental factors on human health. Recently developed targeted MS methods and tools are capable of generating statistically relevant data sets that can correlate to specific disease states and assess wellness. Prof. Skip Kingston will discuss targeted MS and data analysis tools.

09. The Roles of Metal in Ion Chemistry and Structure: In Honor of the Late Robert C. Dunbar
(Metal Ion Coordination Chemistry Interest Group)
Presiding: Eric Dodds, Nicolas Polfer
Room 10

A great role model, both as a scientist and as a human being, Robert C. Dunbar (Case Western Reserve University) sadly passed away in late 2017. His astute observations on fundamental ion structure, and particularly the intricate role of metals, will be sorely missed by the metal ion coordination community. We will therefore run a broadly themed workshop in his honor, with new experimental and theoretical insights that are inspired by some of Rob's work. It is expected that the discussions will give a historical perspective on old and new ideas how metals affect and even direct ion chemistry.

10. Environmental MS: New Trends in Sampling and Separations
(Environmental Applications Interest Group)
Presiding: Achille Cappiello, Imma Ferrer, Andrew Ottens
Room 9

The workshop will be centered upon two topic areas: new and miniaturized sample preparation techniques, with a particular emphasis on the "green" ones; new separation approaches, including stationary phases and comprehensive chromatography for improving MS sensitivity and selectivity. Three or four members of the environmental mass spectrometry community will informally present a few slides to generate discussion within the working group.

11. MassIVE Big Data: Revealing, Sharing and Reusing Discoveries of Deep Proteome Diversity in Repository-Scale Mass Spectrometry Data
Presiding: Nuno Bandeira, Mingxun Wang
Room 8

The growing volume of mass spectrometry data available in the public domain continues to expand the range of tissues, fluids, species and clinical conditions covered by multiple datasets and experimental protocols, thereby constituting a valuable resource for reanalysis and generation of new testable hypotheses. This workshop will focus on the systematic discovery of novel proteomics events in repository-scale big data, as well as discuss ways to aggregate the resulting discoveries into open community resources designed to facilitate i) exploration of novel events across hundreds of millions of identifications and b) reutilization of public discoveries for the design and analysis of new experiments.

12. Bioanalysis of Intact Biotherapeutics by Hybrid LBA/LCMS: Challenges & Solutions
(Regulated Bioanalysis Interest Group)
Presiding: Fabio Garofolo, Jian Wang
Room 7 AB

This workshop will discuss the Pros/Cons of using HRMS (QTOF & Orbitrap) for bioanalysis of intact therapeutic proteins and/or subunits and why and how intact protein quantification should be performed. The following topics will be discussed in an open and highly interactive panel discussion with opinion leaders and experts in the field: "Bottom-up" (signature peptide) and "Top-down" strategies in Bioanalysis; limitation of signature peptide approach to provide sufficient information on the biotherapeutics measured - "Lost in digestion"; how to preserve the therapeutic protein for intact quantification; identification and quantitation of intact biotherapeutics and their catabolites for a better understanding of the various circulating biotherapeutic forms, biotransformation, glycoforms quantitation and post-translational modifications. Moreover, it will be discussed how to overcome sensitivity issues in therapeutic intact protein quantification by maximizing enrichment via immunoaffinity (IA), deglycosylation and subunits quantification. Finally, the advantages of summing isotope signals will be discussed with a specific emphasis on charge state & isotope effects on S/N; possibility to charge state coalescence with DMSO to gain in signal intensity; optimizing extraction window (XIC) for quantitation, declustering potential, accumulation time and chromatographic options for intact proteins. The workshop will be concluded with sharing current industry standards for applying intact biotherapeutics bioanalysis by Hybrid LBA/LCMS in a fully regulated environment.

13. Forensic ID: Qualitative Identification in Forensic Mass Spectrometry
(Forensics & Homeland Security Interest Group)
Presiding: Kenyon Evans-Nguyen, Christopher Mulligan
Room 33 ABC

Mass spectrometry is integral to forensic science for identification, particularly for drugs, explosives, and ignitable liquids. Because these conclusions must withstand extensive scrutiny in an adversarial court system, the threshold for definitive identification in forensic science substantially exceeds that of most industrial or academic analyses. While forensic DNA analysis has established rigorous statistical methods for assessing certainty in identification, there are no such established criteria in forensic chemistry analyses. Advisory committees, such as the Scientific Working Group for the Analysis of Seized Drugs (SWGDRUG), as well as the standard operating procedures (SOPs) for working forensic laboratories set guidelines for whether analytical techniques could be considered as preliminary, confirmatory, or definitive identification techniques.

In this workshop, the qualitative identification of different evidence types using well-established mass spectrometry techniques (e.g., GC-MS and LC-MS) as well as emerging techniques (i.e., ambient ionization, fieldable instruments) will be discussed. While these emerging techniques can potentially speed up analysis and/or reduce costs, the lack of well-established criteria to determine specificity of identification is a barrier to adoption in forensic laboratories. The coordinators will lead the audience in a discussion with a panel of forensic scientists to discuss the ways in which academic, industrial, and government scientists can collaboratively work with forensic scientists through the challenges currently encountered in forensic identifications with mass spectrometry.

14. Computational Biology and Biology for Metabolomics: Bridging the Gap Matchmaking Session
Presiding: Emmanuel Hatzakis, Rachel Kopec, Ewy Mathe
Room 32 AB

Most of the time, bench scientists (chemists and biologists) and computational biologists speak different languages, yet science nowadays requires collaborative work. While bench scientists seek help with analysis of their data, computational biologists are hungry for data to test out their solutions to analytical problems. However, it is not always easy for researchers to find each other, particularly in a large conference setting.

With this in mind, the goal of this workshop is to promote conversations between computational biology, chemistry, and biology experts and to help bridge the gap between the fields. The session will be split into two parts: 1) 3-4 brief (10-15 min) talks from software developers and tools users; 2) informal, small group discussions (led by speakers), where tool developers/analysis experts interact with bench scientists/ novice researchers to identify common interests and foster future conversations/collaborations. Topics will include broad aspects of metabolomics analysis, including integration of metabolomics data with other omics data, and interpretation of metabolomic profiles (e.g. pathway analysis).

15. Lipidomics: Current Trends in Mass Spectrometry Data Collection
(Lipids & Lipodomics Interest Group)
Presiding: John Bowden, Eva Duchoslav
Room 31 ABC

Non-specific fragmentation techniques allow collection of unbiased MS/MS datasets on a chromatographic time scale. Ongoing advances in liquid chromatography and the advent of ion mobility are enabling greater separation of lipid isomers. At the same time, novel ion activation techniques are enhancing lipid structural characterization. With this expanding number of possibilities for mass spectrometry data collection it can be challenging to decide what approach is the best one for your project. This workshop will review several current techniques and their applications. A group of experts will share their experience with example workflows and answer any questions on how to get the most complete relevant information from the lipidomics MS experiments.

16. FAIMS/DIMS/DMS: Basics and Applications
Presiding: Rian Griffiths
Room 30 DE

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

AFTER 8:00 PM
CORPORATE HOSPITALITY SUITES
HILTON SAN DIEGO BAYFRONT

WEDNESDAY MORNING ORAL SESSIONS

7:00 am Wednesday
CORPORATE BREAKFAST SEMINARS
CONVENTION CENTER AND
HILTON SAN DIEGO BAYFRONT
See page 15 for detailed schedule.
Reservation or RSVP required.

8:30-10:30 am Wednesday
INSTRUMENTATION: MASS ANALYZER INNOVATIONS
Session Chair: Randall E. Pedder (Ardara Technologies)
Hall D ground level

WOA am 08:30 **A New Instrument for Improving the Signal-To-Noise of Mass Spectra**; Andrew N. Krutchinsky[1]; Herbert Cohen[1]; Brian T. Chait[1]; [1]*The Rockefeller University, New York, NY*

WOA am 08:50 **Advancing Digital Waveform Technology**; Margaret Elizabeth Reece[1]; Ashley Marie Moon[1]; Adam Paul Huntley[1]; Bojana Opacic[1]; Zachary Philip Gotlib[1]; Nathan Michael Hoffman[1]; Peter T. A. Reilly[1]; [1]*Washington State University, Pullman, WA*

WOA am 09:10 **inTrap-MALDI Charge Detection Mass Spectrometry for Intact High m/z Molecular Ion Analysis**; Chun-Yen Cheng[1]; Yao-Hsin Tseng[1]; Szu-Wei Chou[1]; Shih Chieh Yang[1]; [1]*AcroMass Technologies, Inc., Taipei, Taiwan*

WOA am 09:30 **Ion Mobility Separation Using a Dual-Trap Instrument**; Jingjin Fan[1]; Xinwei Liu[1]; Xiaoyu Zhou[1]; Zheng Ouyang[1]; [1]*State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instrument, Tsinghua University, Beijing, China*

WOA am 09:50 **Precursor and Neutral Loss Scans on Benchtop and Portable Ion Trap Mass Spectrometers**; Dalton T. Snyder[1]; Lucas J. Szalwinski[1]; Ryan Hilger[1]; Robert L. Schrader[1]; Valentina Pirro[1]; Desmond A. Kaplan[2]; Ryan M. Danell[3]; Veronica T. Pinnick[4]; Paul R. Mahaffy[4]; Mitch Wells[5]; R. Graham Cooks[1]; [1]*Purdue University, West Lafayette, IN;* [2]*KapScience LLC, Tewksbury, MA;* [3]*Danell*

Consulting, Inc., Winterville, NC; [4]NASA Goddard Space Flight Center, Greenbelt, MD; [5]FLIR Systems, Inc., West Lafayette, IN

WOA am 10:10 **Multiplexed Operation of an Orthogonal Multi-Reflecting TOF Instrument to Increase Duty Cycle by Two Orders**; Boris Kozlov[1]; Jeffery M Brown[1]; Viatcheslav Artaev[2]; *[1]Waters Corporation, Wilmslow, UK; [2]LECO Corporation, Saint Joseph, MI*

8:30-10:30 am Wednesday
ION MOBILITY: STRUCTURE
Session Chair: Eric Davis (Department of Biology and Chemistry)
Ballroom 20A upper level

WOB am 08:30 **Mass Spectrometry and Ion Mobility Spectrometry for Investigating the Interlocked Nature of Catenanes**; Anneli Kruve[1]; Kenji Caprice[2]; Christoph A Schalley[1]; Fabien Cougnon[2]; *[1]Free University of Berlin, Berlin, Germany; [2]University of Geneva, Geneva, Switzerland*

WOB am 08:50 **Ion Mobility Spectrometry-Mass Spectrometry Reveals Critical Steps in Thermal and Laser-induced Protein Melting Transitions**; Tarick J. El-Baba[1]; Daniel R. Fuller[1]; Daniel W. Woodall[1]; Shannon A. Raab[1]; Christopher R. Conant[1]; Jonathan M. Dilger[2]; Yoni Toker[3]; Evan R. Williams[4]; David H. Russell[5]; David E. Clemmer[1]; *[1]Department of Chemistry, Indiana University, Bloomington, IN; [2]Spectrum Warfare Systems Department, NSWC Crane Division, Crane, IN; [3]Department of Physics and Inst. of Nanotechnology, Bar-Ilan University, Ramat-Gan, Israel; [4]Department of Chemistry, University of California, Berkeley, Berkeley, CA; [5]Department of Chemistry, Texas A&M University, College Station, TX*

WOB am 09:10 **Native Ion Mobility-Mass Spectrometry and Computational Investigation of Surface-Induced Dissociation of Non-Specific Protein Heterodimer Ions**; Micah T Donor[1]; Daniel Ko[1]; James S Prell[1, 2]; *[1]University of Oregon Department of Chemistry and Biochemistry, Eugene, OR; [2]Materials Science Institute, University of Oregon, Eugene, OR*

WOB am 09:30 **Characterization and Separation of Chiral Isomers by Ion Mobility: An Investigation of Lassopressin Nonapeptides**; James N. Dodds[1]; Shawn T. Phillips[1]; Berkley M. Ellis[1]; Jody C. May[1]; John A. McLean[1]; *[1]Vanderbilt University, Nashville, TN*

WOB am 09:50 **Probing Structures Various Cyclosporin Analogues Using Differential Mobility Spectroscopy, Collision Induced Dissociation and Gas-Phase Hydrogen-Deuterium Exchange**; J. Larry Campbell[1]; K. H. Brian Lam[1, 2]; J. C. Yves Le Blanc[1]; Tim Hoffman[1]; *[1]SCIEX, Concord, ON, Canada; [2]York University, Toronto, ON, Canada*

WOB am 10:10 **Memory of the Condensed-Phase in the Gas-Phase: Effects of Solution, Charge, and Energy on Structures of Serum Albumin Ions**; Meagan Gadzuk-Shea[1]; Matthew F Bush[1]; *[1]University of Washington, Seattle, WA*

8:30-10:30 am Wednesday
QUANTITATIVE ANALYSIS IN DRUG DISCOVERY AND DEVELOPMENT
Session Chair: Wilson Shou (Bristol-Myers Squibb Company)
Ballroom 20BC upper level

WOC am 08:30 **How to Boost Bioanalysis with a Modern Platform for Automated LC-MS/MS**; Tom Bretschneider[1]; Wolfgang Rist[1]; Wolfgang Jörg[1]; Spaeth Christian[1]; Wild Siegfried[1]; Daniel Bischoff[1]; Andreas Harald Luippold[1]; *[1]Boehringer-Ingelheim Pharma GmbH & CO KG, Biberach an der Riß, Germany*

WOC am 08:50 **LCMS-based Quantitation of Tissue Protein Biomarkers – Challenges and Applications**; Petia Shipkova[1]; Bogdan Sleczka[1]; Jacob Zalaznick[1]; Yongxin Zhu[1]; Hongwei Zhang[1]; Timothy Olah[1]; *[1]Bristol Myers Squibb, Princeton, NJ*

WOC am 09:10 **Targeted Proteomic Approaches for Identifying Novel Targets of Clinically Used Kinase Inhibitors**; Weili Miao[1]; Lei Guo[2]; Yinsheng Wang[2]; *[1]University of California, Riverside, CA; [2]UC Riverside, Riverside, CA*

WOC am 09:30 **Quantification of Anticancer Drug in Live Single Cancer Cells Using the Single-Probe MS Technique**; Ning Pan[1]; Shawna Standke[1]; Mei Sun[1]; Naga Rama Kothapalli[1]; Anthony Burgett[1]; Zhibo Yang[1]; *[1]University of Oklahoma, Norman, OK*

WOC am 09:50 **Intact Monoclonal Antibody Quantitation for Preclinical Pharmacokinetic Drug Development**; Lisa A O'Callaghan[1]; Daniel S. Spellman[1]; Kevin P. Bateman[1]; *[1]Merck, West Point, PA*

WOC am 10:10 **Detection of Ionization Suppression in Individual Study Samples**; Richard King[1]; Jacob Barlow[2]; Susan Crathern[1]; William Metzler[1]; Carmen Fernandez-Metzler[1]; *[1]PharmaCadence Analytical Services, LLC, Hatfield, PA; [2]California Institute of Technology, Pasadena, CA*

8:30-10:30 am Wednesday
MS IN CLINICAL ANALYSIS
Session Chair: Ravinder J. Singh (Mayo Clinic)
Ballroom 20D upper level

WOD am 08:30 **Development of Amyloidosis Typing Methods Using Data-Independent Acquisition Mass Spectrometry**; Han-Yin Yang[1]; Dao-Fu Dai[2]; Kelly D. Smith[2]; Andy Hoofnagle[3]; Christine C. Wu[4]; Michael J MacCoss[5]; *[1]University of Washington, Seattle, WA; [2]University of Washington Pathology, Seattle, WA; [3]University of Washington Clinical Chemistry, Seattle, WA; [4]Stratus Biosciences, Seattle, WA; [5]University of Washington Genome Sciences, Seattle, WA*

WOD am 08:50 **Automated and Robust Clinical Glycomics Analysis of Plasma and DBS with Linkage-Specific Sialic Acid Esterification Combined with Ultrahigh Resolution MS**; Gerda C. M. Vreeker[1]; Simone Nicolardi[1]; Marco R. Bladergroen[1]; Corné J. van der Plas[1]; Wilma E. Mesker[1]; Rob A. E. M. Tollenaar[1]; Yuri E. M. van der Burgt[1]; Manfred Wuhrer[1]; *[1]Leiden University Medical Center, Leiden, Netherlands*

WOD am 09:10 **Validation of the MasSpec Pen for Ovarian Cancer Diagnosis**; Marta Sans[1]; Jialing Zhang[1]; John Q. Lin[1]; Noah Giese[1]; Jinsong Liu[2]; Anil K Sood[2]; Livia S Eberlin[1]; *[1]University of Texas at Austin, Austin, TX; [2]MD Anderson Cancer Center, Houston, TX*

WOD am 09:30 **Simultaneous Quantitation of Norelgestromin, Ethinyl Estradiol, Estradiol, and Progesterone in Human Serum by LC-MS/MS**; Steven W. Blue[1]; Andrea J. Winchell[1]; David W. Erikson[1]; *[1]Oregon National Primate Research Center, Beaverton, OR*

WOD am 09:50 **Near Real-Time Diagnosis of Omental Metastases in Patients with Primary Colorectal Cancer Using Rapid Evaporative Ionisation Mass Spectrometry (REIMS)**; Eftychios Manoli[1];

Afeez Adebesin[1,2]; Zsolt Bodai[1]; Julia Balog[3]; Hiromi Kudo[1]; Steven D Pringle[4]; Robert Goldin[1]; Ara Darzi[1,2]; Jamie Murphy[1,2]; James M Kinross[1,2]; Zoltan Takats[1]; *[1]Imperial College London, London, UK; [2]Imperial College Healthcare NHS Trust, London, UK; [3]Waters Research Centre, Budapest, Hungary; [4]Waters Corporation, Wilmslow, UK*

WOD am 10:10 **Development and Validation of a High Sensitivity Assay of Estrogens in Human Plasma by UHPLC-MS/MS without Derivatization**; Mikael Levi[1]; Hironori Kobayashi[2]; Jun Watanabe[1]; *[1]Shimadzu Corporation, MS Business Unit, Kyoto, Japan; [2]Department of Pediatrics, Shimane University Faculty of Medecine, Shimane, Japan*

8:30-10:30 am Wednesday
EXPOSOMICS
Session Chair: Krystal J. Pollitt (University of Massachusetts Amherst)
Ballroom 6A upper level

WOE am 08:30 **Linking Chemo-Environmental Fingerprints of Dusts with Health Status of Household Members**; Yi-Ling Gao[1]; Hsin-Hsiang Chung[2]; Wen-Chi Chang[3]; Ta-Chen Su[3]; Cheng-Chih Hsu[1]; *[1]Department of Chemistry, National Taiwan University, Taipei, Taiwan; [2]National Taiwan University, Taipei, Taiwan; [3]Department of Internal Medicine, National Taiwan University Hospital, Taipei, Taiwan*

WOE am 08:50 **Measuring Human Exposure to Glyphosate Using a Rapid Urinary LC-MS/MS Assay**; Marissa McGilvrey[1]; Khyatiben V Pathak[1]; Mary Ellen Ahearn[1]; Russ Brandt[1]; Patrick Pirrotte[1]; *[1]Collaborative Center for Translational Mass Spectrometry, Translational Genomics Research Institute (TGen), Phoenix, AZ*

WOE am 09:10 **Metabolomics –A Key Technology for Deciphering Exposure and Effect**; Benedikt Warth[1,2]; Gary Siuzdak[2]; *[1]University of Vienna, Vienna, Austria; [2]The Scripps Research Institute, La Jolla, CA*

WOE am 09:30 **Improving High Throughput Exposomics through EPA's Non-Targeted Analysis Collaborative Trial (ENTACT)**; Randolph R Singh[1]; Alex Chao[1]; Xin Rui Xia[2]; Damian Shea[2]; Jon Sobus[1]; Elin Ulrich[1]; *[1]US Environmental Protection Agency, RTP, NC; [2]North Carolina State University, Raleigh, NC*

WOE am 09:50 **Targeted and Non-Targeted Analysis of the Serum Exposome Using Comprehensive Two-Dimensional Gas Chromatography (GCxGC) Coupled to High Resolution Mass Spectrometry**; Karl J Jobst[1]; Alicia Mell[1,2]; Robert Di Lorenzo[2]; Eric J Reiner[3]; John G Sled[2]; *[1]McMaster University, Hamilton, ON, Canada; [2]Hospital for Sick Children, Toronto, ON, Canada; [3]University of Toronto, Toronto, ON, Canada*

WOE am 10:10 **Serum Proteomics Using Microflow UHPLC and Data-Independent Acquisition**; Matthew Foster[1]; J. Will Thompson[1]; Elizabeth Petzold[1]; Sarah Rains[1]; Rose Asrican[1]; Emily Ko[1]; Thomas Burke[1]; Christopher Woods[1]; M. Arthur Moseley[1]; *[1]Duke University, Durham, NC*

8:30-10:30 am Wednesday
MACROMOLECULAR COMPLEXES
Session Chair: William Russell (University of Texas Medical Branch)
Ballroom 6B upper level

WOF am 08:30 **Resolving Subpopulations in High and Low-Density Lipoproteins**; Corinne Lutomski[1]; Scott M Gordon[2]; Alan T Remaley[2]; Martin F Jarrold[1]; *[1]Indiana University, Bloomington, IN; [2]National Institutes of Health, Bethesda, MD*

WOF am 08:50 **Conformational Switching of the MLKL Pseudokinase Domain Promotes MLKL Tetramerization and Cell Death by Necroptosis**; Jarrod Sandow[1]; Emma Petrie[1]; Annette Jacobsen[1]; Michael Griffin[2]; Brian Smith[3]; Isabelle Lucet[1]; Katherine Davies[1]; Ahmad Wardak[1]; John Silke[1]; Peter Czabotar[1]; James Murphy[1]; Andrew I. Webb[1]; *[1]The Walter & Eliza Hall Institute, Parkville, Australia; [2]Bio21 Molecular Science and Biotechnology Institute, The University of Melbourne, Melbourne, Australia; [3]La Trobe University, Bundoora, Australia*

WOF am 09:10 **Compositional Heterogeneity of Ribosomal Particles Probed In-Depth by a Combination of Top-Down, Bottom-Up and Native Mass Spectrometry**; Sem Tamara[1]; Michiel van de Waterbeemd[1]; Kyle L. Fort[2]; Eugen Damoc[2]; Vojtech Franc[1]; Philipp Bieri[3]; Martin Itten[3]; Alexander Makarov[2]; Nenad Ban[3]; Albert J.R. Heck[1]; *[1]Utrecht University, Utrecht, Netherlands; [2]Thermo Fisher Scientific, Bremen, Germany; [3]ETH Zurich, Zurich, Switzerland*

WOF am 09:30 **Global Measurement of Ribosomal Fidelity Under Genetic and Antibiotic Stress**; Camille N Pierre[1]; Matthew M Champion[1]; *[1]University of Notre Dame, Notre Dame, IN*

WOF am 09:50 **Hydrogen-Deuterium Exchange of Challenging Macromolecular Protein Complexes**; Sheena D'arcy[1]; Lokeshwar Bhenderu[1]; Kyle W Murray[1]; *[1]The University of Texas at Dallas, Richardson, TX*

WOF am 10:10 **HX MS Details Binding and Dynamics in the 19S Proteasome Base Subcomplex upon Deubiquitinase Interaction**; Jamie A. Moroco[1]; Ka Ying Hung[2]; Geng Tian[2]; Suzanne Elsasser[2]; Duco van Dalen[3]; Huib Ovaa[3]; Daniel Finley[2]; John R. Engen[1]; *[1]Northeastern University, Boston, MA; [2]Harvard Medical School, Boston, MA; [3]Leiden University Medical Center, Leiden, Netherlands*

8:30-10:30 am Wednesday
INFORMATICS: PEPTIDE AND PROTEIN IDENTIFICATION, PROTEOMICS
Session Chair: John S. Cottrell (Matrix Science, Ltd.)
Ballroom 6CF upper level

WOG am 08:30 **Maestro: Multi-Stage Discovery of Hypermodified Peptides and Deep Proteome Diversity**; Julie S Wertz[1]; Seungjin Na[1]; Laurence Bernstein[1]; Jeremy Carver[1]; Benjamin Pullman[1]; Jian Wang[1]; Mingxun Wang[1,2]; Nuno Bandeira[1,2]; *[1]Department of Computer Science and Engineering, University of California, San Diego, La Jolla, CA; [2]Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA*

WOG am 08:50 **Enhanced Global PTM Discovery (G-PTM-D) and Label-Free Quantification with MetaMorpheus**; Michael R. Shortreed[1]; Stefan K. Solntsev[1]; Lei Lu[1]; Zach Rolfs[1]; Robert J. Millikin[1]; Rachel M. Miller[1]; Leah V. Schaffer[1]; Connor V. Hoffmann[1]; Xanrun Qu[1]; Brian L. Frey[1]; Lloyd M. Smith[1]; *[1]University of Wisconsin, Madison, WI*

WOG am 09:10 **Database Independent Protein Sequencing (DiPS) Enables Full-Length *de-novo* Protein and Antibody Sequence Determination**; Alon Savidor[1]; Rotem Barzilay[1]; Dalia Elinger[1]; Yosef Yarden[1]; Moshit Lindzen[1]; Alexandra Gabashvili[1]; Ophir Adiv Tal[1]; Yishai Levin[1]; *[1]Weizmann Institute, Rehovot, Israel*

WOG am 09:30 **Symmetric Binomial Score and Tag-Enhanced Scoring Significantly Improve Sensitivity of the Andromeda Search Engine**; Petra Gutenbrunner[1]; Shivani Tiwary[1]; Favio Salinas[1]; Roie Levy[2]; Kanna Palaniappan[2]; Peter Cimermancic[2]; Jürgen Cox[1]; *[1]Max-Planck Institute of Biochemistry, Martinsried, Germany; [2]Verily Life Sciences, South San Francisco, CA*

WOG am 09:50 **The Pitfalls of Empirical FDR Cross Validation for the Targeted Analysis of DIA or SWATH**; Oliver M Bernhardt[1]; Tejas Gandhi[1]; Lynn Verbeke[1]; Sira Echevarria-Zomeno[1]; Florian Marty[1]; Roland Bruderer[1]; Lukas Reiter[1]; *[1]Biognosys AG, Schlieren, Switzerland*

WOG am 10:10 **Proteometools: Progress on the Generation of Reference Peptides and Spectra for the Human Proteome**; Daniel P Zolg[1]; Mathias Wilhelm[1]; Siegfried Gessulat[1, 2]; Tobias K Schmidt[1]; Patroklos Samaras[1]; Karsten Schnatbaum[3]; Johannes Zerweck[3]; Tobias Knaute[3]; Ulf Reimer[3]; Hans-Christian Ehrlich[2]; Stephan Aiche[2]; Pedro Navarro[4]; Bernard Delanghe[4]; Andreas Huhmer[5]; Bernhard Kuster[1, 6, 7]; *[1]Technical University of Munich, Chair of Proteomics and Bioanalytics, Freising, Germany; [2]SAP SE, Potsdam, Germany; [3]JPT Peptide Technologies GmbH, Berlin, Germany; [4]Thermo Fisher Scientific, Bremen, Germany; [5]Thermo Fisher Scientific, San Jose, CA; [6]Center for Integrated Protein Science (CIPSM), Munich, Germany; [7]Bavarian Center for Biomolecular Mass Spectrometry, Freising, Germany*

8:30-10:30 am Wednesday
FUNDAMENTALS: ION SPECTROSCOPY (IN MEMORY OF ROB DUNBAR)
Session Chair: Victor Ryzhov (Northern Illinois University)
Ballroom 6DE upper level

WOH am 08:30 **Metal Ion Coordination Elucidated by IR Ion Spectroscopy: Dunbar's legacy**; Jos Oomens[1]; Giel Berden[1]; Jonathan Martens[1]; Nicolas C Polfer[2]; *[1]Radboud University Nijmegen, Nijmegen, Netherlands; [2]University of Florida Department of Chemistry, Gainesville, FL*

WOH am 08:50 **Inverse Sandwich Cyclopentadienyl Complexes of Sodium in the Gas Phase**; Terry B McMahon[1]; Joshua Featherstone[1]; Jonathan Martens[3]; Jos Oomens[3]; *[1]University of Waterloo, Waterloo, ON, Canada; [3]Radboud University, FELIX Laboratory, Nijmegen, Netherlands*

WOH am 09:10 **Electronic Circular Dichroism Ion Spectroscopy**; Steven Daly[1]; Nina Khristenko[1]; Frédéric Rosu[2]; Valerie Gabelica[1]; *[1]INSERM, CNRS & University of Bordeaux (ARNA Laboratory), Pessac, France; [2]CNRS, INSERM & University of Bordeaux (IECB), Pessac, France*

WOH am 09:30 **Gas-Phase Spectroscopy and Chemistry of the Long-Lived Triplet Cation of Rhodamine 6G**; Richard A. J. O'hair[1]; Luke Mac Aleese[2]; Mathilde Bouakil[2]; Philippe Dugourd[2]; *[1]University of Melbourne, Victoria, Australia; [2]Institut Lumière Matière, UMR5306 CNRS & UCBL, Lyon, France*

WOH am 09:50 **Investigating Electronic and Structural Changes Imposed by Zwitterionic Pairing in Model Peptide Systems Using IR-UV Double Resonance Spectroscopy**; Christopher Harrilal[1]; Anthony M Pitts-McCoy[2]; Timothy S. Zwier[2]; Scott A McLuckey[2]; *[1]Purdue University, Lafayette, IN; [2]Purdue University, West Lafayette, IN*

WOH am 10:10 **A Dunbaresque Study of the IRMPD Spectra of Aspartic Acid Complexes with Zn2+ and Cd2+**; Georgia C. Boles[1]; Randy L. Hightower[1]; Rebecca A. Coates[1]; Christopher P. McNary[1]; Giel Berden[2]; Jos Oomens[2]; Peter B. Armentrout[1]; *[1]University of Utah, Salt Lake City, UT; [2]Radboud University, Nijmegen, Netherlands*

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

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

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

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

WEDNESDAY AFTERNOON ORAL SESSIONS

2:30-4:30 pm Wednesday
INSTRUMENTATION: INNOVATIONS IN FT-BASED MASS ANALYZERS
Session Chair: Jon Amster (University of Georgia)
Hall D ground level

WOA pm 02:30 **Progress in Development of FT Mass Spectrometer on the Bases of Multiple Electrode Harmonized Kingdon Trap**; Eugene (Evgeny) Nikolaev[1]; Gleb Vladimirov[1, 2]; Oleg Kharybin[1]; Yuri Kostyukevich[1]; Luis Fernando Velasquez-Garcia[3]; *[1]Skolkovo Institute of Science and Technology, Moscow, Russia; [2]Moscow Institute of Physics and Technology, Moscow, Russia; [3]Massachusetts Institute of Technology, Cambridge, MA*

WOA pm 02:50 **Ultrahigh Resolving Power Ion Isolation by 21 T FT-ICR MS**; Donald F. Smith[1]; Greg T. Blakney[1]; Steve C. Beu[2]; Christopher L. Hendrickson[1, 3]; *[1]National High Magnetic Field Laboratory, Tallahassee, FL; [2]S. C. Beu Consulting, Austin, Texas; [3]Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL*

WOA pm 03:10 **Towards Increasing the Performance of FTICR-MS with Signal Detection at Frequency Multiples: Signal Theory and Numerical Study**; Qinghao Wu[1]; Mikhail Gorshkov[2]; Jared B. Shaw[3]; Ljiljana Pasa Tolic[3]; *[1]Pacific Northwest National Laboratory, Richland; [2]V.L. Talrose Institute for Energy Problems of Chemical Physics, Moscow, Russia; [3]PNNL, Richland, WA*

WOA pm 03:30 **CRAFTI Collision Cross Sections at Extended m/z Using Low Energy Dissociation: Cucurbit[5]uril Complexes Containing Cesium by Variable Energy Techniques**; Tina H. M. Farzan[1]; Andrew J. Arslanian[1]; David V. Dearden[1]; *[1]Brigham Young University, Provo, UT*

WOA pm 03:50 **Complex Mixtures in Native Mass Spectrometry: Rapid, Simultaneous Measurements of Mass, Charge and Mobility One Ion at a Time**; Conner C Harper[1]; Andrew G Elliott[1]; Haw-Wei Lin[1]; Evan R Williams[1]; *[1]University of California, Berkeley, Berkeley, CA*

WOA pm 04:10 **Less is More: Low Ion Count Scans Lead to Increased Resolution**; Jared O. Kafader[1]; Michael W. Senko[2]; Rafael D. Melani[1]; Alexander Makarov[3]; Neil L. Kelleher[1]; Philip D. Compton[1]; *[1]Northwestern*

University, Evanston, IL; [2]Thermo Fisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific, Bremen, Germany

2:30-4:30 pm Wednesday
MICROORGANISMS AND THE MICROBIOME
Session Chair: Trent Northen (Lawrence Berkeley National Laboratory)
Ballroom 20A upper level

WOB pm 02:30 **Global Analysis of the Chemistry Associated with the Microbiome**; Mingxun Wang[1]; Ricardo da Silva[1]; Madeleine Ernst[1]; Nuno Bandeira[1]; Rob Knight[1]; Pieter Dorrestein[2]; *[1]UCSD, San Diego, CA; [2]University of California, San Diego, Skaggs School, La Jolla, CA*

WOB pm 02:50 **Lipidomic Dissection of Immunomodulatory Mediator Biosynthesis by Gut Microbiota-Diet Interaction**; Sungwhan F Oh[1, 2]; Heebum Song[3]; Wen Zheng[1]; Naama Geva-Zatorsky[1]; Charlie C Lee[1]; Seung Bum Park[3]; Dennis L Kasper[1]; *[1]Harvard Medical School, Boston, MA; [2]Brigham and Women's Hospital, Boston, MA; [3]Seoul National University, Seoul, South Korea*

WOB pm 03:10 **Application of Dynamic Silac to Determine Protein Turnover During Toxin-Induced Persistence and Resuscitation in *E.Coli***; Maja Semanjski[1]; Elsa Germain[2]; Szabolcs Semsey[3]; Kenn Gerdes[3]; Boris Macek[1]; *[1]Quantitative Proteomics, University of Tuebingen, Tuebingen, Germany; [2]Laboratoire de Chimie Bacterienne UMR 7283, Aix Marseille University, Marseille, France; [3]Department of Biology, University of Copenhagen, Copenhagen, Denmark*

WOB pm 03:30 **Elucidation of Metabolic Networks by Large Scale, Non-Targeted Metabolomics**; Nicola Zamboni[1]; Tobias Fuhrer[2]; Daniel Sévin[2]; Uwe Sauer[2]; *[1]ETH Zürich, Zürich, Switzerland; [2]ETH Zürich, Zurich, Switzerland*

WOB pm 03:50 ***De novo* Sequencing of Tandem Mass Spectra Reveals a Vast Dark Matter of Cyclopeptidomics**; Bahar Behsaz[1]; Hosein Mohimani[2]; Alexey Gurevich[3]; Andrey Prjibelski[3]; Mark F Fisher[4]; Larry Smarr[5]; Pieter C. Dorrestein[6]; Joshua S Mylne[4]; Pavel A Pevzner[7]; *[1]Bioinformatics and Systems Biology Program, University of California San Diego, La Jolla, CA; [2]Computational Biology Department, School of Computer Science, Carnegie Mellon University, Pittsburgh, PA; [3]Center for Algorithmic Biotechnology, Institute of Translational Biomedicine, Saint Petersburg State University, St Petersburg, Russia; [4]School of Molecular Sciences and ARC Centre of Excellence in Plant Energy Biology, The University of Western Australia, Crawley, Australia; [5]Department of Computer Science and Engineering, University of California, San Diego, La Jolla, CA; [6]Skaggs School of Pharmacy & Pharmaceutical Sciences, University of California San Diego, San Diego, CA; [7]Computer Science and Engineering, University of California, San Diego, La Jolla, CA*

WOB pm 04:10 **Characterization of the Central Pacific Oxygen Minimum Zone: The Results of the ProteOMZ Expedition**; Jaclyn Saunders[1]; Matthew McIlvin[1]; Dawn Moran[1]; Noelle Held[1]; Joe Futrelle[1]; Eric Webb[2]; Alyson Santoro[3]; Chris Dupont[4]; Mak Saito[1]; *[1]Woods Hole Oceanographic Inst., Woods Hole Ma 02543, MA; [2]University of Southern California, Los Angeles, CA; [3]University of California, Santa Cruz, CA; [4]J. Craig Venter Institute, La Jolla, CA*

2:30-4:30 pm Wednesday
MS IN EXTRACTABLE AND LEACHABLE ANALYSIS
Session Chair: Kate Comstock (Thermo Fisher Scientific)
Ballroom 20BC upper level

WOC pm 02:30 **Component Identification Beyond "EI Library Search". USP <1663> in Practice**; Gyorgy Vas[1]; Louis Fleck[1]; Howard Carpenter[1]; Jiun-Tang Huang[1]; Jason Cole[2]; *[1]Intertek, Whitehouse, NJ; [2]Thermo Fisher Scientific, San Jose, CA*

WOC pm 02:50 **Characterization and Visualization of Complex Mixtures of Extractables/Leachables and Pharmaceutically Relevant Compounds Using High Resolution 2-D and 3-D Mass Mapping**; Douglas E. Kiehl[1]; Scott Campbell[2]; David Stranz[2]; Diane Paskiet[3]; George Maydwell[2]; *[1]Eli Lilly & Company, Indianapolis, IN; [2]Sierra Analytics, Inc., Modesto, CA; [3]West Pharmaceutical Services, Inc., Exton, PA*

WOC pm 03:10 **Large Scale Assessment of E&L's from Single Use Bioreactors for Biopharmaceutical Manufacture**; Noemi Dorival-Garcia[1]; Sara Carillo[1]; Christine Ta[1]; Jonathan Bones[1]; *[1]The National Institute for Bioprocessing Research & Training, Dublin, Ireland*

WOC pm 03:30 **Ion Mobility Spectrometry (IMS) Analysis for Extractable and Leachable Compounds from Prefilled Syringe (PFS)**; Dujuan Lu[1]; Danny Hower[1]; Gordon Fujimoto[2]; Chris Stumpf[3]; *[1]SGS Life Science Services, Fairfield, NJ; [2]Waters Corporation, Beverly, MA; [3]Waters Corporation, Milford, MA*

WOC pm 03:50 **A Quick Approach of Identification of Extractables by LC/Q/TOF**; Jin Ren[1]; Wenan Lu[2]; Benben Song[1]; *[1]Pall Biotech, Westborough, MA; [2]Pall Biotech, Portsmouth, UK*

WOC pm 04:10 **Comparison of Library Generated CCS Values for Extractable and Leachable Components, Using LC-Ion-Mobility-Mass Spectrometry Using Different Chromatographic Conditions**; Jane Cooper[1]; Patricia Wright[2]; Sarah Dowd[3]; Baiba Cabovska[4]; *[1]Waters Corporation, Wilmslow, UK; [2]Smithers Rapra, Shawbury, UK; [3]Waters Corp., Beverly, MA; [4]Waters Technologies Corporation, Milford, MA*

2:30-4:30 pm Wednesday
QUANTITATIVE PROTEOMICS IN SYSTEMS BIOLOGY
Session Chair: Emily Chen (Thermofisher Scientific Precision Medicine Science Center)
Ballroom 20D upper level

WOD pm 02:30 **Systems Proteomics of Gene Expression**; Georg Kustatscher[1]; Juri Rappsilber[1]; *[1]Wellcome Trust Centre for Cell Biology, Edinburgh, UK*

WOD pm 02:50 **Multi-Omic Characterization of the Kinome in Lung and Upper Airway Cancer**; Emily M Cousins[1]; Naim Rashid[2]; Heejoon Jo[2]; Xiaobei Zhao[2]; Erica Cloer[2]; Dennis Goldfarb[2]; Paul Little[2]; Scott Randell[2]; Gary Johnson[2]; Neil Hayes[2]; Ben Major[1]; *[1]University of North Carolina Chapel Hill, Chapel Hill, NC; [2]UNC-Chapel Hill, Chapel Hill, NC*

WOD pm 03:10 **A Systematic Map of Protein-Metabolite Interactions Reveals Principles of Chemical Communication**; Ilaria Piazza[1]; Paola Picotti[2]; *[1]ETH Zurich, Zurich, Switzerland; [2]ETH Zürich, Zurich, Switzerland*

WOD pm 03:30 **Activity Landscapes of Cancer Cell Lines Predict Drug Response**; Martin Heinrich Frejno[1]; Benjamin Ruprecht[1, 2]; Chen Meng[1]; Alexander Hogrebe[1, 3]; Jana Zecha[1, 4, 5]; Dominic Helm[1, 6];

Thomas Oellerich[7, 8]; Sebastian Scheich[8]; Hans-Michael Kvasnicka[9]; Enken Drecoll[10]; Wilko Weichert[10]; Bernhard Kuster[1, 11, 12]; *[1]Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; [2]Chemical Biology and Discovery Proteomics, Merck & Co., Boston, MA; [3]Novo Nordisk Foundation Center for Protein Research, University of Copenhagen, Copenhagen, Denmark; [4]German Cancer Consortium (DKTK), Munich, Germany; [5]German Cancer Research Center (DKFZ), Heidelberg, Germany; [6]Proteomics Core Facility, EMBL, Heidelberg, Germany; [7]Department of Haematology, Cambridge University, Cambridge, UK; [8]Department of Medicine II, Goethe University, Frankfurt, Germany; [9]Department of Pathology, Goethe University, Frankfurt, Germany; [10]Department of Pathology, Technical University of Munich, Munich, Germany; [11]Center for Integrated Protein Science (CIPSM), Munich, Germany; [12]Bavarian Center for Biomolecular Mass Spectrometry, Freising, Germany*

WOD pm 03:50 **Exploring Cell-Type Specificity across Thousands of Human Protein Complexes**; Edward L. Huttlin[1]; Raphael J Bruckner[1]; Joe Cannon[1]; Jose Navarrete-Perea[1]; Fana Gebreab[1]; Kurt Baltier[1]; Melanie Gygi[1]; Alexandra Panov[1]; Devin K. Schweppe[1]; Joao A. Paulo[1]; J. Wade Harper[1]; Steve Gygi[1]; *[1]Harvard Medical School, Boston, MA*

WOD pm 04:10 **Development of Quantitative MRM Assays for the Measurement of 3,000 Proteins Across 20 Mouse Tissues**; Sarah A. Michaud[1]; Andrea L. Palmer[1]; Nicholas J.T. Sinclair[1]; Helena Pětrošová[1]; Ingo Feldmann[2]; Yassene Mohammed[1, 3]; Albert Sickmann[2]; Christoph H. Borchers[1, 4, 5, 6]; *[1]University of Victoria - Genome BC Proteomics Centre, Victoria, BC; [2]Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Dortmund, Germany; [3]Center for Proteomics and Metabolomics, Leiden University, Leiden, Netherlands; [4]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC; [5]Jewish General Hospital Proteomics Centre, McGill University, Montreal, QC, Canada; [6]Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC, Canada*

2:30-4:30 pm Wednesday
ENVIRONMENTAL: INNOVATIVE APPROACHES AND INSTRUMENTATION
Session Chair: Kevin R. Tucker (Southern Illinois University Edwardsville)
Ballroom 6A upper level

WOE pm 02:30 **Planetary Scale Metabolomics - Molecular Imaging of the Pacific Ocean**; Daniel Petras[1, 2]; Irina Koester[1, 2]; Jeremiah J. Minich[2, 3, 4]; Ricardo Da Silva[1]; Madeleine Ernst[1]; Brandon M. Stephens[2]; Andreas Haas[5, 6]; Craig E. Nelson[7]; Linda W. Kelly[8]; Rob Knight[3, 4]; Lihini I. Aluwihare[2]; Pieter C. Dorrestein[1]; *[1]University of California San Diego, Skaggs School of Pharmacy and Pharmaceutical Sciences, La Jolla, CA; [2]University of California San Diego, Scripps Institution of Oceanography, La Jolla, CA; [3]University of California San Diego, Department of Pediatrics, La Jolla, CA; [4]University of California San Diego, Department of Computer Science and Engineering, La Jolla, CA; [5]NIOZ Royal Institute for Sea Research, Texel, Netherlands; [6]Utrecht University, Utrecht, Netherlands; [7]University of Hawaii at Manoa, Department of Oceanography, Honolulu, HI; [8]San Diego State University, Department of Biology, San Diego, CA*

WOE pm 02:50 **Metabolic Profiling of Water and Plants from Wastewater Treatment Areas by FT-MS and MALDI Imaging**; Claire Villette[1, 2]; Maximilien Nuel[1]; Julien Delecolle[2]; Adrien Wanko[1]; Dimitri Heintz[2]; *[1]Département de mécanique des fluides et rhéologie, ICUBE Laboratoire des sciences de l'ingénieur, de l'informatique et de l'imagerie – UNISTRA/CNRS/ENGEES/INSA, Strasbourg, France; [2]Plant Imaging and Mass Spectrometry, Institut de Biologie Moléculaire des Plantes, CNRS, Université de Strasbourg, Strasbourg, France*

WOE pm 03:10 **Ion Mobility Mass Spectrometry of All Mono to Deca-Chlorinated Biphenyl Isomers: Correlation with Known Structures and Toxicities**; Jerry Hart[1]; Gareth Rhys Jones[2]; David Smith[1]; Malcolm Clench[1]; *[1]Sheffield Hallam University, Sheffield, UK; [2]Waters Corporation, Wilmslow, UK*

WOE pm 03:30 **LC and LC-MS/MS Studies of the Sorption and Decomposition Kinetics of Pesticides Interacting with Soils**; Donald S. Gamble[1]; Marc Lamoureux[1]; Hanan Malibari[1]; Heather Gamble[2]; Josh Ye[3]; *[1]St. Mary's University, Halifax, NS; [2]Perkin Elmer Health Sciences, Woodbridge, ON, Canada; [3]PerkinElmer Inc., Woodbridge, ON, Canada*

WOE pm 03:50 **Capillary Electrophoresis with Electrospray Ionization (CESI) Mass Spectrometry for the Analysis of Polar Pesticide Residues and Comparison with Liquid Chromatography**; Wiley Albanus Hall[1]; Spencer Walse[2]; Erik Rivera[2]; *[1]Safe Food Alliance, Kingsburg, CA; [2]USDA-ARS-SJVASC, Parlier, CA*

WOE pm 04:10 **Development of Thin Film Microextraction Techniques for On-Site Sampling and Determination of Pesticides Using Benchtop and Hand Portable GC/MS Instrumentation**; Jonathan J Grandy[1]; Hamed Piri-Moghadam[2]; Emanuela Gionfriddo[3]; Ezel Boyacı[4]; Janusz Pawliszyn[5]; *[1]Univeristy of Waterloo, Waterloo, ON, Canada; [2]Memorial University of Newfoundland, St John's, NL; [3]University of Toledo, Toledo, OH; [4]Middle East Technical University, Ankara, Turkey; [5]University of Waterloo, Waterloo, ON, Canada*

2:30-4:30 pm Wednesday
COVALENT LABELING AND CHEMICAL CROSSLINKING
Session Chair: Lisa Jones (University of Maryland)
Ballroom 6B upper level

WOF pm 02:30 **Identification of the Fondaparinux Binding Site of JR-FL gp120 by High Resolution Hydroxyl Radical Protein Footprinting and Blind Computational Docking**; Sandeep K. Misra[1]; Amika Sood[2]; Paulo A. Soares[3]; Vitor H. Pomin[1, 3]; Robert J. Woods[2]; Joshua S. Sharp[1]; *[1]Department of BioMolecular Sciences, School of Pharmacy, University of Mississippi, Oxford, MS; [2]Complex Carbohydrate Research Center, University of Georgia, Athens, GA; [3]Institute of Medical Biochemistry Leopoldo de Meis, University Hospital Clementino Fraga Filho, Federal University of Rio de Janeiro, Rio de Janeiro, Brazil*

WOF pm 02:50 **A New Beautiful Friendship: Solution Thermal Melting and Nanospray-MS for the Characterization of Intermolecular Conjugates Produced by Bifunctional Crosslinking**; Alice Sosic[1, 2]; Botros Toro[1]; Richard Goettlich[3]; Pan Li[4]; Barbara Gatto[2]; Daniele Fabris[4]; *[1]University at*

Albany, Albany, NY; [2]University of Padova, Padova, Italy; [3]Institute of Organic Chemistry, Justus Liebig University, Giessen, Germany; [4]The RNA Institute, University at Albany, Albany, NY

WOF pm 03:10 **Protein-DNA Interactions Analyzed by Cross-Linking of Recombinant and Native Chromatin Samples**; Alexandra Stuetzer[1]; Aleksandar Chernev[1]; Timo Sachsenberg[2]; Maria Tauber[1]; Wolfgang Fischle[1]; Oliver Kohlbacher[2]; Henning Urlaub[1]; *[1]MPI for Bbiophysical Chemistry, Goettingen, Germany; [2]University Tuebingen, Tuebingen, Germany*

WOF pm 03:30 **High-Throughput Structural Proteomics to Measure Aberrant Protein Folds *in vivo***; Casimir Bamberger[1]; Sandra Pankow[1]; Salvador Martínez-Bartolomé[1]; John Yates[1]; *[1]The Scripps Research Institute, La Jolla, CA*

WOF pm 03:50 **A New *in vivo* Cross-Linking Mass Spectrometry Workflow to Characterize Protein–Protein Interactions in Bacterial Pathogens**; Martial Rey[1]; Youxin Kong[2]; Guillaume Duménil[2]; Julia Chamot-Rooke[1]; *[1]Mass Spectrometry for Biology Unit, CNRS USR 2000, Institut Pasteur, France; [2]Pathogenesis of Vascular Infections Unit, INSERM, Institut Pasteur, France*

WOF pm 04:10 **Integrated Experimental and Computational Pipeline for Proteome-Wide in Tissue Crosslinking Analysis**; Karl A.T. Makepeace[1]; Yassene Mohammed[1, 2]; Elena L. Rudashevskaya[3]; Rachael D. Brown[1]; Evgeniy V. Petrotchenko[1]; Albert Sickmann[3]; Christoph H. Borchers[1, 4, 5, 6]; *[1]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [2]Center for Proteomics and Metabolomics, Leiden University, Leiden, Netherlands; [3]Leibniz-Institut für Analytische Wissenschaften-ISAS-e.V., Dortmund, Germany; [4]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada; [5]Jewish General Hospital Proteomics Centre, McGill University, Montreal, QC, Canada; [6]Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC, Canada*

2:30-4:30 pm Wednesday
INFORMATICS: METABOLOMICS
Session Chair: Xiaoyu Yang (NIST)
Ballroom 6CF upper level

WOG pm 02:30 **Propagating Annotations on Molecular Networks Using in Silico Fragmentation**; Ricardo Silva[1, 2]; Mingxun Wang[1]; Louis-Félix Nothias[1]; Justin J. J. van der Hooft[1, 3]; Andrés Mauricio Caraballo-Rodríguez[1]; Evan Fox[4]; Marcy J. Balunas[5]; Jonathan L. Klassen[4]; Norberto Peporine Lopes[2]; Pieter C. Dorrestein[1]; *[1]Collaborative Mass Spectrometry Innovation Center, Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California, San Diego, CA; [2]NPPNS, Department of Physics and Chemistry, School of Pharmaceutical Sciences of Ribeirão Preto, University of São Paulo, Ribeirão Preto, Brazil; [3]Bioinformatics Group, Department of Plant Sciences, Wageningen University, Wageningen, Netherlands; [4]Department of Molecular and Cell Biology, University of Connecticut, Storrs, CT; [5]Division of Medicinal Chemistry, Department of Pharmaceutical Sciences, University of Connecticut, Storrs, CT*

WOG pm 02:50 **Construction and Application of a High-Resolution MS/MS Retention Time Library for Rapid Identification of Endogenous Metabolites in Metabolomics**; Shuang Zhao[1]; Xian Luo[1]; Wan Chan[1]; Ulrike Schweiger-Hufnagel[2]; Aiko Barsch[2]; Liang Li[1]; *[1]University of Alberta, Edmonton, AB, Canada; [2]Bruker Daltonik GmbH, Bremen, Germany*

WOG pm 03:10 **DataSet-Dependent Acquisition Enables Comprehensive Tandem Mass Spectrometry Coverage of Complex Samples**; Corey Broeckling[1]; Emmy Hoyes[2]; Jeffery M. Brown[2]; Jessica Prenni[1]; *[1]Colorado State University, Fort Collins, CO; [2]Waters Corporation, Wilmslow, UK*

WOG pm 03:30 **ADAP-GC 4.0: Application of Non-Negative Matrix Factorization to Spectral Deconvolution of Gas Chromatography-Mass Spectrometry Metabolomics Data**; Aleksandr Smirnov[1]; Wei Jia[2]; Douglas I. Walker[3]; Dean P. Jones[3]; Xiuxia Du[1]; *[1]University of North Carolina at Charlotte, Charlotte, NC; [2]University of Hawaii Cancer Center, Honolulu, HI; [3]Emory University, Atlanta, GA*

WOG pm 03:50 **MassBank of North America: An Open-Access, Auto-Curating Mass Spectral Repository for Compound Identification**; Sajjan Singh Mehta[1]; Gert Wohlgemuth[1]; Diego Pedrosa[1]; Matthew Mueller[1]; Oliver Fiehn[1]; *[1]University of California, Davis, Davis, CA*

WOG pm 04:10 **Collisional Cross Section Prediction Directly From SMILES Using Deep Neural Network**; Pier-Luc Plante[1, 2, 3]; Élina Francovic-Fontaine[1, 3]; Erin S. Baker[4]; Jacques Corbeil[1, 2, 3]; *[1]Universite Laval, Quebec, QC, Canada; [2]Infectious Disease Research Center, Québec, QC, Canada; [3]Universite Laval Big Data Research Center, Québec, QC, Canada; [4]Pacific Northwest National Laboratory, Richland, WA*

2:30-4:30 pm Wednesday
FUNDAMENTALS: ION ACTIVATION AND DISSOCIATION
Session Chair: Rachel O. Loo (UCLA)
Ballroom 6DE upper level

WOH pm 02:30 **Radical-Induced Dissociation of Isomeric Compounds Using Various Gas-phase Radical Species (H•, OH•, N•, O)**; Hidenori Takahashi[1]; Yuji Shimabukuro[2]; Daiki Asakawa[3]; Shinichi Iwamoto[1]; Motoi Wada[2]; Koichi Tanaka[1]; *[1]Shimadzu corp., Kyoto, Japan; [2]Doshisha University, Kyotanabe, Japan; [3]AIST, Tsukuba, Japan*

WOH pm 02:50 **Implementing an Electrostatic ECD Cell on a Q-Exactive Enabling ECD and EChcD Fragmentation**; Kyle Fort[1]; Christian N. Cramer[2]; Valery G. Voinov[3]; Yury V. Vasil'ev[3]; Nathan I. Lopez[3]; Joseph S. Beckman[3]; Albert J.R. Heck[1]; *[1]Utrecht University, Utrecht, Netherlands; [2]University of Copenhagen, Copenhagen, Denmark; [3]Oregon State University, Corvallis, Oregon*

WOH pm 03:10 **Electron Transfer Dissociation Versus Collisionally Activated Dissociation of Sodium Cationized Polymethacrylates**; Jialin Mao[1]; Chrys Wesdemiotis[1]; *[1]University of Akron, Akron, OH*

WOH pm 03:30 **The Presence of B Ions in Electron Capture/ Transfer Dissociation of Supercharged Peptides**; Qingyi Wang[1]; Kristina Hakansson[1]; *[1]University of Michigan, Ann Arbor, MI*

WOH pm 03:50 **UVPD Joins the FTMS Ion Activation and Dissociation Toolbox for Sulfated Glycosaminoglycan Oligosaccharide Gas-Phase Ion Sequencing**; Franklin E. Leach III[1]; Dustin R.

Klein[2]; Jennifer S Brodbelt[2]; I. Jonathan Amster[1]; *[1]University of Georgia, Athens, GA; [2]University of Texas at Austin, Austin, TX*

WOH pm 04:10 **A New Paradigm for Glycan Sequencing: Why Fundamentals Matter**; Yang Tang[1]; Juan Wei[2]; Yiqun Huang[2]; Pengyu Hong[3]; Catherine E. Costello[1, 2]; Cheng Lin[2]; *[1]Boston University, Boston, MA; [2]Boston University School of Medicine, Boston, MA; [3]Brandeis University, Waltham, MA*

4:45-5:30 pm Wednesday
ASMS MEETING
Vicki H. Wysocki (The Ohio State University), presiding
Enjoy a beverage and hear the latest ASMS news.
Ballroom 20A upper level

5:45 - 7:00 PM WEDNESDAY WORKSHOPS

There are light refreshments in Sails Pavilion upper level 5:30 - 5:45 pm.

01. How New Methods are Enabling the Characterization of Isomeric Glycans
Presiding: Ron Orlando
Room 14 AB

Glycosylation of proteins is one of the most common protein posttranslational modifications (PTM). A correlation between changes in the glycan moieties of glycoproteins and many mammalian diseases, including hereditary disorders, immune deficiencies, cardiovascular disease, and cancer has been suggested. The diverse biological roles of glycans and their implications in diseases have created a demand for reliable glycomic strategies, permitting sensitive monitoring of isomeric glycans in biological systems. These strategies are needed to better understand the roles and attributes of glycan in biological systems. In this workshop, the use of different strategies, such as multistage MS, electron dissociation techniques, ion mobility, separations, for the compressive characterization of glycan isomers will be critically described and discussed.

02. Using R for Mass Spectrometry Data Analysis and Workflows
Presiding: Ryan Benz, Jeffrey Jones
Room 15 AB

This workshop will focus on the various ways that R can be used for mass spectrometry data processing and analysis. An overview of several R packages for mass spectrometry data access and analysis will be shown, along with example workflows going from raw MS data all the way to data analysis and final analysis reports. Time will also be given for questions and input from the participants. The goal of the workshop is to provide a foundation for anyone to access and analyze their own mass spectrometry data and help broaden analysis possibilities beyond canned routines in existing software packages.

03. Multi-MS-Omics Data Integration (Bioinformatics MS Interest Group)
Presiding: Isabell Bludau, Sam Payne
Room 16 AB

A diversity of molecules exist in living systems and a characterization of each of these molecular types constitutes 'omics' sciences. Although each individual omics discipline can reveal valuable insights into the architecture and functionality of biological systems, cellular processes are more completely described by the diversity and interplay of all different types of molecules. As technologies in proteomics, metabolomics and lipidomics improve, it is critical to remain connected as a community. The purpose of this workshop will be to bring together people with expertise in different MS-based omics fields and to discuss approaches to integrate and benefit from multi-omics data. We plan to discuss the current status of proteomics, metabolomics and lipidomics research and data analysis with their specific benefits and limitations. We will further highlight and discuss current strategies to perform multi-omics data integration to increase biological insights. Finally, we would like to stimulate cross-omics discussions on how to best benefit from each other's experience and how to design novel analysis workflows to investigate cross-omics interaction networks, such as recent strategies for determining protein-metabolite interactions.

04. Metabolomics: Best Practices for Standardization and Data Exchange (Metabolomics Interest Group)
Presiding: John Bowden, Gary Patti
Room 17 AB

The success of any omic science relies upon establishing standardized practices for sample handling, data acquisition, data processing, and data sharing. Such standardized practices are important for several reasons such as: they facilitate interpretation of the data by other laboratories, they enable meta-comparisons of existing datasets, they promote efficiency by preventing multiple laboratories from having to repeat the same experiment, and they generally make data more accessible to researchers from other fields with less expertise in metabolomics. Standardization is particularly critical in untargeted metabolomics, where datasets commonly contain thousands of unidentified features or signals. The objective of this workshop is to highlight recent progress for standardization and data exchange in metabolomics. Additionally, ideas to improve harmonization going forward will be explored.

Specific topics to be covered include: (i) discussion of the successes and pitfalls of previous ring trials, (ii) consideration of ongoing ring trials, (iii) overview of current resources for data sharing, (iv) discussion of the role of commercial kits in standardizing metabolomic pipelines, (v) specific needs for standardizing targeted metabolomics vs untargeted metabolomics vs lipidomics, and (vi) brainstorming about current gaps and challenges that have limited standardization and data sharing in metabolomics.

05. The NIH and NSF Review and Funding Process
Presiding: Kelsey Cook, Salvatore Sechi, Douglas Sheeley
Room 5B

Many ASMS members and conference participants are supported by the National Institutes of Health or the National Science Foundation. During this workshop the general funding and review process of grant applications/proposals will be presented. Issues like identifying the best contacts, writing an effective application/proposal, and responding to the reviewers' criticisms will be discussed. Speakers will explore these issues from the perspectives of the applicant, reviewer, and administrator, with some emphasis on new investigators and training opportunities. A "mock" NIH study section presentation will provide additional insight into the review process and opportunity for discussion with NIH and NSF staff. 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.

There are light refreshments in Sails Pavilion upper level 5:30 - 5:45 pm.

06. Photoionization as a Powerful Analytical Tool in Mass Spectrometry: Back to the Roots (Photoionization MS Interest Group)
Presiding: Sven Ehlert, Eleanor Riches
Room 5A

Photoionization is a powerful tool for soft ionization mass spectrometry (PI-MS) in research and routine analytical applications. In this year's workshop we want to concentrate on the fundamentals of atmospheric pressure (APPI) and vacuum (SPI and REMPI) photoionization for mass spectrometry. Two stimulating talks from experts in these fields will introduce you to the world of photoionization and will open the floor for interesting discussions about the roots of these techniques, from research to industrial applications. We want to give the attendees the opportunity not only to discuss challenges but also to ask questions to the experts and experienced users. The general idea of a "back to the roots" session is to refocus, from time to time, on the basics and fundamentals to support new users and other interested scientists with their first steps into these new techniques and into the community of PI users. The aim is to help attendees understand more about the techniques and to have the chance to troubleshoot any specific issues they have encountered.

Even though the focus is on fundamentals of APPI, SPI and REMPI there will also be the chance to discuss novel and exciting developments with the PI community. Together with the attendees, we want to reveal the advantages of photoionization mass spectrometry to support its dissemination into laboratories worldwide.

07. Trans-Proteomic Pipeline: Current Applications and Future Directions
Presiding: Dave Campbell, Eric Deutsch, Luis Mendoza
Room 4

The workshop will begin with a brief overview of the Trans-Proteomic Pipeline (TPP) and its newest features and capabilities. We will then focus on 5 individual topics, fostering a discussion with workshop participants on the current strengths, weaknesses, and future directions for the TPP. The workshop will enable participants to describe challenges in proteomic data analysis and help drive directions in software approaches through needs of the community. The topic leads for discussion are: proteogenomics & PEFF applications, spectrum library creation, statistical analysis & visualization tools, label-free quantification, and DIA data analysis approaches. Each topic will be introduced with a brief summary of features and ideas. Then feedback and discussion by the workshop participants will be promoted.

09. Food Safety & Security: HRMS Applications (Flavor, Fragrance & Foodstuff Interest Group)
Presiding: Sara Kern, Melanie Downs
Room 10

Food, Flavor and Fragrance High Resolution Mass Spectrometry (HRMS) applications and developments discussion continuation. A panel of scientists from academia, government, and industry will offer insight and guide the group discussion regarding food contaminants, pesticides, non-targeted analyte identification, food packaging safety, food allergens, proteomics, and natural product authenticity strategies.

10. Applications of Solid Phase Microextraction in Mass Spectrometry
Presiding: Barbara Bojko, German Gomez Rios, Janusz Pawliszyn
Room 9

The workshop is targeted at both new and current SPME users. The primary goal of the workshop is to provide the interested participants with deeper insight into the main principles of this technique, which will enhance the productivity and the quality of analytical results. This workshop will be of interest to analytical chemists, laboratory supervisors, scientists and industry regulators in the environmental, food and beverage, pharmaceutical, clinical, cosmetic, industrial hygiene and many other fields. High throughput capabilities of the technology will be emphasized in the discussions including SPMESH devices used in DART and coated blade spray (CBS) in direct coupling many MS formats. The unique features of in vivo SPME sampling technologies will be of particular interest to researchers in life sciences. Different devices will be discussed with matrix compatible coatings including BioSPME fibres. Concepts behind SPME-DESI, SPME-MOI/OPP and coated blade spray technologies will be introduced.

11. Improving Scientific Writing Skills
Presiding: Chris Petucci
Room 8

A scientist's ability to clearly communicate ideas in written form has a major impact on his or her scientific reputation, obtaining grants, and publishing manuscripts. This workshop will be a hands-on session that includes essential grammar for scientists, writing grammatically correct sentences, and principles of logical paragraph development. At the conclusion of this session, you will have an increased knowledge of vital writing skills to prepare high quality manuscripts and other documents.

12. Career and Collaboration Opportunities in China
Presiding: Jun Qu, Andy Tao
Room 7 AB

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

13. ADC Research and Development: The Role of Mass Spectrometry in ADC Biotherapeutic Development (Pharmaceuticals Interest Group)
Presiding: Andrew Dawdy, John Valliere-Douglass
Room 33 ABC

Recognizing the recent significant clinical and commercial success of ADCs, the pharmaceutical interest group initiated this workshop to explore the role of mass spectrometry in ADC R&D. The format of the workshop will consist of a short informal presentation (less than 15 minutes) followed by an audience driven discussion with peers and a panel of experts. The short presentation will include a primer on ADCs, for those practicing MS but unfamiliar with ADC therapeutics and their conjugates, and then provide a snapshot of current applications of MS analysis in the industry for ADC R&D. The organizers will have backup questions prepared for the panel and audience to start or prompt the discussion is needed. Potential areas of discussion may include initial mAb and drug assessments, bioanalytical assay development and the scaling range of characterization required for ADCs as they progress through clinical development. Discussion may focus on MS method development, optimization, data analysis, and how this information is being applied within industry paradigms or changing them.

There are light refreshments in Sails Pavilion upper level 5:30 - 5:45 pm.

14. Imaging Mass Spectrometry Data Analysis and Interpretation: Are You Getting the Most out of Your Data? (Imaging MS Interest Group)
Presiding: Reid Groseclose, Martina Marchetti-Deschmann
Room 32 AB

Over the past several years, advancements in instrumentation and efforts for automated sample preparation have greatly enhanced the speed and depth with which imaging mass spectrometry (IMS) datasets can be acquired. The vast size and dimensionality of these datasets makes manual extraction of relevant information impractical and superficial in many cases. As a result, users must rely on computational methods for automated analysis and interpretation of data. This is a rapidly growing area in the field of IMS and numerous bioinformatic approaches have been reported and several tools (open-source and commercial) are now available to users.
In this workshop, we will discuss some of the latest developments and strategies in computational analysis of IMS data including statistical methods, anatomical/histological correlation, and molecular annotation. We will also seek input on the challenges and limitations that users face when employing these methods in their own research. The workshop will consist of a series of seed presentations by experts to initiate open discussions for future developments.

15. Top Down Proteomics: Strategies for Analysis (Top-Down Proteomics Interest Group)
Presiding: Paul Thomas, Nicolas Young
Room 31 ABC

Top down protein mass spectrometry allows comprehensive analysis of intact, multiply modified proteoforms from complex mixtures. While the technique is simple in concept, its implementation is often fraught with technical challenges not present in the analysis of peptides or small molecules. In this workshop, we will discuss multiple, diverse topics around a central theme of analyzing intact proteoforms including: Strategies for sample preparation and separation of proteoforms from complex mixtures in LC-MS experiments; An update on Pilot Project 2 on the top down characterization of antibodies from the Consortium for Top Down Proteomics, Metrics for identification and accurate quantitation of proteoforms; Proteoform notation and language; and new large-scale projects to increase engagement from the community at large. Each topic will be introduced by a brief talk followed by audience discussion and input. We will also review and discuss common roadblocks to successful top down proteomics experiments from sample preparation to data acquisition to data analysis in a panel format. A limited number of 5 minute 'lightning talks' will be available for researchers to provide rapid-fire updates on findings relevant to the entire top down mass spectrometry community and worthy of community discussion. Contact workshop chairs if you are interested in presenting.

16. Implicit Bias
Presiding: Jenny Brodbelt
Room 30 DE

Implicit bias is defined by attitudes or stereotypes, typically harbored unintentionally, that affect our decisions and actions in an unconscious manner. These types of influences lead to both favorable and unfavorable evaluations and are recognized as occurring beyond a person's intentional awareness. Implicit biases may shape attitudes about other people based on race, ethnicity, age, and appearance, among others. It has been found that the roots of many of these biased associations are established at a very early age via exposure to both direct and indirect messages as well as via multi-media inputs. This workshop will feature a discussion about implicit bias in science.

AFTER 8:00 pm
CORPORATE HOSPITALITY SUITES
HILTON SAN DIEGO BAYFRONT

THURSDAY MORNING ORAL SESSIONS

7:00 am Thursday
CORPORATE BREAKFAST SEMINARS
CONVENTION CENTER
See page 15 for detailed schedule.
Reservation or RSVP required.

8:30-10:30 am Thursday
INSTRUMENTATION: ION DETECTION
Session Chair: Michael W. Senko (Thermo Fisher Scientific)
Hall D ground level

ThOA am 08:30 **Miniaturized, Crossed-Field Ion Detector Enabled by Cycloidal Electron Trajectories**; Toby Shanley[1]; Dick Stresau[1]; *[1]ETP Ion Detect, Sydney, Australia*

ThOA am 08:50 **A Quantitative Measurement of Secondary Electron Yield with High Kinetic Energy Ion Beam**; Szu-Hsueh Lai[1]; Jung-Lee Lin[1]; Chung-Hsuan Chen[1]; *[1]Academia Sinica, Taipei, Taiwan*

ThOA am 09:10 **Improving the Spatial Resolution of Microscope-Mode Ion Imaging Mass Spectrometry**; Robert Burleigh[1]; Ang Guo[1]; Michael Burt[1]; Steve Thompson[2]; Mark Brouard[1]; *[1]University of Oxford, Oxford, UK; [2]Scientific Analysis Instruments, Manchester, UK*

ThOA am 09:30 **Studies of Surface Collision Phenomena of Micron-Sized Charged Particles**; Morgan E C Miller[1]; Michelle P Mezher[1]; Robert E Continetti[1]; *[1]University of California San Diego, San Diego, CA*

ThOA am 09:50 **A Two-Dimensional Trajectory Analyzer Based on Printed Circuit Board Image-Charge Detectors**; Jiuzhi Gao[1]; Daniel E. Austin[1]; *[1]Brigham Young University, Provo, UT*

ThOA am 10:10 **Charge Detection Mass Spectrometry for Megadalton Polymer Characterization and Measurement of Charged Droplet Size Distribution at the Rayleigh Limit**; David Hrabovsky[1]; Bérengère Argence[1]; Denis Lesage[1]; Philippe Colomby[1]; Michel Surugue[1]; Richard B. Cole[1]; *[1]Sorbonne Université - Paris 06, Paris, France*

8:30-10:30 am Thursday
IMAGING: INSTRUMENTATION & METHOD DEVELOPMENT
Session Chair: Jeffrey M. Spraggins (Vanderbilt University)
Ballroom 20A upper level

ThOB am 08:30 **Chemical and Topographical 3D-Surface Imaging of Plant Leafs Using Autofocusing AP MALDI MSI**; Mario Kompauer[1]; Domenic Dreisbach[1]; Sven Heiles[1]; Bernhard Spengler[1]; *[1]University of Giessen, Giessen, Germany*

ThOB am 08:50 **Mid-level Data Fusion and Pan Sharpening of MALDI-FT-ICR MS by Infrared Imaging for Enhanced Chemical Analysis of the Rodent Hippocampus**; Elizabeth Kathleen Neumann[1, 2]; Troy J Comi[2, 3]; Nicolas Spegazzini[2, 3]; Jennifer Mitchell[2, 4]; Stanislav S Rubakhin[1, 2]; Rohit

Bhargava[1, 2, 3]; Martha U Gillette[2, 3, 4, 5]; Jonathan V Sweedler[1, 2, 5]; *[1]Department of Chemistry University of Illinois at Urbana-Champaign, Urbana, IL; [2]Beckman Institute University of Illinois at Urbana-Champaign, Urbana, IL; [3]Department of Bioengineering University of Illinois at Urbana-Champaign, Urbana, IL; [4]Department of Cell and Developmental Biology University of Illinois at Urbana-Champaign, Urbana, IL; [5]Neuroscience Program, University of Illinois at Urbana-Champaign, Urbana, IL*

ThOB am 09:10 **1 µm Spatial Resolution Imaging MS of Intracellular Molecules Using Atmospheric Pressure Laser Ionization with a Transmission Geometry Optical System**; Hayato Kawai[1]; Hisanao Hazama[1]; Kunio Awazu[1, 2, 3]; *[1]Graduate School of Engineering, Osaka University, Suita, Japan; [2]Graduate School of Frontier Biosciences, Osaka University, Suita, Japan; [3]Global Center for Medical Engineering and Informatics, Osaka University, Suita, Japan*

ThOB am 09:30 **DESI-UVPD-MS for Characterization of Phospholipid Isomers Within Biological Tissue Sections**; Dustin Klein[1]; Clara L. Feider[1]; Livia S. Eberlin[1]; Jennifer S. Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX*

ThOB am 09:50 **Multiple Modes And Multiple Sensors for Enhanced Information on Analyte Distributions - Molecular and Elemental Imaging from one Tissue Section**; Martina Marchetti-Deschmann[1]; Holzlechner Matthias Holzlechner[1]; Anastasiya Svirkova[1]; Maximilian Bonta[1]; Anna Turyanskaya[1]; Hans Lohninger[1]; Christina Streli[1]; Andreas Limbeck[1]; *[1]TU Wien, Vienna, Austria*

ThOB am 10:10 **Where Do Drug Molecules Go Inside of Cells? A New Method to Probe the Composition of Cellular Organelles**; Gregory L Fisher[1]; Corryn E Chini[2]; Ben Johnson[3]; Michael M Tamkun[3]; Mary L Kraft[2]; *[1]Physical Electronics, Chanhassen, MN; [2]University of Illinois at Urbana-Champaign, School of Chemical Sciences, Urbana, IL; [3]Colorado State University, Department of Biomedical Sciences, Fort Collins, CO*

8:30-10:30 am Thursday
FOOD SAFETY & CHEMISTRY: INNOVATIONS
Session Chair: Sara C. McGrath (FDA/CFSAN)
Ballroom 20BC upper level

ThOC am 08:30 **Fast "Dilute-and-Shoot" Quantitative Detection of Targeted Compounds with a Liquid-EI (LEI) LC-MS Interface in Food, Forensic, and PCP Applications**; Maurizio Piergiovanni[1]; Marco Agostini[2]; Giorgio Famiglini[3]; Pierangela Palma[3]; Veronica Termopoli[3]; Achille Cappiello[3]; *[1]University of Urbino, Urbino, Italy; [2]A.S.U.R. AV1, Pesaro, Italy; [3]University of Urbino, Urbino, Italy*

ThOC am 08:50 **MALDI Imaging and Laser Ablation Sampling for Analysis of Fungicide Distribution in Apples**; Igor Pereira[1]; Bijay Banstola[2]; Kelin Wang[2]; Boniek G Vaz[1]; Fabrizio Donnarumma[2]; Kermit K Murray[2]; *[1]Federal University of Goias, Goiania, Brazil; [2]Louisiana State University, Baton Rouge, LA*

ThOC am 09:10 **Multiclass Capillary Electrophoresis-Tandem Mass Spectrometry Method for Analysis of Polar Marine Toxins**; Daniel G Beach[1]; Elliott S Kerrin[1]; Krista M Thomas[1]; Michael A Quilliam[1]; Pearse McCarron[1]; *[1]National Research Council Canada, Halifax, Nova Scotia*

ThOC am 09:30 **Determination of Hexavalent Chromium in Dietary Supplements**; James Henderson[1]; Lauren Stubbert[1]; Weier Hao[1]; Logan Miller[1]; Matt Pamuku[2]; Larry Tucker[3]; Diego Cortesi[4]; H. M. Skip Kingston[1]; *[1]Duquesne University, Pittsburgh, PA; [2]Applied Isotope Technologies, Pittsburgh, PA; [3]Metrohm USA, Inc, Riverview, FL; [4]Milestone SLR, Bergamo, Italy*

ThOC am 09:50 **Profiling Free Milk Oligosaccharides with Isobaric Labeling and Quadrupole Time-Of-Flight Mass Spectrometry**; Randall Robinson[1]; Nina A. Poulsen[2]; Daniela Barile[1]; *[1]UC Davis, Davis, CA; [2]Aarhus University, Tjele, Denmark*

ThOC am 10:10 **Artificial Intelligence Enables the Detection of Pathogens in Food by Mass Spectrometric Analysis of RNA Modifications**; Daniele Fabris[1]; Colin Aldrich[2]; Mehraveh Salehi[3]; Reza Nemati[2]; Botros Toro[2]; Waqas Awan[2]; Lucas Davison[2]; *[1]The RNA Institute, University at Albany, Albany, NY; [2]University at Albany, Albany, NY; [3]Yale University, New Haven, CT*

8:30-10:30 am Thursday
BIOMARKERS: QUALITATIVE ANALYSIS
Session Chair: Young Ah Goo (Northwestern University)
Ballroom 20D upper level

ThOD am 08:30 **Serial-Omics: From Breast Tumors to Bodily Fluids to Dried Blood Spots**; Susanne B Breitkopf[1]; Min Yuan[1]; He Huang[1]; Gerburg M Wulf[1]; John M Asara[1]; *[1]Beth Israel Deaconess Medical Center/Harvard Medical School, Boston, MA*

ThOD am 08:50 **Changes in Epidermal Lipids Detected by Multiple-Reaction Monitoring Profiling Can Predict Dermatitis Progression in a Mouse Model**; Jackeline Franco[1]; Christina R Ferreira[1]; Bartek Rajwa[1]; John P Sundberg[2]; Harm HogenEsch[1]; *[1]Purdue University, West Lafayette, IN; [2]The Jackson Laboratory, Bar Harbor, ME*

ThOD am 09:10 **Breast Cancer Detection Using Targeted Plasma Metabolic Profiling**; Paniz Jasbi[1]; Dongfang Wang[2]; Dan Du[3]; Sunny Cheng[4]; Qiang Fei[4]; Julia Yue Cui[4]; Daniel Raftery[4]; Haiwei Gu[1]; *[1]Mayo Clinic, Scottsdale, Scottsdale, AZ; [2]Peking University, Beijing, China; [3]West-China Hospital/Medical School, Chengdu, China; [4]University of Washington, Seattle, WA*

ThOD am 09:30 **Integrated Glycomic and Intact Glycopeptide Analysis of Prostate Cancer Tissue**; Sarah M Totten[1]; Abel Bermudez[1]; Andrés Guerrero[2]; John Yan[2]; Aled Jones[2]; James D Brooks[3]; Sharon J Pitteri[1]; *[1]Canary Center at Stanford for Cancer Early Detection, Department of Radiology, Stanford University School of Medicine, Palo Alto, CA; [2]ProZyme, Hayward, California; [3]Department of Urology, Stanford University School of Medicine, Stanford, CA*

ThOD am 09:50 **Investigation of a Targeted Protein Panel of Diagnostic and Prognostic Value to ALS in Biological Fluids**; Jeffrey R. Enders[1]; Joshua Beri[2]; Lucas Vu[3]; Jiyan An[3]; Robert Bowser[3]; Michael S. Bereman[1, 2, 4]; *[1]Center for Human Health and the Environment, North Carolina State University, Raleigh, NC; [2]Department of Biological Sciences, North Carolina State University, Raleigh, NC; [3]Barrow Neurological Institute, Phoenix, AZ; [4]Department of Chemistry, North Carolina State University, Raleigh, NC*

ThOD am 10:10 **Classification of Plasma Cell Disorders by 21 Tesla FT-ICR Top-Down and Middle-Down MS/MS Analysis of Monoclonal Immunoglobulins in Human Serum**; Lidong He[1, 2]; Lissa C Anderson[2]; David R Barnidge[3]; David L Murray[4]; Surendra Dasari[4]; Angela Dispenzieri[4]; Christopher L Hendrickson[1, 2]; Alan G Marshall[1, 2]; *[1]Florida State University, Tallahassee, FL; [2]National High Magnetic Field Laboratory, Tallahassee, FL; [3]The Binding Site, Rochester, MN; [4]Mayo Clinic, Rochester, MN*

8:30-10:30 am Thursday
LIPIDOMICS: LIPIDS AND PROFILING
Session Chair: Candice Z. Ulmer (Centers for Disease Control and Prevention)
Ballroom 6A upper level

ThOE am 08:30 **Guidelines for Lipidomics Analysis and Reporting – the Lipidomics Standards Initiative (LSI)**; Gerhard Liebisch[1]; John A. Bowden[2]; William J. Griffiths[3]; Robert Ahrends[4]; Todd W Mitchell[5]; Makoto Arita[6]; Christer Ejsing[7]; Michal Holčapek[8]; Markus R. Wenk[9]; Kim Ekroos[10]; *[1]Institute of Clinical Chemistry and Laboratory Medicine, University of Regensburg, Regensburg, Germany; [2]Chemical Sciences Division, Hollings Marine Laboratory, National Institute of Standards and Technology, USA, Charleston, SC; [3]Swansea University Medical School, ILS1 Building, Singleton Park, Swansea, UK; [4]Leibniz-Institut für Analytische Wissenschaften-ISAS-e.V., Dortmund, Germany; [5]School of Medicine, Illawarra Health and Medical Research Institute, University of Wollongong, NSW 2522, Wollongong, Australia; [6]Laboratory for Metabolomics, RIKEN Center for Integrative Medical Sciences (IMS), Tsurumi, Kanagawa 230-0045, Yokohama, Japan; [7]Department of Biochemistry and Molecular Biology, VILLUM Center for Bioanalytical Sciences, University of Southern Denmark, DK-5230, Odense, Denmark; [8]Department of Analytical Chemistry, Faculty of Chemical Technology, University of Pardubice, Pardubice, Czech Republic; [9]Singapore Lipidomics Incubator (SLING), Department of Biochemistry, YLL School of Medicine, National University of Singapore, Singapore; [10]Lipidomics Consulting Ltd., FI-02230, Esbo, Finland*

ThOE am 08:50 **UV-Photodissociation for Structural Elucidation of the 'Hidden' Lipidome: Toward Understanding the Role of Aberrant Lipid Metabolism in Colorectal Cancer**; Yepy H Rustam[1]; Michelle Palmieri[2]; Dmitri Mouradov[2]; Mengxuan Fang[1]; Oliver Sieber[2]; Gavin E Reid[1]; *[1]University of Melbourne, Parkville, Australia; [2]Walter and Eliza Hall Institute of Medical Research, Parkville, Australia*

ThOE am 09:10 **Sensitive Lipid Profiling of Bovine Gametes and Embryos by Direct Sample Injection and Tailored Monitoring Using MRM Scans**; Camila B de Lima[1]; Marcella P Milazzotto[2]; Tiago Jose P Sobreira[3]; Alessandra Vireque[4]; Christina R. Ferreira[3]; Graham R. Cooks[3]; *[1]University of Sao Paulo, Sao Paulo, Brazil; [2]Universidade Federal do ABC, Santo Andre, Brazil; [3]Purdue University, West Lafayette, IN; [4]Invitra, Assisted Reproductive Technologies Ltd., Ribeirao Preto, Brazil*

ThOE am 09:30 **Determining the Time-Course of Lipidome Alterations in Mild Traumatic Brain Injury**; Scott Hogan[1]; Eric Gaupp[1]; Kyle Milligan[1]; Michelle LaPlaca[1]; Facundo M. Fernandez[1]; *[1]Georgia Institute of Technology, Atlanta, GA*

ThOE am 09:50 **Rapid Diagnosis of Pancreatic Ductal Adenocarcinoma Tissue Using the MasSpec Pen**; Mary King[1]; Jialing Zhang[1]; John Q. Lin[1]; Wendong Yu[2]; James Suliburk[2]; Hop Tran Cao[2]; George Van Buren[2]; Livia S Eberlin[1]; *[1]University of Texas at Austin, Austin, TX; [2]Baylor College of Medicine, Houston, TX*

ThOE am 10:10 **Mass Spectrometry Approaches for Lipidomic Quantitation: Applications in Cancer Biomarker Research**; Michal Holcapek[1]; Denise Wolrab[1]; Eva Cífková[1]; Robert Jirásko[1]; Ondřej Peterka[1]; Tereza Hrnčiarová[1]; Miroslav Lísa[1]; Roman Hrstka[2]; David Vrána[3]; Bohuslav Melichar[3]; *[1]University of Pardubice, Pardubice, Czech Republic; [2]Masaryk Memorial Cancer Institute, Regional Centre for Applied Molecular Oncology, Brno, Czech Republic; [3]Palacký University, Faculty of Medicine and Dentistry, Department of Urology, Olomouc, Czech Republic*

8:30-10:30 am Thursday
GLYCOPEPTIDES AND GLYCOPROTEINS
Session Chair: Weiguo Andy Tao (Purdue University)
Ballroom 6B upper level

ThOF am 08:30 **Reliable Quantitation of Glycan and Glycopeptide Isomers to Acquire a Better Understanding of Biological Roles of Glycoproteins**; Yehia Mechref[1]; Wenjing Peng[1]; Yifan Huang[1]; Xue Dong[1]; Jingfu Zhao[1]; *[1]Texas Tech University, Lubbock, TX*

ThOF am 08:50 ***De novo*-and Database-Driven Mass Spectrometric Sequencing Approaches Allow Fast and Accurate Mapping of Variable Domain Glycosylation of Polyclonal Antibodies**; Olivier Lardinois[1]; Leesa J. Deterding[1]; *[1]National Institute of Environmental Health Sciences, Research Triangle Park, NC*

ThOF am 09:10 **Mapping of Sialic Acid-Protein Interaction on Cell Membranes by Oxidative Reactions**; Qiongyu Li[1]; Yixuan Xie[1]; Gege Xu[1]; Carlito B. Lebrilla[2]; *[1]University of California, Davis, Davis, CA; [2]University of California Davis, Davis, CA*

ThOF am 09:30 **A Mucin-Specific Protease Improves Mass Spectrometric Analysis of Mucin-Type O-Glycoproteins**; Stacy A. Malaker[1]; Kayvon Pedram[1]; Carolyn R. Bertozzi[1, 2]; *[1]Stanford University, Stanford, CA; [2]Howard Hughes Medical Institute, Stanford, CA*

ThOF am 09:50 **Novel Chemical Labeling for MS-Based N-Glycome Identification and Quantitation**; Ying Zhang[1]; Lijun Yang[2]; Haojie Lu[2]; *[1]Fudan University, Shanghai, China; [2]Fudan Universiry, Shanghai, China*

ThOF am 10:10 **Identification of Intact Glycopeptides from EThcD Data Using SugarQb**; Johannes Stadlmann[1]; David M Hoi[2]; Jasmin Taubenschmid[1]; Karl Mechtler[1, 2]; Josef M Penninger[1]; *[1]IMBA - Institute of Molecular Biotechnology of the Austrian Academy of Sciences, Vienna, Austria; [2]Institute of Molecular Pathology (IMP), Vienna, Austria*

8:30-10:30 am Thursday
INFORMATICS: DATA-INDEPENDENT ACQUISITION: INNOVATIVE METHODS AND APPLICATIONS
Session Chair: Jeremy Koelmel (University of Florida)
Ballroom 6CF upper level

ThOG am 08:30 **Using Data Independent Acquisition to Expedite the Development of a Quantitative Triple Quadruple Assay in Cerebrospinal Fluid**; Deanna

Plubell[1]; Sandra E Spencer[1]; Tom Montine[2]; Michael J MacCoss[1]; *[1]University of Washington Genome Sciences, Seattle, WA; [2]Stanford University, Palo Alto, CA*

ThOG am 08:50 **Discovery DIA: All Ion fragmentation on the timsTOF Pro**; Daryl Wilding-McBride[1]; Giuseppe Infusini[1]; Markus Lubeck[2]; Oliver Raether[2]; Andrew I. Webb[1]; *[1]The Walter & Eliza Hall Institute, Parkville, Australia; [2]Bruker Daltonik GmbH, Bremen, Germany*

ThOG am 09:10 **Discussion of the Pros and Cons of Isobaric Labelling Compared to Single Shot Data-Independent Acquisition**; Jan Muntel[1]; Roland Bruderer[1]; Joanna M Kirkpatrick[2]; Oliver M. Bernhardt[1]; Lynn Verbeke[1]; Tejas Gandhi[1]; Ting Huang[3]; Olga Vitek[3]; Alessandro Ori[2]; Lukas Reiter[4]; *[1]Biognosys AG, Schlieren, Switzerland; [2]Leibniz Institute on Aging, Jena, Germany; [3]Northeastern University, Boston, MA; [4]Biognosys, Schlieren, Switzerland*

ThOG am 09:30 **PTMIdentification and Quantification Using Exclusively DIA (PIQED) Reveals Dichotomous Mitochondrial Protein Acylation from Excess Dietary Sugar and Fat**; Jesse Meyer[1]; Samir Softic[2]; Natan Basisty[1]; Matthew Rardin[3]; Eric Verdin[1]; Bradford W Gibson[3]; Olga Ilkayeva[4]; Chris Newgard[4]; C. Ronald Kahn[2]; Birgit Schilling[1]; *[1]The Buck Institute For Research On Aging, Novato, CA; [2]Joslin Diabetes Center, Harvard Medical School, Boston, MA; [3]Amgen, South San Francisco, CA; [4]Duke University, Durham, NC*

ThOG am 09:50 **Deep Learning Enables De novo Peptide Sequencing from DIA data**; Hieu Tran[1]; Xin Chen[2]; Chuyi Liu[3]; Rui Qiao[3]; Lei Xin[2]; Kun Xiong[3]; Paul Shan[2]; Ming Li[1]; *[1]University of Waterloo, Waterloo, ON, Canada; [2]Bioinformatics Solutions Inc., Waterloo, ON; [3]RSVP Technologies Inc., Waterloo, ON, Canada*

ThOG am 10:10 **High Quality Peptide MS/MS Spectrum Prediction Using Deep Learning and Its Application in DIA Data Analysis**; Peter Cimermancic[1]; Roie Levy[1]; Kanna Palaniappan[1]; Favio Salinas[2]; Shivani Tiwary[2]; Petra Gutenbrunner[2]; Jürgen Cox[2]; *[1]Verily Life Sciences, South San Francisco, CA; [2]Max Planck Institute of Biochemistry, Martinsried, Germany*

8:30-10:30 am Thursday
MEMBRANE PROTEIN MS
Session Chair: Yansheng Liu (Yale University School of Medicine, Cancer Biology Institute)
Ballroom 6DE upper level

ThOH am 08:30 **Development of a Novel Cleavable Surfactant for Top-Down Membrane Proteomics**; Kyle Brown[1]; Bifan Chen[2]; Tania Guardado[2]; Ziqing Lin[3, 4]; Ying Ge[3, 4, 5]; *[1]Department of Chemistry, University of Wisconsin–Madison, Madison, WI; [2]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [3]Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI; [4]Human Proteomics Program, School of Medicine and Public Health, University of Wisconsin-Madison, Madsion, WI; [5]Department of chemistry University of Wisconsin Madison, Madison, WI*

ThOH am 08:50 **Exploring the Co-Evolution of Membrane Protein-Lipid Interactions with Orbitrap Native Mass Spectrometry Above and Beyond the Resolution Limit**; Joseph Gault[1]; Idlir Liko[2]; Dmitriy Boll[3]; Maria Reinhardt-Szyba[3]; Alexander Makarov[3]; Carol V Robinson[1]; *[1]University Of Oxford, Oxford, UK; [2]OMass Technologies Ltd., Oxford, UK; [3]Thermo Fisher Scientific, Bremen, Germany*

ThOH am 09:10 **GPCR-Ligand Interactions: Does Native Mass Spectrometry and HDX Give the Full Picture for Efficient Drug Design?**; Krzysztof Okrasa[1]; Stacey Southall[1]; James Errey[1]; Robert Cooke[1]; *[1]Heptares Therapeutics Ltd., Welwyn Garden City, UK*

ThOH am 09:30 **Mass Spectrometry-Based Identification and Quantitation of a Novel Cell Surface Marker Panel for Primary Human B-lymphocytes**; Matthew Waas[1]; Jeannnie M. Caramillo[2]; Jacek W. Sikora[2]; Paul Martin Thomas[2]; Neil L. Kelleher[2]; Rebekah L. Gundry[1]; *[1]Medical College of Wisconsin, Milwaukee, WI; [2]Northwestern University, Evanston, IL*

ThOH am 09:50 **A New Role for Post-Translational Modifications in Membrane Protein Biogenesis and Misfolding Disease**; Sandra Pankow[1]; Casimir Bamberger[1]; Robin Park[1]; John R Yates[1]; *[1]The Scripps Research Institute, La Jolla, CA*

ThOH am 10:10 **Comparative Proteomics Analysis of Exosomes Derived from Mammary Epithelial Cells with Different Metastatic Abilities**; Chengjian Tu[1]; Shen He[2]; Jun Li[1]; Jianmin Zhang[2]; Jun Qu[1]; *[1]University at Buffalo, Buffalo, NY; [2]Roswell Park Comprehensive Cancer Center, Buffalo, NY*

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

Odd-number posters present:
10:30 - 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

2:30-4:30 pm Thursday
INSTRUMENTATION: NEW DEVELOPMENTS IN IONIZATION AND SAMPLING
Session Chair: Julia Laskin (Purdue University)
Hall D ground level

ThOA pm 02:30 **Orbitrap-Synchronized Triboelectric Nanogenerators: A Better Alternative to Power-Pulsed Ion Sources**; Marcos Bouza[1]; Anyin Li[1]; Zhong Lin Wang[1]; Facundo M. Fernandez[1]; *[1]Georgia Institute of Technology, Atlanta, GA*

ThOA pm 02:50 **Online Reaction Monitoring in Non-Aqueous Solutions by Condensed Phase Membrane Introduction Mass Spectrometry-Liquid Electron Ionization (CP-MIMS-LEI)**; Veronica Termopoli[1]; Gregory W. Vandergrift[2, 3]; Maurizio Piergiovanni[1]; Giorgio Famiglini[1]; Pierangela Palma[1, 2]; Erik T. Krogh[2, 3]; Achille Cappiello[1, 2]; Christopher G. Gill[2, 3, 4, 5]; *[1]University of Urbino Carlo Bo, Urbino, Italy; [2]Appl. Env. Res. Labs. (AERL), Nanaimo, BC, Canada; [3]Chemistry, University of Victoria, Victoria, BC, Canada; [4]Chemistry, Simon Fraser University, Burnaby, BC; [5]University of Washington, Seattle, WA*

ThOA pm 03:10 **Mechanism and Application of Droplet Assisted Ionization (DAI) for Characterization of Airborne Nanoparticles**; Murray V Johnston[1]; Michael A Apsokardu[1]; Devan E Kerecman[1]; *[1]University of Delaware, Newark, DE*

ThOA pm 03:30 **Development and Validation of a Microfluidic Open Interface with Flow-Isolated Desorption Volume for the Direct Coupling of SPME to MS**; Marcos Tascon[1]; Nikita Looby[1]; German Augusto Gomez-Rios[1]; Md. Nazmul Alam[1]; Emir Nazdrajic[1]; Daniel Rickert[1]; Janusz Pawliszyn[1]; *[1]University of Waterloo, Department of Chemistry, Waterloo, Ontario, Canada*

ThOA pm 03:50 **Application for Nanofluidic Devices towards Single-Cell Proteomics to Enable Study of Xenopus laevis Embryonic Development**; Anumita Saha-Shah[1]; Melody Esmaeili[1]; Peter S Klein[1]; Benjamin A. Garcia[1]; *[1]University of Pennsylvania School of Medicine, Philadelphia, PA*

ThOA pm 04:10 **Sub-Atmospheric Pressure Matrix-Assisted Ionization (MAI) Provides Simplicity, Sensitivity, and Robustness**; Sarah Trimpin[1, 2]; I-Chung Lu[3]; Chuping Lee[1]; Santosh Karki[1]; James Wager-Miller[4]; Ken Mackie[4]; *[1]Department of Chemistry, Wayne State University, Detroit, MI; [2]Cardiovascular Research Institute, Wayne State University School of Medicine, Detroit, MI; [3]Department of Chemistry, National Chung Hsing University, Taichung City, Taiwan; [4]Psychology and Brain Sciences, Indiana University, Bloomington, IN*

2:30-4:30 pm Thursday
IMAGING: COMPUTATIONAL METHODS AND ANALYSIS
Session Chair: Shane Ellis (Maastricht Multimodal Molecular Imaging institute (M4I))
Ballroom 20A upper level

ThOB pm 02:30 **Big Data Driven Mass Recalibration for Imaging Mass Spectrometry**; Andrew Palmer[1]; Artem Tarasov[1]; James McKenzie[2]; Zoltan Takats[2]; Theodore Alexandrov[1]; *[1]European Molecular Biology Laboratory, Heidelberg, Germany; [2]Imperial College London, London, UK*

ThOB pm 02:50 **Machine Learning Classification of Clinical Tumoral Tissues with Mass Spectrometry Imaging Datasets and Morphometric Characteristics**; Gaël Picard de Muller[1]; Thibault Ballier[2]; Fabien Pamelard[1]; Rima Ait-Belkacem[1]; Quentin de Smedt[2]; José Corral Gallego[2]; Jonathan Stauber[1]; *[1]Imabiotech, Loos, France; [2]Skapane, Lille, France*

ThOB pm 03:10 **Assessing Deep Learning for Reliable, Repeatable Compression and Decompression of Mass Spectrometry Imaging Data**; Spencer Thomas[1]; Rory T. Steven[1]; Alex Dexter[1]; Efstathios Elia[1]; Gregory Hamm[2]; Richard Goodwin[2]; Ian S Gilmore[1]; Josephine Bunch[1, 3]; *[1]National Physical Laboratory, Teddington, UK; [2]AstraZeneca, UK, Cambridge, UK; [3]Imperial College, London, UK*

ThOB pm 03:30 **High Spatial Resolution Ambient Ionization Mass Spectrometry Imaging Using Microscopy Image Fusion**; Chih-Lin Chen[1]; Li-En Lin[1]; Ying-Chen Huang[1]; Hsin-Hsiang Chung[1]; Yu-Ju Peng[2]; Chiao-Wei Lin[3]; Ko-Chien Chen[3]; Chiao-Hui Hsieh[4]; Tang-Long Shen[3]; Hsueh-Fen Juan[4]; Cheng-Chih Richard Hsu[1]; *[1]Department of Chemistry, National Taiwan University, Taipei, Taiwan; [2]Department of Animal Science and Technology, National Taiwan University, Taipei, Taiwan; [3]Department of Plant Pathology and Microbiology, National Taiwan University, Taipei, Taiwan; [4]Department of Life Science, National Taiwan University, Taipei, Taiwan*

ThOB pm 03:50 **A Novel Cross-Normalization Method for MALDI TOF Peptide Imaging for Improved Inter-Lab Comparability and Multi-Center Studies**; Tobias Boskamp[1, 2]; Rita Casadonte[3]; Lena Hauberg-Lotte[1]; Delf Lachmund[1]; Janina Oetjen[4]; Yovany Cordero Hernandez[1]; Dennis Trede[2]; Jörg Kriegsmann[3, 5]; Peter Maass[1, 2]; *[1]University of Bremen, Center for Industrial Mathematics, Bremen, Germany; [2]SCiLS, Bremen, Germany; [3]Proteopath GmbH, Trier, Germany; [4]University of Bremen, MALDI Imaging Lab, Bremen, Germany; [5]Center for Histology, Cytology and Molecular Diagnostic, Trier, Germany*

ThOB pm 04:10 **Combining Machine Learning and Multivariate Curve Resolution for Mass Spectrometry Imaging Data Analysis: From Spheroids to Tumors**; Xiang Tian[1]; Genwei Zhang[1]; Wen Yang[1]; Chuanbin Mao[1]; Zhibo Yang[1]; *[1]University of Oklahoma, Norman, OK*

2:30-4:30 pm Thursday
FOOD SAFETY & CHEMISTRY: FOODOMICS, ALLERGENS, BACTERIA, FOODS
Session Chair: Melanie Downs (Melanie Downs)
Ballroom 20BC upper level

ThOC pm 02:30 **Prolyl Endopeptidase, Is It Cut out for Gluten Reduction? Using LC-MS to Uncover the Hidden Gluten in Craft Beers**; Michelle Colgrave[1]; Keren Byrne[1]; Crispin A Howitt[1]; *[1]CSIRO, St Lucia, Australia*

ThOC pm 02:50 **A Multi-Laboratory Ring Trial for the Detection of Peanut Protein in a Food Matrix Using Targeted LC-MS/MS**; Victoria J Lee[1]; Rebekah L Sayers[1]; Ivona Baricevic-Jones[1]; Carol-ann Costello[1]; Anuradha Balasundaram[1]; Chiara Nitride[1]; Christine H. Parker[2]; Sabine Baumgartner[3]; Gavin O'Connor[4]; Philip Johnson[5]; Alexander Gillert[6]; Andreas Reuter[7]; Emanuele Scollo[8]; Linda Monaci[9]; Martin Roeder[10]; Nathalie Gillard[11]; Reka Haraszi[12]; Rosario Romero[13]; EN Clare Mills[1]; *[1]University of Manchester, Manchester, UK; [2]FDA-CFSAN, College Park, MD; [3]BOKU, Universitaet f. Bodenkultur Wien, Tulln, Austria; [4]Joint Research Centre (JRC), Geel, Belgium; [5]Food Allergy Research and Resource Program, Department of Food Science and Technology, University of Nebraska-Lincoln, Lincoln, NE; [6]Institut Kirchhoff*

Berlin GmbH, Berlin, Germany; [7]Paul-Ehrlich Institut (PEI), Langen, Germany; [8]Reading Scientific Services Ltd, Reading, UK; [9]ISPA-CNR, Bari, Italy; [10]Insitut fur Produktqualitaet (ifp), Berlin, Germany; [11]CER Groupe, Marloie, Belgium; [12]Campden BRI, Campden, UK; [13]Fera Science Ltd, York, UK

ThOC pm 03:10 **LC-HRMS Workflows for Algal Toxin Reference Material Profiling and Stability Assessment**; Elliott J Wright[1]; Daniel G Beach[1]; Melanie MacArthur[1]; Pearse McCarron[1]; *[1]National Research Council of Canada, Halifax, NS*

ThOC pm 03:30 **Small Molecule Interactions from the Cheese Microbiota:Pseudomonas vs. Candida**; Melissa M. Galey[1]; Emily Pierce[2]; Rachel J. Dutton[2]; Laura M. Sanchez[1]; *[1]University of Illinois at Chicago, Chicago, IL; [2]University of California San Diego, San Diego, CA*

ThOC pm 03:50 **A High-Throughput UHPLC/QqQ-MS Monosaccharide Analysis for Monitoring Host-Microbiome Interactions in the Infant Gut**; Matthew J. Amicucci[1]; Ace G. Galermo[1]; Eshani Nandita[1]; Carlito B. Lebrilla[1]; *[1]University of California Davis, Davis, CA*

ThOC pm 04:10 **In-situ Analysis of Food Flavors Using Portable Mass Spectrometry**; Fred Paul Mark Jjunju[1]; Stamatios Giannoukos[1]; Alan Marshall[2]; Stephen Taylor[2]; *[1]University Of Liverpool, Liverpool, UK; [2]Department of Electrical Engineering and Electronics University of Liverpool, Liverpool, UK*

2:30-4:30 pm Thursday
THERAPEUTIC PROTEINS, ANTIBODIES, AND ANTIBODY/DRUG CONJUGATES
Session Chair: Jon Fitchett (Lilly Biotech Center-San Diego)
Ballroom 20D upper level

ThOD pm 02:30 **A Suite of Liquid Chromatography Strategies Coupled Online to Top-down High-resolution Mass Spectrometry for Comprehensive Analysis of Antibody Drug Conjugates**; Bifan Chen[1]; Ziqing Lin[1]; Qingge Xu[1]; Cexiong Fu[2]; Qunying Zhang[2]; Ying Ge[1]; *[1]University of Wisconsin-Madison, Madison, Wisconsin; [2]Abbvie Inc., North Chicago, IL*

ThOD pm 02:50 **Coupling Ion-Exchange Chromatography to Native Spray Mass Spectrometry for the Charge-Based Separation and Characterization of Intact Therapeutic Proteins**; Andrew W Dawdy[1]; Aaron O Bailey[2]; Jason C Rouse[3]; Olga V Friese[1]; *[1]Pfizer, St. Louis, MO; [2]Thermo Fisher Scientific, San Jose, CA; [3]Pfizer, Andover, MA*

ThOD pm 03:10 **Does the Knob-Into-Hole Bispecific Construct Impact the Structure and Dynamics of an Antibody?**; Hui-Min Zhang[1]; Peilu Liu[2]; Alan G Marshall[2, 3]; Yung-Hsiang Kao[1]; *[1]Genentech, a member of the Roche group, South San Francisco, CA; [2]Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL; [3]Ion Cyclotron Resonance Program, National High Magnetic Field Laboratory, Tallahassee, FL, United States, Tallahassee, FL*

ThOD pm 03:30 **Novel Hydrogen/Deuterium Exchange Mass Spectrometry Method for Biopharmaceutical Characterization at High Concentrations**; Yuwei Tian[1]; Lihua Huang[2]; Brandon T Ruotolo[1]; Ning Wang[2]; *[1]University of Michigan, Ann Arbor, MI; [2]Eli Lilly and Company, Indianapolis, IN*

ThOD pm 03:50 **Characterization of Bispecific and Mis-Paired Antibodies by Charge-Variant Mass Spectrometry**; Wilson Phung[1]; Aaron O Bailey[2]; Bingchuan Wei[1]; Yonghua Zhang[1]; Michael Dillon[1]; Christoph Spiess[1]; Paul Carter[1]; Wendy Sandoval[1]; Guanghui Han[1]; *[1]Genentech, Inc., South San Francisco, CA; [2]Thermo Fisher Scientific, San Jose, CA*

ThOD pm 04:10 **Characterization of Aspartate Isomerization in Specific Sequence Motifs of Antibodies and Bispecific Antibodies of Therapeutic Interest**; Yuping Zhou[1]; Jason X Tang[1]; *[1]Eli Lilly and Company, Indianapolis, IN*

2:30-4:30 pm Thursday
LIPIDOMICS: NEW MS TECHNOLOGIES AND APPLICATIONS
Session Chair: Kim Ekroos (Lipidomics Consulting Ltd)
Ballroom 6A upper level

ThOE pm 02:30 **Three-Phase Lipid Extraction (3PLE) – A Simple, Fast, and Efficient Method for Lipidomics Workflows**; Goncalo Vale[1]; Bonne Thompson[1]; Kaitlyn Eckert[1]; Sarah Martin[1]; Matthew Mitsche[1]; Jeffrey McDonald[1]; *[1]UT Southwestern, Dallas, TX*

ThOE pm 02:50 **Shotgun Lipidomics Analysis of Monohexosyl Alkyl (Alkenyl)-Acylglycerol in Biological Samples**; Chunyan Wang[1]; Juan Pablo Palavicini[1]; Xianlin Han[1]; *[1]Barshop Institute for Longevity and Aging Studies, San Antonio, TX*

ThOE pm 03:10 **Distinguishing Lipid Isomers with Advanced Separations, Ion-Molecule Reactions and Fragmentation Approaches to Evaluate Their Role in Biochemical Processes**; Erin S. Baker[1]; Xueyun Zheng[2]; Noor Aly[2]; Jennifer E. Kyle[2]; Kristin E. Burnum-Johnson[2]; Berwyck L. J. Poad[3]; Stephen J. Blanksby[3]; Sheher B. Mohsin[4]; Richard D. Smith[2]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]Pacific Northwest National Laboratory, Richland; [3]Central Analytical Research Facility, Institute for Future Environments, Queensland University of Technology, Brisbane, Australia; [4]Agilent Technologies, Inc., Santa Clara, CA*

ThOE pm 03:30 **Evaluating New Fragmentation Technologies in Conjunction with Ion Mobility-Mass Spectrometry for Improved Lipid Structural Characterization**; Rachel Harris[1]; Jody C. May[1]; Craig A. Stinson[2]; Sophie R. Harvey[3]; Yu Xia[4]; Vicki H. Wysocki[3]; John A. McLean[1]; *[1]Vanderbilt University, Nashville, TN; [2]Intel Corporation, Santa Clara, CA; [3]Ohio State University, Columbus, OH; [4]Tsinghua University, Beijing, China*

ThOE pm 03:50 **Relative Quantification of Phospholipid sn-Isomers Using Positive Doubly-Charged Lipid-Metal Ion Complexes**; Sven Heiles[1]; Simon Becher[1]; Patrick Esch[1]; *[1]Justus Liebig University Giessen, Giessen, Germany*

ThOE pm 04:10 **Stable Isotope Labeling with Mass Spectrometry Elucidates Complex Lipid Regulation in Beta-Glucosidase Mutant Cell Models of Parkinson's disease**; Nathan Hatcher[1]; Robert E. Drolet[1]; Lihang Yao[1]; Andres D. Ramirez[1]; Lei Ma[1]; Marla L. Watt[1]; Stephen F. Previs[2]; David G. McLaren[2]; Sean M. Smith[1]; *[1]Merck Research Laboratories, West Point, PA; [2]Merck Research Laboratories, Kenilworth, NJ*

2:30-4:30 pm Thursday
BIOMARKERS: QUANTITATIVE ANALYSIS
Session Chair: Adam Hawkridge (Virginia Commonwealth University)
Ballroom 6B upper level

ThOF pm 02:30 **Quantitative Proteomic Analyses of Uterine Leiomyomas from Hereditary Leiomyomatosis and Renal Cell Cancer Patients**; Nicholas Bateman[1]; Christopher Tarney[1]; Niyati Parikh[1]; Ming Zhao[2]; Kelly Conrads[1]; James Segars[3]; Paul Driggers[3]; Chad Hamilton[1]; George L Maxwell[2];

Thomas Conrads[2]; [1]*Gynecologic Cancer Center of Excellence, Murtha Cancer Center, Uniformed Services University of the Health Sciences, Bethesda, MD;* [2]*Inova Schar Cancer Institute, Annandale, VA;* [3]*Johns Hopkins School of Medicine, Baltimore, MD*

ThOF pm 02:50 **A Novel and Automated LC-MS/MS Assay for Coporporphyrin-I and –III, Emerging Endogenous Biomarkers of OATP, in First-In-Human Clinical Trials**; Amanda King-Ahmad[1]; Ragu Ramanathan[1]; Sara Clemens[2]; Jenny Zhang[1]; Christopher L Holliman[1]; Fumin Li[2]; A David Rodrigues[1]; [1]*Pfizer, Groton, CT;* [2]*PPD, Middleton, WI*

ThOF pm 03:10 **Targeted Proteomics for Pharmacodynamics of Melanoma Patients Treated with a BRAF-HSP90 Inhibitor Combination**; Zeynep Eroglu[1]; Y. Ann Chen[1]; Geoffrey T Gibney[2]; Jeffrey S Weber[3]; Ragini R Kudchadkar[4]; Nikhil I Khushalani[1]; Joseph Markowitz[1]; Andrew Brohl[1]; Leticia F Tetteh[1]; Howida Ramadan[1]; Gina Arnone[1]; Jiannong Li[1]; Xiuhua Zhao[1]; Ritin Sharma[1]; Lancia N.F. Darville-Bowleg[1]; Bin Fang[1]; Inna Smalley[1]; Jane L Messina[1]; John M Koomen[5]; Vernon K Sondak[1]; Keiran SM Smalley[1]; [1]*Moffitt Cancer Center, Tampa, FL;* [2]*Georgetown University Medical Center, Washington, D.C., Washington, D.C.;* [3]*Langone Cancer Center, New York, NY;* [4]*Emory University, Atlanta, GA;* [5]*H. Lee Moffitt Cancer Center, Tampa, FL*

ThOF pm 03:30 **Longitudinal Multi-Omics Profiling in Insulin Resistant and Sensitive Prediabetic Population**; Sara Ahadi[1]; Hannes Röst[2]; Daniel Hornburg[1]; Tejaswini Mishra[1]; Wenyu Zhou[1]; Kevin Contrepois[1]; Reza Sailani[1]; Mike Snyder[1]; [1]*Stanford Medical School, Palo Alto, CA;* [2]*University of Toronto, Toronto, ON, Canada*

ThOF pm 03:50 **Longitudinal and Cross-Panel Analysis of INLIGHT™ N-Linked Glycans in the Avian Model to Predict the Onset of Ovarian Cancer**; David C Muddiman[1]; Elizabeth S. Hecht[2]; Daniel Rotroff[1]; Rebecca Wysocky[1]; James Petitte[1]; Alison Motsinger-Reif[1]; [1]*North Carolina State University, Raleigh, NC;* [2]*Thermo Fisher Scientific, San Jose, CA*

ThOF pm 04:10 **Modeling Septic Shock via Longitudinal Serum Proteomics**; Erin Harberts[1]; Tao Liang[2]; Sung Hwan Yoon[1]; Belita N Opene[1]; Melinda McFarland[3]; David R Goodlett[2]; Robert K. Ernst[1]; [1]*Department of Microbial Pathogenesis, School of Dentistry, University of Maryland, Baltimore, MD;* [2]*Department of Pharmaceutical Science, School of Pharmacy, University of Maryland, Baltimore, MD;* [3]*Center for Food Safety and Applied Nutrition, U.S. Food and Drug Administration, Washington, DC*

2:30-4:30 pm Thursday
INFORMATICS: MULTIOMICS INTEGRATION AND APPLICATIONS
Session Chair: Chris Beecher (IROA Technologies)
Ballroom 6CF upper level

ThOG pm 02:30 **MS-Driven Multi-Omics Innovation in Industrial Life Sciences**; Michiel Akeroyd[1]; Erwin Kaal[1]; Brenda Ammerlaan[1]; Joep Schmitz[1]; Rob van der Hoeven[1]; Maurien Olsthoorn[1]; [1]*DSM Biotechnology Center, Delft, Netherlands*

ThOG pm 02:50 **Characterization of the Human Oral Microbiome in Health and Disease: Integration of 16S, Proteomics, Metabolomics, and Lipidomics Data**; Katherine A. Overmyer[1]; Timothy W. Rhoads[2]; Michael S Westphall[2]; Sanjay K. Shukla[3]; Amit Acharya[3]; Joshua J. Coon[1, 2]; [1]*Morgridge Institute for Research, Madison, WI;* [2]*University of Wisconsin–Madison, Madison, WI;* [3]*Marshfield Clinic Research Foundation, Marshfield, WI*

ThOG pm 03:10 **Multi-Omic Analysis of 384 Mice Maps the Genetic Architecture of Diabetes and Obesity**; Vanessa Linke[1]; Elyse C. Freiberger[2]; Nicholas W. Kwiecien[2]; Edna A. Trujillo[2]; Paul D. Hutchins[2]; Alexander S. Hebert[2]; Thiru Reddy[3]; Jason D. Russell[3]; Brian S. Yandell[2]; Julia H. Kreznar[2]; Lindsay L. Traeger[2]; Eugenio I. Vivas[2]; Kathryn L. Schueler[2]; Donald S. Stapleton[2]; Mary E. Rabaglia[2]; Mark P. Keller[2]; Karl W. Broman[2]; Daniel M. Gatti[4]; Gary A. Churchill[4]; Federico E. Rey[2]; Alan D. Attie[2]; Joshua J. Coon[3, 5, 6, 7]; [1]*University of Wisconsin-Madison, Madison, WI;* [2]*University of Wisconsin, Madison, Madison, WI;* [3]*Morgridge Institute for Research, Madison, WI;* [4]*The Jackson Laboratory, Bar Harbor, ME;* [5]*Department of Chemistry, University of Wisconsin-Madison, Madison, WI;* [6]*Genome Center of Wisconsin, Madison, WI;* [7]*Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI*

ThOG pm 03:30 **Systems Biology Approach for Mechanism of Action Identification in 30 Days**; Akos Vertes[1]; Albert Arul[1]; Peter Avar[1]; Andrew Korte[1]; Camille Lombard-Banek[1]; Peter Nemes[2]; Lida Pavin[1]; Ziad Sahab[1]; Bindesh Shrestha[3]; Sylwia A Stopka[1]; wei Yuan[1]; Deborah Bunin[4]; Merrill Knapp[4]; Andrew Poggio[4]; Carolyn Talcott[4]; Brian Davis[5]; Christine Morton[5]; Christopher Sevinsky[5]; Maria Zavodszky[5]; [1]*George Washington University, Washington, DC;* [2]*University of Maryland, College Park, MD;* [3]*Waters Corp, Beverly, MA;* [4]*SRI International, Menlo Park, CA;* [5]*GE Global Research, Niskayuna, NY*

ThOG pm 03:50 **Tracing Human Brain Development Using an Integrated Multiomics Approach**; Sureyya Ozcan[1]; Daniel Cuthbertson[2]; Jakub Tomasik[3]; Michael S Breen[4]; Jua Lee[5]; Amaury Cazenave-Gassiot[6, 7]; Michelle Lin Kaiqi[6, 7]; Shanshan Ji[7]; Joseph D Buxbaum[4]; Philip Doble[8]; David Bishop[8]; Markus R. Wenk[6, 7]; Maree J Webster[9]; Hyun Joo An[5]; Hee-Sup Shin[10]; Cyndi Shannon Weickert[11]; Rudolf Grimm[2]; Sabine Bahn[1]; [1]*Department of Chemical Engineering and Biotechnology, University of Cambridge, Cambridge, UK;* [2]*Agilent Technologies, Inc., Santa Clara, CA;* [3]*University of Cambridge, Cambridge, UK;* [4]*Department of Psychiatry, Genetics and Genomic Sciences, Icahn School of Medicine at Mount Sinai, New York, NY;* [5]*Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, South Korea;* [6]*Department of Biochemistry, Yong Loo Lin School of Medicine, National University of Singapore,, Singapore, Singapore;* [7]*Singapore Lipidomics Incubator (SLING), Life Sciences Institute, National University of Singapore, Singapore;* [8]*Elemental Bio-imaging Facility, University of Technology Sydney, Broadway, New South Wales, Australia, New South Wales, Australia;* [9]*Stanley Medical Research Institute, Laboratory of Brain Research, Rockville, Maryland;* [10]*Institute for Basic Science, Daejeon, South Korea;* [11]*Neuroscience Research, Schizophrenia Research Institute and University of New South Wales, Sydney, Australia*

ThOG pm 04:10 **HotSpot Analysis in Proteometabolomics: Integrating Quantitative Staphylococcus Aureus Proteomics and Metabolomics, from Experimentally Defined Mutants to Recent Clinical Isolates**; Manor Askenazi[1]; Beatrix M. Ueberheide[2]; Avantika Dhabaria[2]; Drew R. Jones[2]; Victor Torres[2]; Bo Shopsin[2]; William Sause[2]; Irnov Irnov[2]; Bernard Delanghe[3]; Kai Fritzemeier[3]; Christoph Henrich[3]; *[1]Biomedical Hosting LLC, Arlington, MA; [2]School of Medicine, New York University, New York, NY; [3]Thermo Fisher Scientific, Bremen, Germany*

2:30-4:30 pm Thursday
FUNDAMENTALS: COMPUTATIONAL METHODS IN ION MOBILITY AND MS
Session Chair: Mary Rodgers (Wayne State University)
Ballroom 6DE upper level

ThOH pm 02:30 **Towards Realistic Mobile Proton MD Strategies for Modeling ESI Droplets and Gaseous Protein Ions: Inclusion of Intramolecular Charge Solvation**; Lars Konermann[1]; Haidy Metwally[2]; Maryam Bakhtiari[2]; *[1]Univ. of Western Ontario, London, ON, Canada; [2]University of Western Ontario, London, ON, Canada*

ThOH pm 02:50 **Computational Protein Structure Prediction Guided by Covalent Labeling and SID Mass Spectrometry Data**; Melanie Aprahamian[1]; Justin Seffernick[1]; Samantha Hinckley[1]; Sophie R. Harvey[1]; Lisa M. Jones[2]; Vicki H. Wysocki[1]; Steffen Lindert[1]; *[1]Ohio State University, Columbus, OH; [2]University of Maryland, Baltimore, MD*

ThOH pm 03:10 **Effect of Different Activation Methods on CID: Experiments and Chemical Dynamics Simulations on the L-Cysteine Sulfate Anion**; Veronica Macaluso[1]; Debora Scuderi[2]; M. Elisa Crestoni[3]; Simonetta Fornarini[3]; Barbara Chiavarino[3]; Emilio Martinez-Nunez[4]; William L. Hase[5]; Riccardo Spezia[6]; *[1]Universite Paris Saclay, Univ Evry, CNRS, LAMBE, France; [2]Laboratoire de Chimie Physique, UMR 8000, Université Paris Sud, Orsay, France; [3]Dipartimento di Chimica e Teconologie del Farmaco, Università di Roma La Sapienza, Rome, Italy; [4]Departamento de Química Física, Universidate de Santiago de Compostela, Santiago of Compostela, Spain; [5]Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX; [6]Sorbonne Université, Laboratoire de Chimie Théorique, UMR 7616 CNRS, Paris, France*

ThOH pm 03:30 **How Do Proteins Unfold in the Gas Phase?**; Christian Bleiholder[1]; Fanny Caroline Liu[1]; Mengqi Chai[1]; Tyler Cropley[1]; *[1]Florida State University, Tallahassee, FL*

ThOH pm 03:50 **Machine Learning Metabolite Collision Cross Section Prediction Without Energy Minimization**; Molly T. Soper-Hopper[1]; Xueyun Zheng[2]; Erin S. Baker[2]; Facundo M. Fernandez[1]; *[1]Georgia Institute of Technology, Atlanta, GA; [2]Pacific Northwest National Laboratory, Richland, WA*

ThOH pm 04:10 **Ion Mobility-Mass Spectrometry and Hybrid Computational Modeling Reveal Detailed Models of Amyloid Peptide Membrane Interactions**; Sugyan M. Dixit[1]; Hua Pan[2]; Brandon T. Ruotolo[1]; *[1]University of Michigan, Ann Arbor, MI; [2]Nankai University, Tianjin, China*

4:45-5:30 pm Thursday
PLENARY LECTURE
Richard A. Yost (University of Florida)
Hall D ground level

The Fight Against Doping: From Strychnine to Turinabol

Larry Bowers
LD Bowers, LLC

6:30-9:00 pm Thursday
CLOSING EVENT
USS Midway
Advance purchase ticket is required ($30).

NEW! Poster Presentation Schedule
Odd-number posters present: 10:30 am - 11:30 am PLUS 12:30 – 2:30 pm
Even-number posters present: 10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm

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

NEW! Poster Presentation Schedule
Odd-number posters present: 10:30 am - 11:30 am PLUS 12:30 – 2:30 pm
Even-number posters present: 10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm

WEDNESDAY POSTERS

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

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

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

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

THURSDAY POSTERS

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

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

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

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

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

AMBIENT IONIZATION: APPLICATIONS I
001-036

MP 001 **A Novel Approach for Rapid, On-Site Agrochemical Screening of Neat Soil Samples Utilizing Paper Cone Ionization-Mass Spectrometry**; Shahnaz Mukta[1]; Christopher C. Mulligan[1]; *[1]Illinois State Unversity, Normal, IL*

MP 002 **Rapid Analysis of Abused Drugs in Urine Using a Miniature Mass Spectrometry Analysis System**; Manqing Kang[1]; Xiaoxiao Ma[2]; Wanru Zhang[3]; Honge Li[3]; Qiang Cai[4]; Jinfeng Xue[5]; Zheng Ouyang[6, 7]; *[1]Tsinghua University, Beijing, China; [2]State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instrument, Tsinghua University, Beijing, China; [3]PURSPEC Technologies, Inc., Beijing, China; [4]Yangtze Delta Region Institute of Tsinghua University, Jiaxing, China; [5]Public Security Bureau, Jiaxing, China; [6]State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instruments, Tsinghua University, Beijing, China; [7]Weldon School of Biomedical Engineering and Department of Chemistry, Purdue University, West Lafayette, IN*

MP 003 **Accelerated Heterogeneous, Copper Catalysed Coupling Reactions in Micro Droplets and Thin Films**; Kiran Iyer[1]; Jing Yi[2]; Andrew Bogdan[3]; Nari P Talaty[3]; Steven W. Djuric[3]; R. Graham Cooks[2]; *[1]Purdue University, West Lafayette, IN; [2]Purdue University, West Lafayette; [3]Abbvie Inc., North Chicago, IL*

MP 004 **Diode Laser Assisted Desorption Low Temperature Plasma Mass Spectrometry for Direct Analysis of Compounds Separated by Thin-Layer Chromatography**; Xiaoxia Gong[1]; Songyue Shi[1]; Inah Bianca Embile[1]; Gerardo Gamez[1]; *[1]Texas Tech University, Lubbock, TX*

MP 005 **Analysis of Zinc(Ii) Formamidinate Complexes Through a Linear Ion Trap Mass Spectrometer**; Michael B Pastor[1]; Qinliang Zhao[1]; David O Sparkman[1]; *[1]University of the Pacific, Stockton, CA*

MP 006 **Broadening the Application of Paper Spray Mass Spectrometry: Performing Enzyme Reactions on the Spray Substrate**; Dan Carmany[1]; Gabrielle Boyd[1]; Phillip M. Mach[1]; Elizabeth Dhummakupt[2]; Paul S Demond[1]; Trevor Glaros[3]; *[1]Excet, Inc., Springfield, VA; [2]National Research Council, APG-EA, MD; [3]US Army ECBC, Aberdeen Proving Ground, MD*

MP 007 **A Rapid Screening Method for Authenticity of Vanilla Extract by Desorption Atmospheric Pressure Chemical Ionization (Dapci)-Mass Spectrometry**; Ciara N Pitman[1]; Joshua Wilhide[1]; William R. LaCourse[1]; *[1]University of Maryland Baltimore County, Baltimore, MD*

MP 008 **Production of Water Radical Cations Through Dapci-Ms and Their Catalytic Property of Reacting with Volatile Non-Polar Substances Such as Benzene**; Dongbo Mi[1]; Xiaofei Gao[1]; Shuanglong Wang[1]; Wei Liu[1]; Huanwen Chen[1]; *[1]East China University of Technology, Jiangxi Key Laboratory for Mass Spectrometry and Instrumentation, NanChang, China*

MP 009 ***In vivo* Real-Time Monitoring System for Metabolites in a Living Mouse Brain Using Probe Electrospray Ionization/Tandem Mass Spectrometry (PESI/MS/MS)**; Kei Zaitsu[1, 2]; Yumi Hayashi[1, 3]; Tasuku Murata[4]; Kazumi Yokota[4]; Tomomi Ohara[2]; Maiko Kusano[2]; Tetsuya Ishikawa[3]; Hitoshi Tsuchihashi[2]; Akira Ishii[2]; Koretsugu Ogata[4]; Hiroshi Tanihata[4]; *[1]In Vivo Real-Time Omics Laboratory, Institute for Advanced Research, Nagoya University, Nagoya, Japan; [2]Department of Legal Medicine and Bioethics, Nagoya University Graduate School of Medicine, Nagoya, Japan; [3]Pathophysiological Laboratory Sciences, Department of Radiological and Medical Laboratory Sciences, Nagoya University Graduate School of Medicine, Nagoya, Japan; [4]Shimadzu Corporation, Kyoto, Japan*

MP 010 **Study of Paal-Knorr Reaction in Micro-droplet Phase Using Extractive Electrospray Ionization Mass Spectrometry**; Xiao-Fei Gao[1]; Dongbo Mi[1]; Huanwen Chen[1]; *[1]East China University of Technology, Jiangxi Key Laboratory for Mass Spectrometry and Instrumentation, Nanchang, China*

MP 011 **Carbon Fiber Ionization Mass Spectrometry Coupled with Solid Phase Micro-extraction for Analysis of Small Organics**; Min-Li Wu[1]; Te-Yu Chen[2]; Yu-Chie Chen[2]; *[1]National Chiao Tung University, Hsinchu, Taiwan; [2]National Chiao Tung University, Hsinchu, Taiwan*

MP 012 **Rapidly Identify Toxicants by Extractive Electrospray Ionization Mass Spectrometry and Construct Toxicants Data Bank**; Shuanglong Wang[1]; Wei Liu[2]; Huanwen Chen[2, 3]; *[1]East China University of Technology, Jiangxi Key Laboratory for Mass Spectrometry and Instrumentation, nanchang, China; [2]East China University of Technology, Jiangxi Key Laboratory for Mass Spectrometry and Instrumentation, NanChang, China; [3]State Key Laboratory of Inorganic Synthesis and Preparative Chemistry, College of Chemistry, Jilin University, Changchun, China*

MP 013 **Integrated Mass Spectrometry Platform Enables Picomole-Scale Real-time Electrosynthetic Reaction Screening and Discovery**; Qiongqiong Wan[1]; Suming Chen[2]; Abraham K. Badu-Tawiah[3]; *[1]The Ohio State University, Columbus, OH; [2]The Johns Hopkins University, Baltimore, Maryland; [3]The Ohio State University, Columbus, Ohio*

MP 014 **Enhanced Ionization and Detection of Explosives on a Waters Qda Mass Spectrometer Equipped with a Helium-Plasma-Ionization (HePI) Source**; Athula B. Attygalle[1]; Julius Pavlov[1]; David Douce[2]; Steve Bajic[3]; *[1]Stevens Institute of Technology, Hoboken, NJ; [2]Waters Corporation, Wilmslow, UK; [3]Waters Corporation, Wilmslow, UK*

MP 015 **High Yield Accelerated Reactions in Stable Thin Film for Derivatization in Ultra-Small Volumes**; Zhenwei Wei[1]; Xiaochao Zhang[2]; Jinyu Wang[2]; Sichun Zhang[2]; Xinrong Zhang[2]; R. Graham Cooks[1]; *[1]Purdue University, West Lafayette, IN; [2]Tsinghua University, Beijing, China*

MP 016 **Rapid Screening the Alkaloids of Poppy Shell in Hot Pot Bottom, Beef Soup and Seasoning by DART Tandem Mass Spectrometry**; Yingshuang Xie[1]; Xiaoping Zhou*[1]; Huan Zhang[1]; Baile Zhang[1]; Xiaokun Duan[2]; Charles C. Liu[2]; *[1]Gansu Entry-Exit Inspection and Quarantine Bureau, Lanzhou, China; [2]ASPEC Technologies Limited, Beijing, China*

MP 017 **Effects of Analyte Concentration on the Protonation Sites of 4-Aminobenzoic Acid Ionized Using Positive Mode APCI**; Rashmi Kumar[1]; Hilkka I. Kenttämaa[2]; *[1]Purdue University, West Lafaytte; [2]Purdue University, West Lafayette*

MP 018 **Veterinary Drug Analysis in Seafood Tissue: A Novel Method**; Cheryl Lassitter[1]; Sheher B. Mohsin[2]; Joan M. Stevens[3]; Gregory L. Feister[1]; Angela D. Ruple[1]; Jon W. Bell[1]; *[1]NOAA, Pascagoula, MS; [2]Agilent Technologies, Inc., Santa Clara, CA; [3]Agilent Technologies, Wilmington, DE*

MP 019 **A New Strategy for Analysis of Emerging Contaminants in Industrial Residual Waters by Paper Spray Ionization Mass Spectrometry (PSI-MS)**; Marcella Ferreira Rodrigues[1]; Igor Pereira da Silva[1]; Germán Sanz Lobón[1]; Ruiter Lima Morais[1]; Boniek G Vaz[1]; *[1]Universidade Federal de Goias, Goiânia, Brazil*

MP 020 **Ultrafast Pre-Screening of Phthalate Diesters Using DART-MS**; Motoshi Sakakura[1]; Teruhisa Shiota[1]; Jun Watanabe[2]; Fumihiko Usui[1]; *[1]AMR Inc., Meguro-ku, Japan; [2]Shimadzu corp., Kyoto, Japan*

MP 021 **Accurate Quantification of Fipronil and its Metabolites in Egg by Stable Isotope Dilution DART Coupled with Quadrupole Time-of-Flight Mass Spectrometry**; You Li[1]; Xiaojun Deng*[1]; Xionghai Yi[1]; Yiyin Shi[1]; Xiaokun Duan[2]; Yue Song[3]; Charles C. Liu[2]; Jianzhong Li[3]; *[1]Shanghai Entry-Exit Inspection and Quarantine Bureau, Shanghai, China; [2]ASPEC Technologies Limited, Beijing, China; [3]Agilent Technology, Inc., Shanghai, China*

MP 022 **Direct Analysis of UV Filters in Sun Cream Using TLC-MS and Minimized Sample Preparation**; Michaela Oberle[1]; Falk-Thilo Ferse[2]; Stephan Altmaier[1]; Michael Schulz[1]; *[1]Merck KGaA, Darmstadt, Germany; [2]Waters GmbH, Eschborn, Germany*

MP 023 **Reaction Acceleration in Field Desorption Mass Spectrometry**; Xingshuo Chen[1]; R. Graham Cooks[1]; *[1]Purdue University, West Lafayette*

MP 024 **Desorption Easy Ambient Sonic-Spray Ionization Mass Spectrometry for Lipidomic Analysis of Cyanobacteria and Green Algae During Growth and Stress Conditions**; Leonidas Mavroudakis[1]; Nikos Lydakis - Simantiris[2]; Spiros Pergantis[1]; *[1]University of Crete, Heraklion, Greece; [2]Technological Education Institute of Crete, Chania, Greece*

MP 025 **Evaluation of the Discoloration Mechanism of Eosin in Oil Paint by Direct Analysis in Real Time-Mass Spectrometry**; Alba Alvarez Martin[1, 2]; Koen Janssens[2]; Gwénaëlle Kavich[3]; G. Asher Newsome[3]; *[1]Museum Conservation Institute, Smithsonian Institution, Suitland, MD; [2]AXES, Department of Chemistry, University of Antwerp, Antwerp, Belgium; [3]Museum Conservation Institute. Smithsonian Institution, Suitland, MD*

MP 026 **Diagnosing Non-Small Cell Lung Cancer Subtype from Fine Needle Aspiration Biopsies with Desorption Electrospray Ionization Mass Spectrometry**; Alena Bensussan[1]; Tanweer Zaidi[2]; Ruth Katz[2]; Erik Cressman[2]; Livia S Eberlin[1]; *[1]The University of Texas at Austin, Austin, TX; [2]MD Anderson Cancer Center, Houston, TX*

MP 027 **Rapid Screening for Veterinary Drug Residues in Food and Companion Animal Tissues Using Liquid Microjunction Surface Sampling Probe Mass Spectrometry**; Laura Burns[1]; DAVID J. BORTS[1, 2]; *[1]Interdepartmental Toxicology Program, Iowa State University, Ames, IA; [2]Department of Veterinary Diagnostic & Production Animal Medicine, Iowa State University College of Veterinary Medicine, Ames, IA*

MP 028 **Rapid Methods for Identification of Microorganisms by Paper Spray and Nanoelectrospray Ionization**; Zhuoer Xie[1]; Pu Wei[1]; Rafal M. Pielak[2]; R. Graham Cooks[1]; *[1]Purdue University, West Lafayette, IN; [2]L'Oréal California Research Center, San Francisco, CA*

MP 029 **Glovebox APPI-FT-ICR-MS for Air-Sensitive F-Block Metal Complexes**; Faye L Cruickshank[1]; Polly L Arnold[1]; C.Logan Mackay[1]; *[1]university of edinburgh, Edinburgh, UK*

MP 030 **Hydrogen Flame Desorption Ionization Mass Spectrometry Analysis of Picoliter Samples**; Yinlong Guo; *National Center for Organic Mass Spectrometry in Shanghai, Shanghai Institute of Organic Chemistry Chinese Academy of Sciences, Shanghai, China*

MP 031 **Ambient Ionization for Direct Food Analysis by (Trans) Portable Mass Spectrometry**; Marco Blokland[1]; Arjen Gerssen[1]; Michel Nielen[1]; *[1]RIKILT Wageningen University & Research, Wageningen, Netherlands*

MP 032 **Cheap and Re-Usable 3D-printed Plates for Efficient DESI-MS Analysis of Bio- and Synthetic Polymers**; Salomé Poyer[1]; Fabio Ziarelli[2]; Laurence Charles[1]; *[1]Aix Marseille Université, CNRS, UMR 7273, Institut de Chimie Radicalaire, Marseille, France; [2]Aix Marseille Université, CNRS, Fédération des Sciences Chimiques de Marseille (FR 1739), Marseille, France*

MP 033 **Probe Electrospray Ionization Using Graphite as Sampling Needle: Simultaneous Determination of Illicit Drugs in Saliva**; Carla S de Freitas[1]; Thaís Pontes Pereira Mendes[1]; Thays Colletes Carvalho[1]; Renata Pereira Limberger[2]; Wanderson Romão[3]; Boniek G Vaz[1]; *[1]Federal University of Goias, Goiania, Brazil; [2]Federal University of Rio Grande do Sul, Porto Alegre, Brazil; [3]Federal University of Espirito Santo, Vitória, Brazil*

MP 034 **Real-Time Authentication of Food and Beverages Using DART-QDa LiveID Analysis**; Kenneth Rosnack[1]; Sara

Stead[2]; Kari Organtini[1]; David Douce[2]; *[1]Waters Corporation, Milford, MA; [2]Waters Corporation, Wilmslow, UK*

MP 035 **Rapid Discrimination of Liver Cancer Tissue by Mass Spectrometry Based on Differences in Phospholipid Metabolism**; Xiao Yipo[1]; Haiyan Lu[2]; Canhong Xie[3]; Chao Dai[3]; Sharon S. Chen[2, 4]; *[1]Nachang University, Nanchang, China; [2]State Key Laboratory of Inorganic Synthesis and Preparative Chemistry, College of Chemistry, Jilin University, Changchun, China; [3]Department of Cardiothoracic Surgery to Second Affiliated Hospital of Nanchang University, Nanchang, China; [4]East China University of Technology, Jiangxi Key Laboratory for Mass Spectrometry and Instrumentation, NanChang, China*

MP 036 **Analysis of 18 Kinds of Polycyclic Aromatic Hydrocarbons in Edible Oil by GCMS**; Wang Yong; *Shimadzu, Beijing, China*

ANTIBODIES & ANTIBODY DRUG CONJUGATES I
037-069

MP 037 **Reliable Identification of Low Levels of Oxidation, Deamidation, Glycosylation, and Glycation in IgG-Based Biotherapeutics with the NISTmAb Spectral Library**; Qian Dong[1]; Yuxue Liang[1]; Xinjian Yan[1]; Sanford P. Markey[1]; Yuri A. Mirokhin[1]; Dmitrii V. Tchekhovskoi[1]; Tallat H Bukhari[1]; Stephen E. Stein[1]; *[1]NIST, Gaithersburg, MD*

MP 038 **Middle-Down Analysis of Antibody Drug Conjugates Using 193 nm UVPD-MS**; Eleanor C. Watts[1]; M. Montana Quick[1]; Jon D. Williams[2]; Robert W. Johnson[2]; Laura J. Miesbauer[2]; Jennifer S. Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX; [2]AbbVie, North Chicago, IL*

MP 039 **Quantitative Microflow HPLC-MS/MS Analysis of the Antibody Drug Conjugate SigmaMAb Extracted from Rat Plasma**; Chad Christianson[1]; Jennifer S. Zimmer[1]; Shane R. Needham[1]; *[1]Alturas Analytics, Moscow, ID*

MP 040 **Consequences of Biotherapeutic Age on Higher Order Structure: Insights from Accelerated Aging Studies**; Richard A Kerr[1]; Hongping Ye[1]; *[1]FDA Department of Pharmaceutical Analysis, St Louis, MO*

MP 041 **A Paradigm Shift for FT-ICR MS: Accurate Native-MS Measurements of mAbs, Polydisperse ADCs and PEGylated Proteins**; Iain D. G. Campuzao[1]; DAVID P. A. KILGOUR[2]; Steve Van Orden[3]; Michael Nshanian[4]; Jennifer L. Lippens[1]; Chawita Netirojjanakul[5]; Joseph A. Loo[4]; *[1]Amgen Inc., Thousand Oaks, CA; [2]Nottingham Trent University, Nottingham, UK; [3]Bruker Daltonics Inc., Billerica, MA; [4]UCLA, Los Angeles, CA; [5]Amgen, Thousand Oaks, CA*

MP 042 **Catabolic Characterization of Calicheamicin-Containing Antibody-Drug Conjugate**; Chunang (christine) Gu[1]; Vince Tong[1]; Rolf Kern[1]; Hetal Sarvaiya[1]; Alex Schammel[1]; Johannes Hampl[1]; Jack Tibbitts[1]; Tony Cano[1]; *[1]Abbvie Stemcentrx LLC, South San Francisco, CA*

MP 043 **DOE Optimization/Validation of a Platform Identity Assay for mAbs/ADCs Using Sub-Unit Mass Analysis on a QTOF in a GMP/QC Setting**; Claire J Bramwell[1]; Jennifer Wang[1]; Omar M Hamdy[1]; *[1]AbbVie Stemcentrx, South San Francsico, CA*

MP 044 **Characterization of Intact Monoclonal Antibodies Under Native and Reverse Phase Conditions Using High Resolution Mass Spectrometry**; Ryo Yokoyama[1]; Sibylle Heidelberger[2]; Annu Uppal[3]; *[1]SCIEX, Shinagawa-ku, Japan; [2]SCIEX, Warrington, UK; [3]SCIEX, Gurugram, India*

MP 045 **Development of NISTmAb-Derived Homogeneous Antibody-Drug Conjugate (ADC) Standards**; Shanhua Lin[1]; Terry Zhang[2]; Brian Agnew[3]; Trina Mouchahoir[4]; John Schiel[4]; *[1]Thermo Fisher Scientific, Sunnyvale, CA; [2]Thermo Fisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific, Eugene, OR; [4]NIST, Gaithersburg, MD*

MP 046 **Discovery and Confirmation of Glucuronylation as a New Acidic Post-Translational Modification on Therapeutic Monoclonal Antibodies**; Yuetian Yan[1]; Anita Liu[1]; Shunhai Wang[1]; Thomas Daly[1]; Ning Li[1]; *[1]Regeneron Pharmaceuticals, Tarrytown, NY*

MP 047 **Achieving 100% Sequence Coverage of Monoclonal Antibodies by Tryptic Digestion Using a Dual-Column LC-MS System**; Anita Liu[1]; Shunhai Wang[1]; Thomas Daly[1]; Ning Li[1]; *[1]Regeneron Pharmaceuticals, Tarrytown, NY*

MP 048 **Routine Analysis of Host Cell Proteins in Antibody Preparations using PASEF**; Stuart Pengelley[1]; Guillaume Tremintin[2]; Waltraud Evers[1]; Detlev Suckau[1]; *[1]Bruker Daltonics, Bremen, Germany; [2]Bruker Daltonics, Billerica, MA*

MP 049 **Ultrasensitive Characterization of Size and Charge Heterogeneity of Therapeutic Monoclonal Antibodies by Native Mass Spectrometry**; Shunhai Wang[1]; Yuetian Yan[1]; Anita Liu[1]; Thomas Daly[1]; Ning Li[1]; *[1]Regeneron Pharmaceuticals, Tarrytown, NY*

MP 050 **Two Level Automation of Therapeutic Antibody Characterization by Mass Spectrometry: from Sample Preparation to Report Generation**; Miroslav Nikolov[1]; Hans Rainer Voelger[1]; Verena Knaupp[1]; Urs Hanke[1]; Manuel Endesfelder[1]; Marco Boettger[1]; Holger Kropp[1]; Georg Drabner[1]; Harald Duerr[1]; Hans Koll[1]; *[1]Large Molecule Research (LMR), Roche Pharma Research & Early Development (pRED), Roche Innovation Center Munich (RICM), Penzberg, Germany*

MP 051 **Asparagine Deamidation and Aspartate Isomerization of Clinical-Stage Antibodies**; Xiaojun Lu[1]; Heather Lynaugh[1]; Maximiliano Vásquez[1]; Tushar Jain[1]; Paul Nobrega[1]; Yingda Xu[1]; *[1]Adimab LLC, Lebanon, NH*

MP 052 **Automated Workflow for Clone Selection and Early-Stage Developability Characterization of Novel Biologics in Pre-Clinical Development**; Bo Zhai[1]; Jing Li[2]; Andrew Mahan[1]; Yong J. Kil[2]; Rose Lawler[2]; Andrew Nichols[2]; Sen Ilker[2]; Eric Carlson[2]; Hirsh Nanda[1]; *[1]Janssen Research & Development, Spring House, PA; [2]Protein Metrics Inc., San Carlos, CA*

MP 053 **Monitoring of Sequence Variants by MAM Using High Resolution Mass Spectrometry**; Kerstin Pohl[1]; Yihan Li[2]; Annu Uppal[3]; Sibylle Heidelberger[4]; *[1]SCIEX, Darmstadt, Germany; [2]SCIEX, Redwood City, CA; [3]Sciex India Pvt Ltd, Haryana, India; [4]SCIEX, Warrington, UK*

MP 054 **Development of LC-MS Peptide Mapping Method Using Efficient Sample Preparation for Monoclonal Antibody with Minimization of Sample Preparation-related Modification Artifacts**; Ping Jiang[1]; Jie Ding[1]; *[1]PPD, Middleton, WI*

MP 055 **Improved Middle-Down Characterization of Antibodies Using Multiple Ion Activation Techniques and Proton Transfer Reaction on a Modified Orbitrap Mass Spectrometer**; John E. P. Syka[1]; Christopher Mullen[1]; Stephane Houel[1]; Romain Huguet[1]; Joshua A Silveira[1]; Helene Cardasis[1]; Vlad Zabrouskov[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

MP 056 **Important Considerations for LC/MS-Based Analysis of Tissue Distributions of Therapeutic Monoclonal Antibody**; Chao Xue[1]; Bo An[1]; Ming Zhang[1]; Yang Qu[1]; Jun Qu[1]; *[1]University at Buffalo, Buffalo, NY*

MP 057 **An Accurate TMT-Based Approach to Quantify and Model Conjugation via NHS Esters in a Monoclonal Antibody**; Jennifer J Hill[1]; Tammy-Lynn Tremblay[1]; Traian Sulea[2]; Christopher R. Corbeil[2]; Enrico O. Purisima[2]; *[1]National Research Council Canada, Ottawa, ON, Canada; [2]National Research Council Canada, Montréal, QC, Canada*

MP 058 **Quantitation of Monoclonal Antibody Infliximab in Human Plasma by LC-MS/MS Using Fab-Selective Limited Proteolysis nSMOL Technology**; Alan Barnes[1]; Aurore Jaffuel[2]; Neil Loftus[1]; *[1]Shimadzu Corporation, Manchester, UK; [2]Shimadzu France, Marne la Vallée, France*

MP 059 **Screening Antigen-Specific Nanobodies by Middle-Down Mass Spectrometry**; Junjie Wang[1]; Peter C. Fridy[1]; Yinyin Li[1]; Michael P. Rout[1]; Brian T. Chait[1]; *[1]Rockefeller University, New York, NY*

MP 060 **LC-MS Analysis of Monoclonal Antibody Glycoforms using a Novel FcR Receptor Affinity Stationary Phase Paired with High Resolution Mass Spectrometry**; Daniel Shollenberger[1]; Stacy Shollenberger[1]; Atis Chakrabarti[1]; *[1]Tosoh Bioscience, King of Prussia*

MP 061 **Automated Workflow for Monoclonal Antibody N-linked Glycan Analysis with AssayMAP Bravo and InstantPC Labeling Dye**; Shuai Wu[1]; Zach Van Den Heuvel[1]; Steve Murphy[1]; Justin Hyche[2]; Aled Jones[2]; *[1]Agilent Technologies, Inc., Santa Clara, CA; [2]ProZyme, Hayward, CA*

MP 062 **A Universal Plate-Based Immunoaffinity LC-MS/MS Workflow for Preclinical Monoclonal Antibody Quantification**; Kevin Ray[1]; Yue Lu[1]; pegah jalili[1]; Jeffrey Turner[1]; Nicolas Caffarelli[1]; Tom Juehne[1]; *[1]MilliporeSigma, St. Louis, MO*

MP 063 **Studying the Prevalence of Secondary Light Chains in Research Purpose Monoclonal Antibodies with MS-Based De Novo Protein Sequencing**; Zac McDonald[1]; Qixin Liu[1]; Mingjie Xie[1]; Bin Ma[2]; Paul Taylor[3]; Anthony Stajduhar[1]; *[1]Rapid Novor Inc., Kitchener, ON, Canada; [2]University of Waterloo, Waterloo, ON, Canada; [3]SPARC Biocentre, SickKids Hospital, Toronto, ON, Canada*

MP 064 **Serum Antibody Proteogenomics and the Hidden Pepertoire**; Stefano R Bonissone[1]; Natalie Castellana[1]; Anand Patel[1]; *[1]Digital Proteomics, San Diego, CA*

MP 065 **Charge Hybrid/C18 Bonded Phase Column for Therapeutic Protein and Peptide Analysis**; Veronica Qin[1]; Andrew Coffey[2]; Anne E Blackwell[3]; Suma Ramagiri[3]; *[1]Agilent Technologies, Inc, Wilmington, DE; [2]Agilent Technologies Inc., Brecknell, UK; [3]Agilent Technologies, Inc., Wilmington, DE*

MP 066 **Dendritic Cell Mass Spectrometry Method Development for Protein Therapeutic Immunogenicity Risk Assessment**; Robert J Seward[1]; Carlos Morales Betanzos[1]; Andrea Casasola-LaMacchia[1]; Dilki Wickramarachchi[1]; Sophie Tourdot[1]; Li Xue[1]; Timothy Hickling[1]; Mireia Fernandez Ocana[1]; Hendrik Neubert[1]; *[1]Pfizer Inc., Andover, MA*

MP 067 **Molecular Networking for the Characterization of Glycosylation on Antibodies**; Stefano Bonissone[1]; Anand Patel[1]; Natalie Castellana[1]; *[1]Digital Proteomics, LLC., San Diego, CA*

MP 068 **Comparability and Performance Assessment of Peptide Mapping Analysis for Antibody Biologics Using High Resolution Mass Spectrometers**; Eun Young Choi[1]; Jung-Keun Suh[1]; *[1]Seoul Media Institute of Technology, Seoul, South Korea*

MP 069 **Sequence Variant Analysis by LC-MS/MS to Ensure mAbs Product Quality**; Li Cui[1]; Sybille Galosy[2]; Yuan Zhu[2]; Aston Liu[2]; Greg Kilby[2]; Leandro Santos[2]; Pramthesh Patel[2]; *[1]GlaxoSmithKline, King Of Prussia, PA; [2]GlaxoSmithKline, King of Prussia, PA*

BIOMARKERS: DISCOVERY I
070-096

MP 070 **Quantitative Label-Free Mass Spectrometry Analysis in the Symptomatic Niemann-Pick, typeC1 Mouse Model**; Melissa R Pergande[1]; Thu T. A. Nguyen[1]; Carol Haney-Ball[2]; Stephanie M. Cologna[1]; *[1]University of Illinois at Chicago, Chicago, IL; [2]Agilent Technologies, Santa Clara, CA*

MP 071 **Multiplexed, Quantitative Proteomic Comparison of Tau+ and TDP43+ Behavioral Variant Frontotemporal Dementia Human Tissue Samples**; Amanda L. Edwards[1]; Carrie Wager[1]; Danielle L. Graham[1]; *[1]Biogen, Cambridge, MA*

MP 072 **High-Throughput Detection of Volatile Organic Compounds in Urine for Prostate Cancer Diagnosis**; Qin Gao[1]; Xiaogang Su[1]; Heinric Williams[2]; Michael H. Annabi[3]; Thomas Prince[2]; Brielle Schreiter[2]; Sara Morgas[3]; Valerie Mata[3]; Luisa F Castillo[1]; Wen-Yee Lee[1]; *[1]University of Texas at El Paso, El Paso, TX; [2]Geisinger Medical Center, Danville, PA; [3]The Clinic Internal Medicine, El Paso, TX*

MP 073 **High-Throughput Detection of Volatile Organic Compounds in Urine for Renal Cancer Diagnosis**; Qin Gao[1]; Xiaogang Su[1]; Heinric Williams[2]; Thomas Prince[2]; Brielle Schreiter[2]; Wen-Yee Lee[1]; *[1]University of Texas at El Paso, El Paso, TX; [2]Geisinger Medical Center, Danville, PA*

MP 074 **LIPIDS: Potential Biomarkers Involved in Spontaneous Pre-Term Birth (sp-PTB) – An Untargeted Metabolomics Approach Using Label Free LC-DIA-MS Method**; Shirish Yakkundi[1]; LEE GETHINGS[2]; Aude-Claire Morillon[1]; James Langridge[3]; Louise Kenny[1]; *[1]INFANT Centre, University College Cork, Cork, Ireland; [2]Waters Corporation, Wilmslow, UK; [3]Waters Corporation, Wilmslow, UK*

MP 075 **Proteomic Analysis of Androgen-Regulated Sexually Dimorphic Proteins in the Mouse Hypothalamus**; Houng-Wei Tsai[1]; Yuanyu Lee[1, 2]; *[1]Department of Biological Sciences, California State University, Long Beach, Long Beach, CA; [2]Center for Education in Proteomics Analysis (CEPA), California State University, Long Beach, Long Beach, CA*

MP 076 **Development of Secreted Biomarkers of Cellular Senescence and Surface Markers for Senescent Cell-Targeted Therapies**; Natan Basisty[1]; Therese Payne[1]; Judith Campisi[1]; Birgit Schilling[1]; *[1]The Buck Institute for Research on Aging, Novato, CA*

MP 077 **Secretome Analysis of Cancer Cell Lines for Identifying Glioblastoma Cell Specific Secreted Proteins**; Tomohiro Kohata[1]; Shingo Ito[1, 2]; Takeshi Masuda[1, 2]; Mitsutoshi Nakada[3]; Sumio Ohtsuki[1, 2]; *[1]Kumamoto University, Kumamoto, Japan; [2]AMED-CREST, Tokyo, Japan; [3]Kanazawa University Hospital, Kanazawa, Japan*

MP 078 **A Proteomic Approach to Identify Novel Biomarkers of Metastasis in Skin Cancer**; Andrew Shapanis[1]; Chester Lai[1]; Jeffrey Theaker[1]; Jim Schofield[1]; Erika Parkinson[1]; Eugene Healy[1]; Paul Skipp[1]; *[1]Southampton university, Southampton, UK*

MP 079 **A (Phospho)Proteomic Investigation of the Molecular Mechanisms Underlying Anti-Inflammatory Response of M2 Macrophages to Janus Kinase Inhibition and Steroid Treatment**; Benjamin Ruprecht[1]; Paulina Karabelas[2]; Hyun-Hee Lee[2]; An Chi[1]; Ivan Cornella-Taracido[1]; *[1]Merck Research Laboratories, Chemical Biology Department, Boston, MA; [2]Merck Research Laboratories, Immunology Department, Boston, MA*

MP 080 **Compare of Non-Targeted Metabolomic Approaches Using Gas Chromatography Coupled with Unit Mass Spectrometry and High-Resolution Mass Spectrometry**; Yan-Ping Lin; *Janssen R&D LLC., Spring House, PA*

MP 081 **Large-Scale Identification of Intact N-glycopeptides in Serum for Biomarker Discovery of Heptocellular Carcinoma Using LC-EThcD-MS/MS**; Jie Zhang[1]; Jianhui Zhu[1]; Jing Wu[1]; Marshall Bern[2]; Ilker Sen[2]; Brent Weatherly[2]; St John Skilton[2]; David M. Lubman[1]; *[1]University of Michigan Medical Center, Ann Arbor, MI; [2]Protein Metrics Inc., San Carlos, CA*

MP 082 **Plasma Biomarker Discovery and Verification in Chronic Kidney Disease**; Qin Fu[1]; Lesley Inker[2]; Josef Coresh[3]; Paul Kimmel[4]; Adrienne Tin Tin[5]; Vidya Venkatraman[1]; Jennifer Van Eyk[1]; *[1]Cedars Sinai Medical Center, Los Angeles,, CA; [2]Tuffs Medical School, Boston, MA; [3]Johns Johns Hopkins University, Baltimore, MD; [4]National Institute of Diabetes and Digestive Kidney Diseases (NIDDK),, Bethesda, MD; [5]Johns Johns Hopkins University, Baltimore, MD, Baltimore, MD*

MP 083 **Proteomic Identification of Potential Biomarkers of Human Non-Small Cell Lung Cancer**; Kiyoshi Yanagisawa; *Center for Neurological diseases and Cancer, Nagoya, Japan*

MP 084 **Coupling Precision and Depth for the Protein Landscapes of Three Subtyped Gastric Cancers**; Yang Fan[1, 2]; Xiaomin Lou[3]; Jin Zi[2]; Yan Ren[2]; Siqi Liu[2]; *[1]Beijing Genomics Institute, Beijing Institute of Genomics, Chinese Academy of Sciences, Shenzhen, China; [2]BGI-Shenzhen, Shenzhen, China; [3]Beijing Institute of Genomics, Chinese Academy of Sciences, Beijing, China*

MP 085 **Mass Spectrometry Profiling of Extracellular Vesicles Provides Insight Into Biology of Triple Negative Breast Cancer**; Krystine Garcia-Mansfield[1]; Victoria David-Dirgo[1]; Panieh Terraf[2]; Ritin Sharma[1]; Botond Igyarto[3]; Kendall Van Keuren-Jensen[2]; Patrick Pirrotte[1]; *[1]Collaborative Center for Translational Mass Spectrometry, Translational Genomics Research Institute (TGen), Phoenix, AZ; [2]Center for Noninvasive Diagnostics, Translational Genomics Research Institute (TGen), Phoenix, AZ; [3]Baylor Institute for Immunology Research, Dallas, TX*

MP 086 **Tobacco Specific Carcinogens Induce Hypermethylation, DNA Adducts, and DNA Damage in Bladder Cancer**; Venkatrao Vantaku[1]; Sri Ramya Donepudi[1]; Vasanta Putluri[1]; Chandrashekar R Ambati[1]; Shiva Shankar Ravi[1]; Arun Sreekumar[1]; Nagireddy Putluri[1]; *[1]Baylor College of Medicine, Houston, TX*

MP 087 **Comparative Proteomics of Respiratory Exosomes in Cystic Fibrosis, Primary Ciliary Dyskinesia and Asthma**; Virginie Rollet-Choen[1, 2]; Matthieu Bourderioux[1]; Joanna Lipecka[1]; Thao Nguyen-Khoa[2]; Cerina Chhuon[1]; Alain Schmitt[1]; Aleksander Edelman[1]; Sermet-Gaudelous Isabelle[1, 2]; Chiara Guerrera[1]; *[1]INSERM, Paris, France; [2]Assistance Publique-Hôpitaux de Paris, APHP, Paris, France*

MP 088 **Changes of Urine Proteome in Patient-Derived Xenograft Model**; Yongtao Liu[1]; Youhe Gao[1]; *[1]Beijing Normal University, Beijing, China*

MP 089 **A Culture-Independent Mass Spectrometry Based Assay for the Rapid Detection of Urinary Tract Infections**; Spencer Dylan Wildman[1]; Daniel B Gregson[2]; Heather Semeniuk[2]; Ryan A Groves[1]; Dominique Bihan[1]; Ian A Lewis[1]; *[1]University of Calgary, Calgary, Alberta; [2]Calgary Laboratory Services, Alberta Health Services, Calgary, Alberta*

MP 090 **Urine Proteomics Workflow for the Discovery of Biomarkers in Children with Asthma**; Paulos Chumala[1]; Carol Haney-Ball[2]; Tess Kelly[1]; Brooke Thompson[1]; Oluwafemi Oluwole[1]; Anna Afanasieva[1]; Donna Rennie[1]; Joshua Lawson[1]; George S. Katselis[1]; *[1]University of Saskatchewan, Saskatoon, SK, Canada; [2]Agilent Technologies, Santa Clara, CA*

MP 091 **Secretogenomics, a Multi-Omics Approach to Discover Personalized Breast Cancer Markers for Precision Non-Invasive Prognosis**; J Astor Ankney[1]; Ling Xie[1]; John A Wrobel[1]; Li Wang[1]; Xian Chen[1, 2]; *[1]University of North Carolina - Chapel Hill, Chapel Hill, NC; [2]Fudan University, Shanghai, China*

MP 092 **Mass Spectrometry-Based Proteomics Investigation of Fragile X Syndrome**; Kelly L Wormwood[1]; Emmalyn J Dupree[1]; Alisa G Woods[1]; Leonard J Abbeduto[2]; Costel C. Darie[1]; *[1]Clarkson University, Potsdam, NY; [2]UC Davis, Davis, CA*

MP 093 **Integration of Phosphoproteomics and Kinome Profiling Reveals Protein Signatures Controlling Cell Signaling in Solid Tumors**; Ritin Sharma[1]; Krystine Garcia-Mansfield[1]; Aurelein Schrapp[1]; Kristin Leskoske[1]; Apurva M Hegde[1]; Victoria David-Dirgo[1]; Patrick Pirrotte[1]; *[1]Collaborative Center for Translational Mass Spectrometry, Translational Genomics Research Institute (TGen), Phoenix, AZ*

MP 094 **Proteomic Analysis of the Heterogeneity of Similarly Diagnosed Acute Spinal Cord Injuries: Biomarkers for Efficient Translational Medicine**; Jason C Rogalski[1]; Karina Nielsen[1]; Shalini Chaudhary[1]; Anna Prudova[1]; Jaihyun Jeong[1]; Alexandra Nastasa[1]; Femke Streijger[1]; Brian Kwon[1]; Leonard J Foster[1]; *[1]University of British Columbia, Vancouver, BC, Canada*

MP 095 **Peptidomic Protocol for Small and Large Undigested Peptide Determination or Discovery Using an Original Column Switching Set-Up and HRMS Detection**; Bertrand Rochat[1, 2]; Patrice Waridel[1]; Jachen Barblan[1]; Manfredo Quadroni[1]; *[1]Université de Lausanne, Lausanne, Switzerland; [2]Centre Hospitalier Universitaire Vaudois, CHUV, Lausanne, Switzerland*

MP 096 **Longitudinal Plasma Profiling with Stable Isotope Standards and Data-Independent Acquisition Analysis**; Sebastian Müller[1]; Oliver M. Bernhardt[1]; Tejas Gandhi[1]; Lukas Reiter[1]; *[1]Biognosys AG, Schlieren, Switzerland*

CARBOHYDRATES I
097-116

MP 097 **Tandem Mass Spectrometry Coupled to Capillary Electrophoresis for the Structural Analysis of Glycosaminoglycan Mixtures**; Patience Sanderson[1]; Morgan Stickney[1]; Franklin E. Leach III[1]; James Xia[2]; Fuming Zhang[3]; Robert J Linhardt[3]; I. Jonathan Amster[1]; *[1]University of Georgia, Athens, GA; [2]CMP Scientific, Corp., Brooklyn, NY; [3]Rensselaer Polytechnic Institute, Troy, NY*

MP 098 **Novel Ionic Liquid Matrices for Qualitative and Quantitative Detection of Carbohydrates by Matrix Assisted Laser Desorption/Ionization Mass Spectrometry**; Xiaoyong Zhao[1]; Yuanjiang Pan[1]; *[1]Department of Chemistry, Zhejiang University, Hangzhou, China*

MP 099 **Gas-Phase Hydrogen/Deuterium Exchange with Ion Mobility Spectrometry: a New Addition to the Glycan MS Toolkit**; Rick Harkewicz[1]; Sanjit S. Uppal (Sunny)[1]; Yuge H Bryner[1]; Abhigya Mookherjee[1]; Miklos Guttman[1]; *[1]University of Washington, Seattle, WA*

MP 100 **Differentiation and Relative Quantification of Isomeric Glycans by Gated-TIMS MS and Gated-TIMS ExD FTICR MS/MS**; Juan Wei[1]; Yang Tang[1]; Jiandong Wu[1]; Joseph Zaia[1]; Catherine Costello[1]; Cheng Lin[1]; *[1]Boston University, Boston, MA*

MP 101 **Discovering Intact Glycosaminoglycan Sequence Motifs from Proteoglycans: A Database Independent Method for Interpretation of Glycan MS2**; Jiana Duan[1]; Yanlei Yu[2]; Franklin E. Leach III[1]; Fuming Zhang[2]; Robert J Linhardt[2]; I. Jonathan Amster[1]; *[1]University of Georgia, Athens, GA; [2]Rensselaer Polytechnic Institute, Troy, NY*

MP 102 **The Effects of Permethylation on the Fragmentation of Metal-Adducted Oligosaccharides**; Ranelle Schaller-Duke[1]; Carolyn J. Cassady[1]; *[1]The University of Alabama, Tuscaloosa, AL*

MP 103 **LC/MS/MS Assay for Immunogenicity Screening in a Therapeutic Glycoprotein: Identification and Characterization of Non-Human Glycan Epitope**; Myung Jin Oh[1, 2]; Nari Seo[1, 2]; Youngsuk Seo[1, 2]; Unyong Kim[3]; Jeong Hee Baek[4]; Chiyoung Ahn[4]; Hyun Joo An[1, 2]; *[1]Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, South Korea; [2]Asia-Pacific Glycomics Reference Site, Daejeon, South Korea; [3]Glycan Co. Ltd., Sungnam, South Korea; [4]Advanced Therapy Product Research Division, National Institute of Food and Drug Safety Evaluation, Cheongju-si, South Korea*

MP 104 **Neuroglycomic Mapping of Developing Human and Mouse Prefrontal Cortex Using LC-MS/MS**; Jua Lee[1, 2]; Jaekyung Yun[1, 2]; Heeyoun Hwang[1, 2]; Sureyya Ozcan[3]; Sabine Bahn[3]; Hee-Sup Shin[4]; Hyun Joo An[1, 2]; *[1]Chungnam*

National University, Daejeon, South Korea; [2]Asia-Pacific Glycomics Reference Site, Daejeon, South Korea; [3]University of Cambridge, Cambridge, UK; [4]Institute for Basic Science, Daejeon, South Korea

MP 105 **pGlycoNovo: A Database-Free Algorithm for Large-Scale Identification of N- and O-Glycopeptides**; Wen-Feng Zeng[1]; Mingqi Liu[2]; Weiqian Cao[3]; Hao Chi[1]; Si-Min He[1]; Pengyuan Yang[3]; *[1]Institute of Computing Technology, Chinese Academy of Sciences, Beijing, China; [2]Fudan University, Shanghai, China; [3]Fudan Universiry, Shanghai, China*

MP 106 **Structural Identification, and Quantitation of Glycans Labeled with Dual Modifications Strategies from Complex Mixtures Using LS-MS Workflows with SimGlycan Software**; Ningombam Sanjib Meitei[1, 2]; Haiying Li[3]; Sohini Saha[1]; Rupanjan Goswami[1]; Arun Apte[2]; Richard S. Lee[3]; *[1]PREMIER Biosoft, Indore, India; [2]PREMIER Biosoft, Palo Alto, CA; [3]Department of Urology, Boston Children's Hospital and Harvard Medical School, Boston, MA*

MP 107 **Effects of Solvent Parameters on the ESI-MS/MS Signal Intensity and Response Factor of Underivatized Saccharides**; Jonathan Thacker[1]; Kevin A. Schug[2]; *[1]University of Texas, Arlington, Arlington, TX; [2]University of Texas At Arlington, Arlington, TX*

MP 108 **A Mixed Isotopic Permethylation Approach for Quantitative Determination of Monosaccharide Branching in Polysaccharides Using UHPLC/QqQ-MS**; Eshani Nandita[1]; Ace G. Galermo[1]; Matthew J. Amicucci[1]; Mariana Barboza[1]; Carlito B. Lebrilla[1]; *[1]UC Davis, Davis, CA*

MP 109 **Isomeric Separation of Permethylated O-Glycans Derived from Glycoproteins Using PGC-LC-MS at High Temperature**; Byeong Gwan "Andrew" Cho[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX*

MP 110 **Microfluidic Chip Enzyme Reactors for Fast Enzymatic Digestion facilitating Peptides and GlycansLC-MS/MS Analyses**; Aiying Yu[1]; Veronica J Lyons[1]; Dimitri Pappas[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX*

MP 111 **Mechanistic Study of Free Radical Activated Glycan Dissociation by 13C Labeled Cellobiose**; Kimberly Fabijanczuk[1]; Kaylee Gaspar[1]; Jose Acosta[1]; Nathaniel Adomako[1]; Tara Otegui[1]; Jinshan Gao[1]; *[1]Montclair State University, Montclair*

MP 112 **Online Post-Column Enzyme Reactors Facilitating Rapid Isomeric Identification of Glycopeptides in Conjunction with PGC-LC-MS/MS**; Yifan Huang[1]; Aiying Yu[1]; Jieqiang Zhong[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX*

MP 113 **Development of a Rapid Glycosidic Linkage Analysis for Oligosaccharides and Polysaccharides**; Ace G. Galermo[1]; Eshani Nandita[1]; Mariana Barboza[1]; Matthew J. Amicucci[1]; Thai-Thanh Vo[1]; Carlito B. Lebrilla[1]; *[1]University of California, Davis, Davis, CA*

MP 114 **De Novo Structural Determination of Glucose Oligosaccharides and Applications on in Situ Structural Determination in LC/MS**; Chi-Kung Ni[1]; Hsu Chen Hsu[2]; Chia Yen Liew[2]; Shih-Pei Huang[2]; Shang-Ting Tsai[2]; *[1]Academia Sinica, Taipei, Taiwan; [2]Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan*

MP 115 **Isobaric Multiplex Reagents for Carbonyl Containing Compound (SUGAR) High-Throughput Quantitative MS Analysis**; Yu Feng[1]; Bingming Chen[1]; Dustin Frost[1]; Qinying Yu[1]; Xuefei Zhong[1]; Miyang Li[1]; Chrysanthy Ikonomidou[1]; Lingjun Li[1]; *[1]University of Wisconsin–Madison, Madison, WI*

MP 116 **Amino Acid-Based Mass Defect Chemical Tags for Glycomics Analysis**; Miyang Li[1]; Yu Feng[2]; Lingjun Li[2]; *[1]University of Wisconsin Madison, Madison, WI; [2]University of Wisconsin-Madison, Madison, WI*

DATA-DEPENDENT ACQUISITION 117-121

MP 117 **Systematic Evaluation of Polyphenolic Natural Products by Mass Spectrometry**; Jeremiah J. Bowers[1]; Harsha P. Gunawardena[2]; Anaëlle Cornu[3]; Ashwini S. Narvekar[1]; Antoine Richieu[3]; Denis Deffieux[3]; Stéphane Quideau[3]; Nishanth Tharayil[1]; *[1]Clemson University, Clemson, SC; [2]The Janssen Pharmaceutical Companies of Johnson and Johnson, Spring House, PA; [3]Université de Bordeaux, Talence, France*

MP 118 **Maximizing Proteome Coverage with the Advanced Peak Determination Algorithm on an Orbitrap Fusion Mass Spectrometer**; Helene Cardasis[1]; Graeme McAlister[1]; Romain Huguet[1]; Derek J Bailey[1]; Shannon Eliuk[1]; Michael W. Senko[1]; Vlad Zabrouskov[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

MP 119 **Data-Dependent Auto-MSMS 3D- Precursor Selection for Bottom-Up Proteomics with Parallel-Accumulation Serial-Fragmentation (PASEF) on a Trapped-Ion-Mobility Quadrupole-Time-Of-Flight Mass Spectrometer (TIMS-QTOF)**; Markus Lubeck[1]; Jens Decker[1]; Michael Krause[1]; Scarlet Koch[1]; Heiner Koch[1]; Niels Goedecke[1]; Florian Meier[2]; Andreas-David Brunner[2]; Oliver Raether[1]; Matthias Mann[2]; *[1]Bruker Daltonik GmbH, Bremen, Germany; [2]Max Planck Institute of Biochemistry, Martinsried, Germany*

MP 120 **New Method Filters for Improved MSn Acquisition for Small Molecule and Proteomics Workflows**; Graeme McAlister[1]; Balaram Barange[1]; Derek J Bailey[1]; Romain Huguet[1]; Reiko Kiyonami[1]; Shannon Eliuk[1]; Vlad Zabrouskov[1]; Seema Sharma[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

MP 121 **Systematic Study of Scan Models for Protein Identification and Label-Free Quantitation**; Charlie Yang; *Rosalind Franklin University, North Chicago, IL*

DATA-INDEPENDENT ACQUISITION 122-142

MP 122 **Polyphenolic Compounds in Forestry Waste Determined by LC-MS2 and LC-MS-IMS.**; Colin M Potter[1]; Bela Paizs[1]; *[1]Bangor University, Bangor, UK*

MP 123 **Large-Scale Analysis of Proteoform-Specific Complex Formation by Complex-Centric Proteome Profiling via SEC-SWATH-MS**; Isabell Bludau[1]; Max Frank[1]; Moritz Heusel[1]; George Rosenberger[1]; Robin Hafen[1]; Amir Banaei Esfahani[1]; Yansheng Liu[2]; Ludovic Gillet[1]; Ben C Collins[1]; Matthias Gstaiger[1]; Vihandha Wickramasinghe[3]; Ashok Venkitaraman[4]; Ruedi Aebersold[1, 5]; *[1]Department of Biology, Institute of Molecular Systems Biology, ETH Zurich, Zürich, Switzerland; [2]Department of Pharmacology, Cancer Biology Institute, Yale University School of Medicine, West Haven, CT 06516; [3]Sir Peter MacCallum Department of Oncology, University of Melbourne, Melbourne, Australia; [4]Medical Research Council Cancer Unit, University of Cambridge, Cambridge, UK; [5]Faculty of Science, University of Zurich, Zurich, Switzerland*

MP 124 **Data-Independent Acquisition (LC-MSE) for the Quantification of RNA Oligonucleotides**; Peter A Lobue[1]; Balasubrahmanyam Addepalli[1]; Manasses Jora[1]; Patrick A Limbach[1]; *[1]University of Cincinnati Chemistry Dept, Cincinnati, OH*

MP 125 **DIA+: A Novel Data-Independent Acquisition Method Combines Multiple Precursor Charges to Boost Peptide Signal**; Eva Borras[1, 2]; Eduard Sabido[1, 2]; *[1]Universitat Pompeu Fabra (UPF), Barcelona, Spain; [2]Centre de Regulació Genòmica (CRG), Barcelona, Spain*

MP 126 **Simplifying the Use of Ion Libraries During Data Processing of Data Independent Acquisition Proteomics Data**; Arianna I Jones[1]; Matt Huebsch[2]; Christie Hunter[3]; Kathleen Lewis[3]; Adam Lau[4]; Nick Morrice[5]; Sara Ahadi[6]; *[1]SCIEX, Framingham, MA; [2]SCIEX, Concord, ON, Canada;*

[3]Sciex, Redwood City, CA; [4]SCIEX, Redwood City, CA; [5]SCIEX, Warrington, UK; [6]Stanford, Palo Alto, CA

MP 127 **Behind DIA Reproducibility**; Carolina Fernandez-Costa[1]; Salvador Martínez-Bartolomé[1]; Daniel B. McClatchy[1]; Sung K Park[1]; Titus Jung[1]; John R. Yates[1]; *[1]Department of Molecular Medicine - The Scripps Research Institute, La Jolla, CA*

MP 128 **Data Independent Acquisition Resource for Deep Phosphoproteome Analysis**; Reta Birhanu Kitata[1]; Pei-Yi Lin[1]; Yun-Chien Chang[1]; Chia-Feng Tsai[2]; Alexey I Nesvizhskii[3, 4]; Yu-Ju Chen[1]; *[1]Institute of Chemistry, Academia Sinica, Taipei, Taiwan; [2]Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, Japan; [3]Department of Computational Medicine and Bioinformatics, University of Michigan, Ann Arbor, MI; [4]Department of Pathology, University of Michigan, Ann Arbor, MI*

MP 129 **Untargeted Study of Pomegranate Juices to Investigate Organoleptic Characteristics Using a Novel Dia Mode and Ion-Mobility Enabled QTof MS**; Sara Stead[1]; Joanne Connolly[1]; Gordon Fujimoto[2]; Kenneth Rosnack[3]; *[1]Waters Corporation, Wilmslow, UK; [2]Waters Corporation, Beverly, MA; [3]Waters Corporation, Milford, MA*

MP 130 **DIA Trade-Offs in Deep Proteomics and Phosphoproteomics**; Christian Kelstrup[1]; Dorte B Bekker-Jensen[1]; Jesper V. Olsen[1]; *[1]CPR, University of Copenhagen, Copenhagen N, Denmark*

MP 131 **Development and Validation of a Multiplex Quantitative Protein Assay for Human Cerebrospinal Fluid**; Lindsay K Pino[1]; Brian C Searle[1]; Andy Hoofnagle[1]; William S Noble[1]; Michael J MacCoss[1]; *[1]University of Washington, Seattle, WA*

MP 132 **Variations of Protein Profile Promoted by Aerobic Exercise on Insulin Resistance (IR) and Insulin Sensitive (IS) Participants**; Jeniffer Quijada[1]; Sara Ahadi[1]; Kevin Contrepois[1]; Kegan Moneghetti[1]; Francois Haddad[1]; Michael Snyder[1]; *[1]Stanford University, Stanford, CA*

MP 133 **Characteristics of Different Multidimensional Data Independent Acquisition Techniques on a Single MS Platform**; Chris Hughes[1]; Keith Richardson[1]; Praveen H[1]; Jonathan P. Williams[1]; *[1]Waters Corporation, Wilmslow, UK*

MP 134 **Best of Both Worlds: A New DIA Workflow in Spectronaut Combines the Depth of Resource with iRT-Precision of Project-Specific Data**; Tejas Gandhi[1]; Lynn Verbeke[1]; Oliver M. Bernhardt[1]; Jan Muntel[1]; Sebastian Müller[1]; Roland Bruderer[1]; Yue Xuan[2]; Lukas Reiter[1]; *[1]Biognosys AG, Schlieren, Switzerland; [2]Thermo Fisher Scientific, Bremen, Germany*

MP 135 **An ABRF Study to Evaluate Data-Independent Acquisition for Protein Quantification in Core Facility Settings**; Yan Wang[1]; Allis Chien[2]; Laura E. Herring[3]; Pratik D Jagtap[4]; LeRoy Martin[5]; Benjamin Neely[6]; Brett S Phinney[7]; Paul Shan[8]; Paul M. Stemmer[9]; *[1]University of Maryland, College Park, MD; [2]Stanford University, Stanford, CA; [3]Department of Pharmacology, UNC-Chapel Hill, Chapel Hill, NC; [4]Department of Biochemistry, Molecular Biology and Biophysics, University of Minnesota, Minneapolis, MN; [5]Waters Corp., Beverly, MA; [6]Chemical Sciences Division, Hollings Marine Laboratory, National Institute of Standards and Technology, Charleston, SC; [7]UC Davis, Davis, CA; [8]Bioinformatics Solutions Inc., Waterloo, ON, Canada; [9]Wayne State University, Detroit , MI*

MP 136 **Data-independent Acquisition-Based Proteomics for Biomarker Quantification in Tumor Biopsies**; Yeoun Jin Kim[1]; Steve M Sweet[1]; Jarrett D Egertson[2]; Wei-li Liao[1]; Andrew J Sedgewick[1]; Sheeno Thyparambil[1]; Charlie Vaske[1]; Sunghee Woo[1]; Gennifer E Merrihew[2]; Michael J MacCoss[2]; Todd Hembrough[1]; *[1]NantOmics, Rockville, MD; [2]University of Washington, Seattle, WA*

MP 137 **Optimizing Experimental Conditions for Generating High Quality DIA Data of Amniotic Fluid Samples**; Hossein Fazelinia[1]; Lynn A. Spruce[2]; Hua Ding[2]; Heather A. Hartman[2]; Heron D. Baumgarten[2]; Aimee G. Kim[2]; Steven H. Seeholzer[2]; *[1]Children's Hospital of Philadelphia, Philadelphia, PA; [2]Children's Hospital of Philadelphia, Philadelphia, PA*

MP 138 **DISCO: TPP Software Tool to Enable Exploration of Light and Dark Molecular Universes in DIA Experiments**; David D. Shteynberg[1]; Samuel L. Bader[1]; Eric W. Deutsch[1]; Michael R. Hoopmann[1]; Mukul K. Midha[1]; Robert L. Moritz[1]; *[1]Institute for Systems Biology, Seattle, WA*

MP 139 **A Protein-Centric Investigation of Human Response to Insulin and Rapamycin With DIA-MS**; Seth Just[1]; Phillip Seitzer[1]; Caleb Emmons[1]; Susan Ludwigsen[1]; Brian C. Searle[1, 2]; *[1]Proteome Software, Portland, OR; [2]University of Washington Genome Sciences, Seattle, WA*

MP 140 **The Application of the Predicted Peptide Retension Time in DIA Analysis**; Xiaohui Liu[1]; Wenyuan Lu[2]; Pengyuan Yang[2]; *[1]Fudan University, Shanghai, China; [2]Fudan Universiry, Shanghai, China*

MP 141 **Development of Ion Library Assessment Tools in SWATHAtlas**; David S Campbell[1]; Samuel L Bader[1]; Mukul K Midha[1]; Robert L Moritz[1]; *[1]ISB, Seattle, WA*

MP 142 **Computational Analysis of Proteomics Data Collected Using Data Independent Acquisition with a Fast Scanning, Unit Resolution Hybrid Quadrupole-Linear Ion Trap**; Austin T Keller[1]; Philip M Remes[2]; Brian C Searle[3]; Jarrett D Egertson[3]; Romain Huguet[2]; Michael J MacCoss[3]; *[1]University of Washington, Seattle, WA; [2]Thermo Scientific, San Jose, CA; [3]University of Washington Genome Sciences, Seattle, WA*

DISEASE BIOMARKERS
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MP 143 **Multi-Omic Characterisation of Bladder and Lung Carcinomas Using a Novel Scanning Quadrupole DIA Acquisition Method**; Lee A Gethings[1]; Adam King[1]; Robert S Plumb[2]; *[1]Waters, Wilmslow, UK; [2]Waters Corporation, Milford, MA*

MP 144 **Quantitative Phosphoproteomics and Global Proteomics investigation Revealed Novel Insights into Myocardial Stunning in a Swine model**; Xue Wang[1]; Xiaomeng Shen[2]; Rebeccah Young[3]; Brian Weil[3]; Jun Li[1]; Jun Qu[1]; *[1]University at Buffalo, Buffalo, NY; [2]Amgen, San Francisco, CA; [3]Clinical and Translational Research Center, Buffalo, NY*

MP 145 **Fecal Metabolomics of a Mouse Model of Autism**; Emily R. Sekera[1]; Troy D. Wood[1]; Heather L. Rudolph[1]; Stephen D. Carro[1]; *[1]University at Buffalo, Buffalo, NY*

MP 146 **Integrated Glycomics, Proteomics and Transcriptomics of Human Parkinson's Disease Pre-Frontal Cortex**; Rekha Raghunathan[1]; John D Hogan[1]; Richard Myers[1]; Joseph Zaia[1]; *[1]Boston University, Boston, MA*

MP 147 **Proteomic Profiling of Breast Cancer-Derived Extracellular Vesicles Allows for Human Breast Cancer Subtype Classification**; Stamatia Rontogianni[1]; Eleni Synadaki[1]; Bohui Li[1]; Wei Wu[1]; A.F. Maarten Altelaar[1]; *[1]Utrecht University, Utrecht, Netherlands*

MP 148 **Stroma Liquid Biopsy – Pan-Cancer Dysregulation of the Serum Proteome**; Matt Kuruc[1]; Roy Swapan[1]; Haiyan Zheng[2]; Amenah Soherwardy[2]; *[1]Biotech Support Group LLC, Monmouth Junction, NJ; [2]Rutgers Center for Proteomics, Piscataway, NJ*

MP 149 **Whole Cell MALDI Fingerprinting Technique as a Robust Tool for Differential Profiling of Mammalian Cells Lines**; Valentina Petukhova; *UIC, Chicago, IL*

MP 150 **Influence of Hepatic Encephalopathy on Bile Acid Content in Brain Tissues of Rats and Mice**; Amy N. W. Schnelle[1]; Luke T Richardson[2]; Michael E Pettit[2]; Sharon DeMorrow[3]; Touradj Solouki[2]; *[1]Baylor University, Waco;*

[2]Baylor University, Waco, TX; [3]Central Texas Veterans Healthcare System, Texas A&M College of Medicine, Temple, TX

MP 151 **Classification and Identification of Lipid Biomarkers in Lung Cancer and Chronic Obstructive Pulmonary Disease**; Jone Garate[1]; Joan Bestard-Escalas[2]; Albert Maimó-Barceló[2]; Roberto Antonio Fernandez[1]; Lucia Martin[1]; Sergio Scrimini[3]; Borja G. Cosio[3]; Jaume Sauleda[3]; Gwendolyn Barcelo-Coblijn[2]; Jose Andres Fernandez[1]; *[1]Dep. of Physical Chemistry, Fac. of Science and Technology, University of the Basque Country (UPV/EHU), Leioa, Spain; [2]Research Unit, Hospital Universitari Son Espases (HUSE), Institut d'Investigació Sanitària Illes Balears (IdISBa), Palma, Spain; [3]Pneumology Unit, Hospital Universitari Son Espases (HUSE), Palma, Spain*

MP 152 **Leukotriene F4 as a Candidate Biomarker for Candidemia Screening**; Carlos Fernando Odir Rodrigues Melo[1]; Luis Felipe Bachur[2]; Mohamed Ziad Dabaja[1]; Cibele Tararam[2]; Ariane Busso-Lopes[2]; Tatiane Melina Guerreiro[1]; Maria Luiza Moretti[2]; Rodrigo Ramos Catharino[1]; *[1]Innovare Biomarkers Laboratory, Campinas, Brazil; [2]Infectious Diseases Division, Department of Internal Medicine, Faculty of Medical Sciences, State University of Campinas, Campinas, Brazil*

MP 153 **Modulation of Endothelial Cells Barrier Tightness by Angiogenic Factors Assessed by Quantitative Phosphoproteomics**; Manuel Tzouros[1, 2]; David Avila[1, 2]; Verena Küppers[1, 3]; Oliv Eidam[1]; Jitao David Zhang[1, 2]; Juliane Siebourg-Polster[1, 2]; Laura Badi[1, 2]; Martin Ebeling[1, 2]; Patric Turowski[4]; Guido Hartmann[1, 3]; *[1]Roche Pharma Research and Early Development, Roche Innovation Center Basel, Hoffmann-La Roche Ltd, Grenzacherstrasse 124, 4070, Basel, Switzerland; [2]Pharmaceutical Sciences, Basel, Switzerland; [3]Neuroscience Ophthalmology and Rare Diseases Discovery and Translational Area, Basel, Switzerland; [4]UCL Institute of Ophthalmology, London, UK*

MP 154 **Identification of Biomarkers for Glioblastoma in Saliva using Ion Mobility Mass Spectrometry**; Amy N. W. Schnelle[1]; Luke T Richardson[2]; Michael E Pettit[2]; Raul A Villacob[2]; Fengfei Wang[3]; Erxi Wu[3]; Touradj Solouki[2]; *[1]Baylor University, Waco; [2]Baylor University, Waco, TX; [3]Baylor Scott & White Health, Dallas, TX*

MP 155 **Molecular Signature of Alzheimer's Disease-Associated Changes Identified in Glaucoma Eyes Using Quantitative Proteomics Analysis**; Mehdi Mirzaei[1, 2]; Vivek Gupta[3]; Joel Chick[4]; Todd M. Greco[5]; Paul A Haynes[2]; Stuart L Graham[3]; *[1]Australian Proteome Analysis Facility - Macquarie University, Sydney, Australia; [2]Department of Molecular Sciences, Macquarie University, Sydney, Australia; [3]Department of Clinical Medicine, Macquarie University, Sydney, Australia; [4]Department of Cell Biology, Harvard Medical School, Boston, MA; [5]Department of Molecular Biology, Princeton University, Princeton, NJ*

MP 156 **Development of a Targeted Mass-Spectrometry Method for Quantification of Cerebrospinal Fluid Biomarkers of Alzheimer's Disease**; Becky C Carlyle[1]; Shannon Leslie[2]; Bianca A Trombetta[1]; Chloe K Nobuhara[1]; Christopher H VanDyck[2]; Angus C Nairn[2]; Steven E Arnold[1]; *[1]Massachusetts General Hospital, Charlestown, MA; [2]Yale University, New Haven, CT*

MP 157 **Method Development for the Assay of Short-Chain Acyl-Coenzyme A Thioesters in Tissues by LC-MS/MS**; Marie-Christine Tang[1]; Hao Yang[2]; Shupei Wang[2]; Grant A. Mitchell[2]; Alexandra Furtos[1]; *[1]Département de Chimie, Université de Montréal, Québec, Canda, Montréal, Québec; [2]Division of Medical Genetics, Département de Pédiatrie et Centre de Recherche, CHU Sainte-Justine, Université de Montréal, Montreal, Québec*

MP 158 **Idnetifying Potential N-glycan Biomarkers for Idiopathic REM Sleep Behavior Disorder by LC-MS/MS**; Xue Dong[1]; Stefania Mondello[2, 3]; Firas Kobeissy[4]; Farid Talih[4]; Raffaele Ferri[2]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX; [2]Oasi Institute for Research on Mental Retardation and Brain Aging, Troina, Italy; [3]University of Messina, Messina, Italy; [4]American University of Beirut, Beirut, Lebanon*

MP 159 **Proteomic Study of Idiopathic REM Sleep Behavior Disorder and Restless Leg Syndrome Using LC-MS/MS for Candidate Biomarker Identification**; Jingfu Zhao[1]; Firas Kobeissy[2]; Firid Talih[2]; Raffaele Ferri[3]; Yehia Mechref[4]; Mondello Stefania[3, 5]; *[1]Texas Tech University, Lubbock, TX; [2]American University of Beirut, Beirut, Lebanon; [3]Oasi Institute for Research on Mental Retardation and Brain Aging, Troina, Italy; [4]Texas Tech University, Lubbock; [5]University of Messina, Messina, Italy*

MP 160 **Microfluidic CE-MS for Newborn Screening: A Single System for Monitoring Small Molecule and Protein Biomarkers**; Erin Redman[1]; Michael P Goodwin[2]; J. Scott Mellors[1]; *[1]908 Devices Inc., Boston, MA; [2]ThermoFisher, San Jose, CA*

MP 161 **Exploring the Lung Interstitial Space Using Hydrogel Nanoparticles and LC-MS/MS on an Orbitrap Fusion Mass Spectrometer**; Paul Russo[1]; Elisa Baldeli[1]; Kianoush Jeiran[1]; Jacopo Vannucci[2]; Francesco Puma[2]; Lucio Crino[3]; Vienna Ludovini[4]; Lance Liotta[1]; Emanuel Petricoin[1]; Mariaelena Pierobon[1]; *[1]George Mason University, Manassas, VA; [2]University of Perugia, Perugia, Italy; [3]Istituto Scientifico Romagnolo per lo Studio e la Cura dei Tumori, Meldola, Italy; [4]S. Maria della Misericordia Hospital, Perugia, Italy*

MP 162 **Urinary Proteomics Reveals Putative Biomarkers for Susceptibility to Infection in Pediatric Patients with Vesicoureteral Reflux**; Dijana Vitko[1]; Patricia S. Cho[2]; Kylie H. Davis[1]; Maggie R. Leary[1]; Shannon DiMartino[1]; Peter Warren[1]; Tanya Logvinenko[1]; John W. Froehlich[1]; Richard S. Lee[1]; *[1]Boston Children's Hospital, Boston; [2]University of Massachusetts Medical School, Worcester, MA*

MP 163 **Lipidomics Analysis of Cultured Human Fibroblasts from Individuals with Autism Spectrum Disorders**; Amy Li[1]; Anne Arnett[2]; Micah Pepper[2]; Raphael Bernier[2]; Libin Xu[1]; *[1]Department of Medicinal Chemistry, University of Washington School of Pharmacy, Seattle, WA; [2]Center on Human Development and Disability, University of Washington, Seattle, WA*

MP 164 **Proteomic Profiling of Cancer Cell Exosomes**; Kelly Servage[1]; Karoliina Stefanius[1]; Kim Orth[1]; *[1]UT Southwestern Medical Center, Dallas, TX*

MP 165 **Alterations of Eicosanoids and Related Mediators in Patients with Schizophrenia**; Dongfang Wang[1]; Bing Cao[1]; Lailai Yan[1]; Qingbin Lu[1]; Jingjing Yan[1]; Xiaoyu Sun[1]; Biao Ren[2]; Haiwei Gu[3]; Jingyu Wang[1]; *[1]Peking University, Beijing, China; [2]Shimadzu (China) Co., Ltd., Beijing, China; [3]Mayo Clinic, Scottsdale, Scottsdale, AZ*

MP 166 **Optimization of Deep Proteome Analysis to Identify Urinary Biomarkers from Pediatric Patient Groups with Kidney Stones**; Joseph A Caruso[1]; Larisa Kovacevic[2]; Nicholas J. Carruthers[3]; Paul M. Stemmer[3]; *[1]Wayne State University, Detroit, MI; [2]Department of Pediatric Urology, Children's Hospital of Michigan, Detroit, MI; [3]Wayne State University, Detroit , MI*

MP 167 **A Proteomic Approach to Monitor the Response of Triple Negative Breast Cancer to Dendritic Cell Vaccination**; Victoria David-Dirgo[1]; Ritin Sharma[1]; Krystine Garcia-Mansfield[1]; Mitchell Kroll[2]; Kendall Van Keuren-Jensen[3]; Botond Igyarto[2]; Patrick Pirrotte[1]; *[1]Collaborative Center for Translational Mass Spectrometry, Translational Genomics Research Institute (TGen), Phoenix, AZ; [2]Baylor Institute for Immunology Research, Dallas, TX; [3]Center for Noninvasive Diagnostics, Translational Genomics Research Institute (TGen), Phoenix, AZ*

MP 168 **Quantitative Characterization of α-Synuclein in Synucleinopathies**; Ying Xiong[1, 2]; Hanno Steen[3, 4]; Judith Steen[1, 2]; *[1]F. M. Kirby Neurobiology Center, Boston Children's Hospital, Boston, MA; [2]Department of Neurology, Harvard Medical School, Boston, MA; [3]Department of Pathology, Boston Children' s Hospital, Boston, MA; [4]Department of Pathology, Harvard Medical School, Boston, MA*

MP 169 **Untargeted and Targeted Lipidomic Analysis of Western Diet-Induced Nonalcoholic Steatohepatitis in Female Ldlr-/- Mice**; Manuel Garcia Jaramillo[1, 2]; Weijian Zhang[1, 2]; Donald B. Jump[1, 2]; *[1]The Nutrition Program, School of Biological and Population Health Sciences, Oregon State University, Corvallis, OR; [2]Linus Pauling Institute, Oregon State University, Corvallis, OR*

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MP 170 **Quantification of a Novel Aldehyde Dehydrogenase Inhibitor in Rat Using Liquid Chromatographic-Quadrupole Time-Of-Flight Mass Spectrometric Method**; Nahye Kim; Min-Ho Park; Seok-Ho Shin; Byeong Ill Lee; Jin-Ju Byeon; Yuri Park; Jangmi Choi; Young G. Shin; Inkyu Hwang; *Chungnam National University, Daejeon, South Korea*

MP 171 **Development and Validation of Brain Exposure Assessment (BEA) Platform**; Lei Yang[1]; Xiang Fu[1]; Chandra Savage[1]; Heather Long[1]; Burgess Freeman[1]; Richard Rahija[1]; Zoran Rankovic[1]; *[1]St. Jude Children's Research Hospital, Memphis, TN*

MP 172 **Determination of Cyclosporin A in Four Different Rabbit Ocular Tissues using Liquid Chromatography–Mass Spectrometry Method**; Weixing Sun[1]; Zhao Heng Ge[1]; John Chapdelaine[1]; Alexandre Brkovic[1]; Adrien Musuku[1]; *[1]Pharmascience.Inc, Montreal, QC, Canada*

MP 173 **Acoustic-Open Port-Mass Spectrometry (AOMS) Enabled HTS: Assay Development for Choline Transporter (CHT) Uptake Function Assessment**; Wenyi Hua[1]; Lorraine Lanyon[1]; Julie Keefer[1]; Claire M Steppan[1]; Chang Liu[2]; Tom Covey[2]; Hui Zhang[1]; *[1]Pfizer Inc., Groton, CT; [2]SCIEX, Concord, ON, Canada*

MP 174 **Ultra Fast Analysis of Dexamethafine and Its Metabolites by Using Nexera MX Parallel Liquid Chromatography Mass Spectrometry System**; Qiang Li[1]; Hongyuan Hao[2]; Taohong Huang[2]; *[1]Shimadzu (China) Co., LTD. Shanghai Branch, Shanghai, China; [2]Shimadzu (China) Co., Ltd,, Shanghai, China*

MP 175 **Method Development and Validation for LCMSMS Quantitation of Octreotide in Porcine Plasma**; P. Patrick Lin[1]; Theresa Q Santos[1]; Bih Hsu[1]; *[1]PHARMout Laboratories, Sunnyvale, CA*

MP 176 **The Use of a New and Versatile Microflow Electrospray Ionization Source for Routine Drug Quantitation in Discovery and Regulated Bioanalysis**; Joseph A Tweed[1]; Jason Barricklow[1]; Christopher L Holliman[1]; *[1]Pfizer Inc., Groton, CT*

MP 177 **Comparison Between the Tandem Quadrupole and Quadrupole Time-Of-Flight Quantification of Exenatide in Rat Plasma**; Gordon J Murray[1]; Jake Y Hsu[2]; David A Johnson[2]; *[1]Waters Corp, Beverly, MA; [2]MicroConstants, Inc, San Diego, CA*

MP 178 **Native MS in Drug Discovery: High-Resolution and Top-Down Analysis of Peptide-RNA Assemblies for Multiplexed Screening of Large Combinatorial Libraries**; Thomas Kenderdine[1]; Daniele Fabris[2]; *[1]University at Albany, Albany, NY; [2]RNA Institute, University at Albany, Albany, NY*

MP 179 **Systems Pharmacology of an Endocannabinoid System Modulator in Zebrafish Larvae**; Vasudev Kantae[1]; Annelot C. M. van Esbroeck[2]; Floor Stevens[2]; Rob C. van Wijk[1]; Amy C. Harms[1]; Piet H. van der Graaf[3, 4]; Mario van der Stelt[2]; Thomas Hankemeier[3]; *[1]Leiden Academic Centre for Drug Research, Leiden University, Leiden, Netherlands; [2]Department of Molecular Physiology, Leiden Institute of Chemistry, Leiden University, Leiden, Netherlands; [3]Leiden University, Leiden, Netherlands; [4]Certara QSP, Canterbury Innovation Centre, Canterbury, UK*

MP 180 **Structural Analysis of Bifunctional Platinum Complexes**; Chao Feng[1]; Yi Chen[2]; Qinliang Zhao[1]; *[1]University of the Pacific, Stockton, CA; [2]Bluevalley Pharmaceutical LLC, Pleasanton, CA*

MP 181 **Analysis of an N-Acetylcysteine Conjugated Prodrug OP-101 in Rat Plasma Using LC-MS/MS**; Forrest Helfrich[1]; Jeff Cleland[2]; Anjali Sharma[2, 3]; Rangaramanujam M Kannan[2, 3]; Mike Buorarati[1]; Dale Schoener[1]; *[1]Intertek Pharmaceutical Services, San Diego, CA; [2]Orpheris, Redwood City, CA; [3]Johns Hopkins School of Medicine, Baltimore, MD*

MP 182 **Development of a Cysteine Reduction Assay for Determination of Disulfide-based Linker Stability in Cysteine-engineered Antibody-Drug Conjugates**; Phillip Chu[1]; Aimee O'Donohue[1]; Katherine Kozak[1]; Yichin Liu[1]; John C. Tran[1]; *[1]Genentech Inc., South San Francisco, CA*

MP 183 **Optimization of a High Throughput PAMPA assay for Peptide Therapeutics**; Bahanu Habulihaz[1]; Bernard K. Choi[1]; Paul J Harradine[1]; Lucinda R Hittle[1]; *[1]Merck & Co., Inc., Rahway, NJ*

MP 184 **Molecular Target Elucidation of Myxobacterial Vioprolide A by an Integrative Proteomics and Metabolomics Approach**; Volker C. Kirsch[1]; Christina Besl[2]; Simone Braig[2]; Angelika M. Vollmar[2]; Stephan A. Sieber[1]; *[1]Center for Integrated Protein Science (CIPSM), Department of Chemistry, Technical University of Munich, Munich, Germany; [2]Pharmaceutical Biology, LMU Munich, Munich, Germany*

MP 185 **UHPLC-MS/MS Analysis of Lanthionine Ketimine Ethyl Ester in Mouse Serum and Tissues**; Ruth Muchiri[1]; Katarzyna Kowal[2]; Kenneth Hensley[3]; Douglas Feinstein[2]; Richard van Breemen[1]; *[1]Oregon State University, Corvallis, OR; [2]University of Illinois at Chicago, Chicago, IL; [3]Arkansas College of Osteopathic Medicine, Fort Smith, AR*

MP 186 **Dose-And Time-Dependent Effects of Hepatotoxicants on ADME Proteins in 3D Human Liver Spheroids by PRM**; Nathalie Selevsek[1]; Witold E. Wolski[1]; Laura Kunz[1]; Henrik Cordes[2]; Vanessa Baier[2]; Lars Kuepfer[2]; Olivia Clayton[3]; Adrian Roth[3]; Ralph Schlapbach[1]; *[1]Functional Genomics Center Zurich, ETH Zurich, Zurich, Switzerland; [2]Institute of Applied Microbiology (iAMB), RWTH Aachen, Aachen, Germany; [3]Roche Pharma Research and Early Development, Roche Innovation Center Basel, Basel, Switzerland*

MP 187 **Comparison of Two LC-MS/MS Protein Quantitation Strategies with Trastuzumab as a Model System in Rat Pharmacokinetics Study**; Zhiren Yu[1]; Zhiyu Li[1]; Weiqun Cao[1]; Yi Tao[1]; Xin Zhang[2]; *[1]Department of DMPK/Non-GLP Bioanalytical Service, WuXi AppTec Co., Shanghai, China; [2]Department of DMPK, WuXi AppTec Co., Shanghai, China*

MP 188 **Bioanalytical Method for Performing both Quantitative and Qualitative Analysis of Drugs in Organovo 3D Bioprinted Human Liver Samplesp**; Emily Adarayan[1]; Ian McIntosh[2]; Andreas Baudy[2]; Elizabeth Mahan[2]; Guangping Bi[2]; Gary Adamson[2]; Rena Zhang[2]; Daniel S. Spellman[2]; *[1]Merck Reseach Labs, West Point, PA; [2]Merck Research Labs, West Point, PA*

MP 189 **Label Free High Throughput Screening of Small Acid-Based Assays Using LDTD-MS/MS in 9 Seconds per Sample**; Jean Lacoursière[1]; Serge Auger[1]; Jonathan Rochon[2]; Pierre Picard[1]; *[1]Phytronix Technologies, Inc., Quebec, QC; [2]Universite Laval, Quebec, QC, Canada*

MP 190 **MS-Based Deep Proteome Profiling in a 7,8-Dihydroxyflavone Treated Mouse Model of Alzheimer's Disease**; Mingming Niu[1]; Hong wang[2]; Yuxin Li[2]; Ji-Hoon Cho[2]; Vishwajeeth R Pagala[2]; Anthony A High[2]; Xusheng Wang[2]; Junmin Peng[1]; *[1]St. Jude Children's Research Hospital, Memphis, TN; [2]St. Jude Proteomics Facility, St. Jude Children's Research Hospital, Memphis, TN*

MP 191 **Design and Integration of a High-Performance Micro-Flow LC-MS/MS system**; Brendon Kapinos[1]; John Janiszewski[1]; Bernhard Nemec[2]; Werner Dobelin[2]; Wayne Lootsma[3]; Steve Ainley[3]; *[1]Pfizer, Groton, CT; [2]Prolab Instruments GmbH, Reinach, Switzerland; [3]Sound Analytics, Niantic, CT*

MP 192 **A High-Throughput Mass Spectrometry Plate-Reader: Acoustic Droplet Ejection to an Open-Port Probe Sampling Interface**; Chang Liu[1]; Hui Zhang[2]; Lucien Ghislain[3]; Jianhua Liu[2]; Wenyi Hua[2]; Timothy Foley[2]; Sammy Datwani[3]; Don Arnold[4]; Thomas R Covey[1]; *[1]SCIEX, Concord, ON, Canada; [2]Pfizer Inc., Groton, CT; [3]Labcyte, San Jose, CA; [4]SCIEX, Redwood City, CA*

MP 193 **Bioactivation of Morpholine Ring in Compound 1: Ring Scission to Potentially Electrophilic Aldehyde Intermediates and Possible Link to the Genotoxicity**; Stephen U Bowlin[1]; Amin Kamel[1]; *[1]Takeda California, San Diego, CA*

MP 194 **Thermal Proteome Profiling to Identify Novel Drug Targets and Mechanisms of Phenobarbital in Human Primary Hepatocytes**; Weiliang Huang[1]; Zhihui Li[1]; Hongbing Wang[1]; Maureen Kane[1]; *[1]University of Maryland, School of Pharmacy, Baltimore, MD*

MP 195 **Target Miner: a Novel Tool for Discovery of Anticancer Drug Targets by a Proteome Signature Library**; Amirata Saei Dibavar[1]; Pierre Sabatier[1]; Bo Zhang[1]; Alexey Chernobrovkin[1]; Roman Zubarev[2]; *[1]Karolinska Institutet, Stockholm, Sweden; [2]Karolinska Institute, Stockholm, Sweden*

MP 196 **Application of High-Throughput RapidFire-MS/MS Assay for Cytochrome P450 Inhibition Studies to Support NCATS Drug Discovery Research**; Dingyin Tao[1]; Pranav Shah[1]; Shyh-Ming Yang[1]; Yuhong Fang[1]; Md Kabir[1]; Amy Q. Wang[1]; Christopher A. LeClair[1]; Xin Xu[1]; *[1]National Center for Advancing Translational Sciences, National Institutes of Health, Rockville, MD*

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MP 197 **Single Cell Analysis by Inductively Coupled Plasma Mass Spectrometry (ICP-MS) for Environmental and Human Health Applications**; Hamid Badiei[1]; Ruth Merrifield[1]; Lauren Amable[2]; Mariko Ikehata[3]; Jamie Lead[4]; Chady Stephan[1]; *[1]PerkinElmer Inc., Woodbridge, ON, Canada; [2]Division of Intramural Research, NIMHD, NIH, Bethesda, MD; [3]Department of Microbiology and Immunology, Life Sciences Centre, University of British Columbia, Vancouver, BC, Canada; [4]Center for Environmental NanoScience and Risk (CENR) Arnold School of Public Health, University of South Carolina, Columbia, SC*

MP 198 **Validation of Quantitative Analysis Method for Determination of Elemental Impurities in Pharmaceutical Products Following USP 232/233 on ICPMS-2030**; Raymond Li[1]; Zhaoqi Zhan[1]; *[1]Application Development and Support Centre, Shimadzu (Asia Pacific) Pte Ltd, 79 Science Park Drive #02-01/08, Singapore 118264, Singapore, Singapore*

MP 199 **Development of Profiling Procedure for Protein Binding Metals in Biofluid Using LC-ICPMS Technique**; Satoshi Yamaki[1]; Yun Zou[1]; Tadashi Taniguchi[2]; Yuki Hashi[3]; Lailai Yan[4]; Siyu Yang[4]; Jingyu Wang[4]; Naoki Hamada[5]; *[1]Shimadzu (China) Co., Ltd., Beijing, China; [2]Shimadzu Corporation, Kyoto, Japan; [3]Shimadzu (China) Co., Ltd,, Shanghai, China; [4]Peking University, Beijing, China; [5]Shimadzu (China) Co., Ltd., Beijing, China*

MP 200 **Elemental Analysis of Stroke Rat Brain By Laser Ablation Inductively Coupled Plasma Quadrupole Mass Spectrometry**; Khalid A. Al-Saad[1]; Mohamad H. Ali[2]; Fazle Rakib[1]; Rick Dijkhuizen[3]; Geralda v Tilborg[3]; Limbeck Andreas[4]; *[1]Qatar University, Doha, Qatar; [2]Qatar Biomedical Research Institute, Doha, Qatar; [3]Utrecht University, Utrecht, Netherlands; [4]Vienna University of Technology, Vienna, Austria*

MP 201 **Trace Metal Analysis of Consumer Products by Flow Injection ICP-MS**; Jennifer Sanderson[1]; Jamey Jones[1]; *[1]Advion Inc., Ithaca, NY*

ELEMENTAL ANALYSIS: ISOTOPE RATIO MS
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MP 202 **Uranium Isotope-Ratio Analysis with Solution-Cathode Glow Discharge Mass Spectrometry (SCGD-MS)**; Garett M. MacLean[1]; George CY Chan[2]; Jake T. Shelley[1]; *[1]Rensselaer Polytechnic Institute, Troy, NY; [2]Lawrence Berkeley Laboratory, Berkeley, CA*

ELEMENTAL ANALYSIS: SIMS AND SURFACE ANALYSIS
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MP 203 **Research of Uncertainty of Key Elements Measurement in Rare Earth Alloy Using Glow Discharge Mass Spectrometry: Continuous Versus Pulsed Mode**; Jianying Zhang[1]; Tao Zhou[2]; Hui Jiao[2]; Dan Song[2]; Lianshan Han[2]; *[1]National Institute of Metrology, China, Beijing, China; [2]National Institute of Metrology, Beijing, China*

MP 204 **A Study on Surface Charge Neutralization of Insulating Samples in TOF SIMS Analysis by Plasma Treatment**; Myoung Choul Choi; *Korea Basic Science Institute, Ochang-Myun, South Korea*

MP 205 **Secondary Ion Yields Produced by 10keV Toluene and Its Cluster Ion Beam Projectiles Generated by UV Laser Ionization**; Chang Min Choi[1]; Ji Young Baek[1]; Sang Ju Lee[1]; Myoung Choul Choi[1]; *[1]Mass Spectrometry & Advanced Instrumentation Research Group, Korea Basic Science Institute, Cheongju-si, South Korea*

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MP 206 **New Mass Spectrometry-Based Strategy for Discovery of Halogenated Peptides in Drinking Water**; Guang Huang[1]; Ping Jiang[1]; Lindsay Jmaiff-Blackstock[1]; Xing-Fang Li[1]; *[1]University of Alberta, Edmonton, AB, Canada*

MP 207 **Development and Evaluation of a Passive Sampling TD-GC-ToFMS Method for VOC Quantification at 24-hour Resolution for Air Quality Compliance Applications**; Nicholas S. Karellas[1]; Robert M. Healy[1]; *[1]Ontario Ministry of the Environment, Toronto, ON, Canada*

MP 208 **Comprehensive Molecular Level Investigation of Oil Contaminated Soils from Gulf War After 30 Years**; Young Hwan Kim[1]; Eunji Cho[2]; Moonhee Park[1]; Sunghwan Kim[2]; *[1]Korea Basic Science Institute, Cheongju, South Korea; [2]Kyungpook National University, Daegu, South Korea*

MP 209 **Uranyl Complexation with Cyclic Peptide Studied by Using Mass Spectrometry and Molecular Dynamics Simulation**; Linnan Li[1]; Sensen Shen[1]; Hexiang Huang[2]; Yu Bai[1]; Huwei Liu[1]; *[1]Peking University, Beijing, China; [2]Sichuan Institute of Materials and Technology, Mianyang, China*

MP 210 **Environmental Transformation of Triclosan Mediated by Plastic Debris in Freshwater Environments**; Kathryn Renyer[1]; Daryl Giblin[2]; Matthew Reichert[1]; Lisa Kim[1]; John Kelly[1]; Timothy Hoellein[1]; Michael L Gross[3, 4]; M. Paul Chiarelli[1]; *[1]Loyola University, Chicago, IL; [2]Washington*

University St Louis, St. Louis, MO; [3]Washington University, St. Louis, St. Louis, MO; [4]Washington University School of Medicine, St Louis, MO

MP 211 **Detection and Quantification of Methylamine and Betaine in Lake Water**; Abdullah Alowaifeer[1]; Qian Wang[1]; Timothy R. McDermott[1]; Brian Bothner[1]; *[1]Montana State University, Bozeman, MT*

MP 212 **Batch Studies of Methylation/Demethylation of Arsenic in Simulated Wetlands**; Young-Soo Han[1]; So-Jeong Kim[1]; Ji-Hyun Park[1, 2]; Dong-Hee Lim[2]; *[1]Korea Institute of Geoscience and Mineral Resources, Daejeon, South Korea; [2]Chungbuk National University, Cheongju, South Korea*

MP 213 **Analysis of 4,4'-Methylenedianiline in Water Extracts Without Sample Preparation Using Liquid Chromatography Mass Spectrometry (LCMS)**; Noelle Elliott[1]; Marshall Henry[1]; *[1]Intertek, Allentown, PA*

MP 214 **Measurement of Harmful Carbonyl Emissions from Variable Power E-Cigarettes**; Nicholas Wallbillich[1]; Gary Glish[1]; *[1]University of North Carolina, Chapel Hill, NC*

MP 215 **Comprehensive Rapid Analysis of Environmental Odors Using SIFT-MS**; Murray J McEwan[1, 2]; Mary Askey[3]; Helena A Barnes[2]; Vaughan S Langford[2]; Daniel B Milligan[2]; James G Olerenshaw[2]; *[1]University of Canterbury, Christchurch, New Zealand; [2]Syft Technologies Ltd, Christchurch, New Zealand; [3]Gelita NZ, Christchurch, New Zealand*

MP 216 **Analysis of Perfluorinated Compounds in Waste Water Using Automated Solid Phase Extraction**; Rudolf Addink[1]; Waleed Hassan[1]; *[1]Toxic Report, Watertown, MA*

MP 217 **Analysis ofPerfluorinatedAlkyl Acids Specified in EPA M537 and Beyond Using LCMS-8045**; Gerard Byrne[1]; Evelyn Wang[1]; Katie Pryor[1]; Christopher Gilles[1]; Brahm Prakash[1]; Tairo Ogura[1]; William Lipps[1]; *[1]Shimadzu Scientific Instrument, Columbia, MD*

MP 218 **High Throughput Analysis of Water for Perfluoroalkyl Substances by Reversed Phase High Performance Liquid Chromatography Tandem Mass Spectrometry**; Jessica M. Morrison[1]; Michael C. Stagliano, Ph.D. [1]; Timothy A. Karrer[1]; Matthew J. Geiger[1]; *[1]MI Dept of Health & Human Services, Lansing, MI*

MP 219 **Optimization and Application of Paper Spray Ionization Mass Spectrometry for the Analysis of Natural Organic Matter**; Donghwi Kim[1]; Sunghwan Kim[1]; *[1]Kyungpook National University, Daegu, South Korea*

MP 220 **Differentiation of Naphthenic Acids from Natural Organic Matter in River Water Using Membrane Sampling and Mass Spectrometric Analysis**; Jeffrey A Hawkes[1]; Kyle D Duncan[1]; Bas Clarijs[1]; Mykelti Berg[2]; Jonas Bergquist[1]; Ingela Lanekoff[1]; Christopher G. Gill[2, 3]; Erik T. Krogh[2, 3]; *[1]Uppsala University, Uppsala, Sweden; [2]Vancouver Island University, Nanaimo, BC, Canada; [3]Department of chemistry, University of Victoria, Victoria, BC, Canada*

MP 221 **Rapid Analysis of Emerging andFugitive Contaminants in Plant Tissues by HPLC-Tandem Mass Spectrometry**; Honglan Shi[1]; Xiaolong He[1]; Haiting Zhang[1]; Runmiao Xue[1]; Wenyan Liu[1]; Joe G. Burken[1]; *[1]Missouri University of Sciense and Technology, Rolla, MO*

MP 222 **Comprehensive Non-Targeted Characterization of Disinfection Byproducts in Chlorinated Seawater Using LC-HRMS/MS and GC-MS**; Noelle J DeStefano[1]; Joshua Allen[2]; Brandie M. Ehrmann[3]; Susan D. Richardson[2]; P. Lee Ferguson[1]; *[1]Duke University, Durham, NC; [2]University of South Carolina, Columbia, SC; [3]University of North Carolina at Chapel Hill, Chapel Hill, NC*

MP 223 **Effects of Mobile Phase pH on Electrospray Ionization Response of Naphthenic Acid Fraction Compounds**; Kerry M Peru[1]; Mary J Thomas[2]; Diana Catalina Palacio Lozano[2]; Dena W McMartin[3]; John V Headley[1]; Mark P Barrow[2]; *[1]Environment and Climate Change Canada, Science and Technology Branch, Saskatoon, SK, Canada; [2]University of Warwick, Coventry, UK; [3]Environmental Systems Engineering, Regina, SK, Canada*

MP 224 **Improved Analysis of Polyfluorinated Alkyl Substances (PFASs) in Environmental Samples by Optimized ASTM Method 7968/7979**; Brahm Prakash[1]; William Lipps[2]; Tairo Ogura[1]; *[1]Shimadzu Scientific Instruments, Inc., Columbia, MD; [2]Shimadzu Scientific Instruments, Inc, Columbia, MD*

MP 225 **Determination of SVOC in Soil by GC-MS/MS Combined with Accelerated Solvent Extraction (ASE)**; Xizhi Wang[1]; Shen Wang[2]; *[1]Thermo Fisher Scientific China (Beijing Branch), Beijing, China; [2]Thermo Fisher Scientific China (Shanghai Branch), Shanghai, China*

MP 226 **Analysis of the Novel PFOA-Replacement Compound, GenX, by High Resolution and Triple Quadrupole Mass Spectrometry**; Simon Roberts[1]; Craig Butt[2]; Robert Di Lorenzo[3]; April Quinn-Paquet[2]; Christopher Borton[1]; Katherine Hyland[4]; *[1]SCIEX, Redwood City, CA; [2]Sciex, Framingham, MA; [3]SCIEX, Concord, ON, Canada; [4]SCIEX, Redwood City, CA*

MP 227 **Automated micro-SPE for the Determination of Perfluoroalkyl Substances**; Thomas Lockwood[1]; David Bishop[1]; Simin D. Maleknia[1]; Andrew Minett[2]; Peter Dawes[2]; Philip Doble[1]; *[1]School of Mathematical and Physical Sciences, University of Technology Sydney, Sydney, Australia; [2]Eprep Pty Ltd, Mulgrave, Australia*

MP 228 **Development of Analytical Method of Melamine in Placenta from Pregnant Women by Isotope Dilution Liquid Chromatography/Tandem Mass Spectrometry**; Chia-Fang Wu[1]; Chiung-I Huang[1]; Yung-Hung Chen[2]; Ming-Tsang Wu[1, 3, 4, 5]; *[1]Research Center for Environmental Medicine, Kaohsiung Medical University, Kaohsiung, Taiwan; [2]Department of Gynecology and Obstetrics, Kaohsiung Municipal Hsiao-Kang Hospital, Kaohsiung, Taiwan; [3]Department of Public Health, College of Health Sciences, Kaohsiung Medical University, Kaohsiung, Taiwan; [4]Graduate Institute of Clinical Medicine, Kaohsiung Medical University, Kaohsiung, Taiwan; [5]Department of Community Medicine, Kaohsiung Medical University Hospital, Kaohsiung Medical University, Kaohsiung, Taiwan*

MP 229 **Quantification of Tobacco Specific Nitrosamines in Cigarette Smoke using LCMSMS**; Chander Mani[1]; Samir Vyas[1]; Saikat Banerjee[1]; *[1]Agilent Technologies, Haryana, India*

MP 230 **Rapid quantitation of 2-hydroxy-4-Methoxybenzophenone (HMB) and Three Metabolites 2,4-Dihydroxybenzophenone (DHB), 2,3,4-Trihydroxybenzophenone (THB), and 2,2-dihydroxy-4-Methoxybenzophenone (DHMB) in Rat Serum**; Estatira Sepehr[1]; Raul A Trbojevich[1]; Matthew S Bryant[1]; *[1]National Center for Toxicological Research, FDA, Jefferson, AR*

MP 231 **Deconvoluted Spectral Matching Improves Target Confirmation for EPA Method 8270D**; Bruce Quimby[1]; Melissa Churley[2]; Dale R. Walker[2]; Michael J. Szelewski[1]; *[1]Agilent Technologies, Inc., Wilmington, DE; [2]Agilent Technologies Inc, Santa Clara, CA*

MP 232 **Investigation of Disinfection By-Product Formation and Toxicity of Swimming Pools Utilizing Cu/Ag Electrolysis and Chlorine**; Joshua M. Allen[1]; Michael J. Plewa[2]; Lucy Quirk[1]; Gretchen Bollar[1]; Susan D. Richardson[1]; *[1]University of South Carolina, Columbia, SC; [2]University of Illinois at Urbana-Champaign, Urbana, IL*

MP 233 **Withdrawn**

MP 234 **Application of GC×GC-HRT-MS Petroleomics Based Spectral Analysis of Two Iconic Oil Spills from the Gulf of Mexico for Environmental Forensics**; Robert K Nelson[1]; Jagoš R. Radović[2]; Christopher M. Reddy[3]; *[1]Woods Hole Oceanographic Inst., Woods Hole, MA; [2]University of Calgary, Calgary, Alberta; [3]Woods Hole Oceanographic Institution, Woods Hole, MA*

MP 235 **Nitroaromatic Pollutants Environmental Fate Characterized by High Resolution Accurate Mass Spectrometry; Understanding Anaerobic Formation of Azo Coupling Products**; Leif Abrell[1]; Warren M Kadoya[1]; Camila L Madeira[1]; Stanley Wong[1]; Reyes Sierra-Alvarez[1]; Eugene A Mash[1]; Jim A Field[1]; *[1]University of Arizona, Tucson, AZ*

MP 236 **Microcosm Approach to the Molecular Understanding of Environmental transformation Products from Macondo Well Oil**; Huan Chen[1]; Amy M McKenna[1]; Sydney F. Niles[1, 2]; Phoebe Zito[3]; Matthew A. Tarr[3]; Ryan P. Rodgers[1, 2]; *[1]National High Magnetic Field Laboratory, Tallahassee, FL; [2]Florida State University, Tallahassee, FL; [3]University of New Orleans, New Orleans, LA*

MP 237 **Characterization of the Complex Dispersant Mixture Corexit®9500 in Seawater Using High-Resolution Mass Spectrometry**; Sarah Choyke[1]; P. Lee Ferguson[1]; *[1]Duke University, Durham, NC*

MP 238 **Analysis of Polycyclic Aromatic Hydrocarbons (PAH) and Hydroxylated PAH Metabolites in Plasma and Urine Using High-Resolution GC/Q-TOF**; Sofia Nieto[1]; Anthony Macherone[2]; Nathan Eno[1]; Michael Armstrong[3]; Marc Elie[3]; Richard Reisdorph[3]; Nichole Reisdorph[3]; *[1]Agilent Technologies, Inc., Santa Clara, CA; [2]Agilent Technologies, Inc., Wilmington, DE; [3]University of Colorado School of Pharmacy, Aurora, CO*

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MP 239 **Nutrients, Flavors, Non-Volatile Chemical Profiles and Chemistry in Daily Consumed Onion Products**; Ying Yang; *Intl Flavors and Fragrances, Union Beach, NJ*

MP 240 **Profiling of Alkylresorcinol Content in Whole Grains Using LC-MS**; Nicole L Burke[1]; Russell W LaClair[1]; *[1]Kellogg, Battle Creek, MI*

MP 241 **Untargeted Metabolomics of Highly Complex Foods**; Nicole C. Sikora[1]; Julia M Gauglitz[1, 2]; Morgan W Panitchpakdi[1]; Christine M. Aceves[1]; Elizabeth A Brown[3]; Pieter C. Dorrestein[1]; *[1]Skaggs School of Pharmacy & Pharmaceutical Sciences, University of California San Diego, San Diego, CA; [2]Center for Microbiome Innovation, University of California San Diego, La Jolla, CA; [3]University of California San Diego, Division of Biological Sciences, La Jolla, CA*

MP 242 **A Comparison of Targeted LC-MS/MS Methods for Multi-allergen Quantification in Foods**; Weili Xiong[1]; Katherine L. Fiedler[1]; Chelsea C. Boo[2]; Timothy R. Croley[1]; Christine H. Parker[1]; *[1]U.S. Food and Drug Administration, Center for Food Safety and Applied Nutrition, College Park, MD; [2]MedImmune, Gaithersburg, MD*

MP 243 **Developing Oligosaccharides Library from Various Plant Sources and in Their Industrial Side Streams Using NanoLC Chip Quadrupole-Time-of-Flight MS**; Tian Tian[1]; Daniela Barile[1]; *[1]Department of Food Science and Technology, University of California, Davis, CA*

MP 244 **Analysis of Glycerolipids in Colombian Cocoa Beans by MALDI-MS**; Deisy Giraldo-Dávila[1]; Juan S. Ramírez-Pradilla[1]; Cristian Blanco-Tirado[1]; Marianny Y Combariza[1]; *[1]universidad Industrial de Santander, Bucaramanga, Colombia*

MP 245 **Proteomic Storage Study of Probiotics**; Barbara S. Larsen; *The DuPont Company, Wilmington, DE*

MP 246 **Characterization and Quantification of Phenolic Compounds in BRS-Moema (Capsicum chinense) by HPLC-ESI-MS/MS**; Ana C Aguiar[1]; Gustavo Araujo Pereira[2]; Cláudia Silva da Costa Ribeiro[3]; Célio Fernando Figueiredo Angolini[4]; Marcos Nogueira Eberlin[4]; Glaucia Maria Pastore[2]; Julian Martínez[1]; *[1]University of Campinas, Campinas, Brazil; [2]University of Campinas, School of Food Engineering, Campinas, Brazil; [3]Embrapa Hortaliças, Brasília, Brazil; [4]ThoMSon Mass Spectrometry Laboratory, University of Campinas, Campinas, Brazil*

MP 247 **Proteomics of Foodcrusts Recovered from Archaeological Ceramics**; Anna Shevchenko[1]; Andrea Schuhmann[1]; Andrej Shevchenko[1]; *[1]MPI of Mol Cell Biology and Genetics, Dresden, Germany*

MP 248 **Proteomic Analysis of Thececal Mucosalof Laying Hens Fed Genetically Modified Mai**; Lilan Zhang[1]; Liang Chen[1]; Ruqing Zhong[1]; Sheng Zhang[2]; Yuxia Chen[1]; Hongfu Zhang[1]; *[1]State Key Laboratory of Animal Nutrition, Institute of Animal Science; Chinese Academy of Agricultural Sciences, Beijing, China; [2]Institute of Biotechnology, Cornell University, Ithaca, NY*

MP 249 **Untargeted Workflow for the Analysis of Cranberry Cultivars and Structural Elucidation of Their Top Discriminating Features**; Chris J Riley[1]; Catherine Neto[1]; *[1]University of Massachusetts Dartmouth, North Dartmouth, MA*

MP 250 **Targeted and Untargeted Metabolomic Profiling of Beer as a Function of Yeast Strain and Fermentation Time**; Kearney M. Foss[1]; Jordyn Palla[1]; Karen Fortmann[2]; Christine A. Hughey[1]; *[1]James Madison University, Harrisonburg, VA; [2]White Labs, San Diego, CA*

MP 251 **Deamidation of Gluten: Identifying Patterns and Preferential Sites, to Support Development of a Targeted Mass Spectrometry Method**; Sophie Bromilow[1, 2]; Lee A Gethings[3]; James Langridge[3]; Michael Buckley[4]; Mike Bromley[5]; Peter Shewry[6]; EN Clare Mills[1]; *[1]Manchester Institute of Biotechnology, School of Biological Sciences, Manchester Academic Health Sciences Centre, University of Manchester, Manchester, UK; [2]Kenneth L. Maddy Equine Analytical Chemistry Laboratory, Davis, CA; [3]Waters Corporation, Wilmslow, UK; [4]Manchester Institute of Biotechnology, School of Chemistry, University of Manchester, Manchester, UK; [5]Synergy Health, Hebden Bridge, UK; [6]Rothamsted Research, Harpenden, UK*

MP 252 **Development and Validation of Non-derivatization LC/MS/MS Method for Fast Determination of Proteinogenic Amino Acids in Fish**; Wan Tung Liw[1]; Zhe Sun[1]; Min Yi Nicole Chan[1]; Jie Xing[1]; Zhaoqi Zhan[1]; *[1]Shimadzu Asia Pacific, Singapore, Singapore*

MP 253 **Profiling the Aroma of Coffee with GC, GCxGC, and TOFMS**; Joseph E Binkley[1]; Elizabeth M Humston-Fulmer[1]; *[1]LECO Corporation, St. Joseph, MI*

MP 254 **Rapid Determination of the Origin of Cocoa Bean and Chocolate with Laser Assisted REIMS – The Bean to Bar Project**; Richard Schäffer[1]; Tamas Karancsi[1]; Steven D Pringle[2]; Zoltan Takats[3]; Viktoria Varga[1]; Zsoka Ath-Horvath[4]; JULIA BALOG[1, 3]; *[1]Waters Research Center, Budapest, Hungary; [2]Waters Corporation, Wilmslow, UK; [3]Imperial College London, London, UK; [4]Harrer Chocolat Ltd., Sopron, Hungary*

MP 255 **Analysis and Comparison of the Natural Product Content of Herbal Supplements Using a Drift Tube Ion Mobility Mass Spectrometer**; Daniel Cuthbertson[1]; Carol Haney-Ball[2]; *[1]Agilent Technologies, Seattle, WA; [2]Agilent Technologies, Inc., Wilmington, DE*

MP 256 **Over 120 Ways to Describe over 2000 Foods, Generating Metadata for Large-Scale Metabolomics Studies**; Morgan W Panitchpakdi[1]; Julia M Gauglitz[1, 2]; Elizabeth A Brown[1, 3]; Austin D Swafford[2]; Christine M Aceves[1]; Francesca Di Ottavio[1, 4]; Nicole C Sikora[1]; Pieter C Dorrestein[1, 2]; *[1]Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California, San Diego, La Jolla, CA; [2]Center for Microbiome Innovation, University of California San Diego, La Jolla, CA; [3]University of California San Diego, Division of Biological Sciences, La Jolla, CA; [4]University of Teramo, Teramo, Italy*

MP 257 **Simultaneous Quantitation of Fat Soluble Vitamins in Infant Milk Formulae Using 5500QTRAP LC-MS/MS System**; Alka Verma[1]; Dr.Anoop kumar[1]; Dr.Jianru Stahl-Zeng[2]; Dr.Manoj Pillai[1]; *[1]Sciex India Pvt Ltd, Gurgaon, India; [2]Sciex, Darmstadt, Germany*

MP 258 **Correlation and Modelling of Wheat Parent:Offspring HMW & LMW Composition by MS-ESI-ToF Analysis with Flour Dough Gluten Strength Parameters**; Dave Hatcher[1]; Ray Bacala[1, 2]; Katherine Cordova[1]; Bin Xiao Fu[1]; *[1]Canadian Grain Commission, Winnipeg, MB; [2]Department of Chemistry, University of Manitoba, Winnipeg, Manitoba*

MP 259 **Comprehensive Cannabisanalysis to Meet the Stringent Limits of Canadian Pesticide Regulations Using the SCIEX QTRAP 6500+ System**; Robert Di Lorenzo[1]; Diana Tran[2]; Katherine Hyland[3]; Simon Roberts[2]; Scott Krepich[4]; Paul Winkler[2]; Craig Butt[5]; April Quinn-Paquet[5]; Christopher Borton[2]; *[1]SCIEX, Concord, ON, Canada; [2]SCIEX, Redwood City, CA; [3]SCIEX, Redwood City, CA; [4]Phenomenex, Torrance, CA; [5]Sciex, Framingham, MA*

MP 260 **Analysis of Carbohydrates in Beer Using Liquid Chromatography Triple Quadrupole Mass Spectrometry**; Michael Volny[1]; Stephanie N. Samra[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

MP 261 **96 Bottles of Beer: Metabolic Profiling of Spent Growth Media Using Rapid, High Throughput Capillary Electrophoresis-Electrospray Ionization-Mass Spectrometry**; Joshua Guerrette[1]; Erin Redman[1]; J. Scott Mellors[1]; *[1]908 Devices, Carrboro, NC*

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MP 262 **Simultaneous Determination of Multi-Residue Pesticides in Tobacco by GPC-GC-MS/MS**; Sun Qian[1]; Fan Jun[2]; Deng Xiao Li[2]; Li Yue qi[3]; Huang Tao Hong[2]; Hashi Yuki; *[1]Shimadzu (China) Co., Ltd., Xian, China; [2]Shimadzu (China) Co., Ltd., Shanghai, China; [3]Shimadzu (China) Co., Ltd., Beijing, China*

MP 263 **Differentiation of Isomeric Food Contaminants by MS/MS Product Ions Characterization**; Alberto Nunez[1]; Yelena Sapozhnikova[1]; *[1]USDA-ARS-ERRC, Wyndmoor, PA*

MP 264 **Reproducible Analysis of Glyphosate, AMPA and 7 Other Polar Pesticides in Food and Water by SAX Chromatography with MS/MS Detection**; Jerry Zweigenbaum[1]; Tarun Anumol[1]; *[1]Agilent Technologies, Wilmington, DE*

MP 265 **Data Analysis Challenges and Strategies for Non-Targeted Screening of Foods Using UPLC/HR-MS and Food Databases**; Ann M. Knolhoff[1]; Christine M. Fisher[1]; *[1]FDA-CFSAN, College Park, MD*

MP 266 **Sensitive Multi-Mycotoxins Analysis with a Single Sample Preparation by LC-MS/MS**; Eishi Imoto[1]; Naoki Mochizuki[2]; Jun Watanabe[1]; *[1]Shimadzu corp., Kyoto, Japan; [2]Yokohama University of Pharmacy, Yokohama city, Japan*

MP 267 **Analysis of Pesticide Residues in Cannabis Regulated by California and Oregon State Using LC/MS/MS with Dual Electrospray and APCI Source**; Avinash Dalmia[1]; Erasmus Cudjoe[2]; Travis Ruthenberg[3]; Josh Ye[2]; Molly Murphy[3]; Feng Qin[2]; Dave Welkie[1]; *[1]Perkinelmer, Shelton, CT; [2]PerkinElmer, Woodbridge, ON, Canada; [3]SC Labs, Santa Ana, CA*

MP 268 **Analysis of β-Agonists by Ultra-High-Performance Liquid Chromatography-Quadrupole-Time-of-Flight Mass Spectrometry and the Study of Their Fragmentation Pathway**; Feng Zhang[1]; Tong Liu[1]; *[1]Institute of Food Safety, Chinese Academy of Inspection and Quarantine, Beijing, China*

MP 269 **Adduct Interference Monitoring Strategies in HRMS for Large Screen Food Safety Applications**; Matthew Standland[1]; Obiadada Ugochukwu[1]; Harrison Ansley[1]; Kevin Hsieh[1]; Walter Hammack[1]; Ghislain Gerard[1]; *[1]Fl. Dept. Ag. Chemical Residue Lab, Tallahassee, FL*

MP 270 **Novel Method for the Sensitive Quantification of Glyphosate, AMPA, Glufosinate and MPPA in Water Without Derivatization**; Aurore Jaffuel[1]; Alban Huteau[1]; *[1]Shimadzu France, Marne la Vallée, France*

MP 271 **Identification and Determination of Cyclopeptide Toxins in Amanita Subpallidorosea, a New Lethal Fungus from China**; Jianfeng Wu[1]; Jiahui Wei[1]; Jia Chen[1]; Bidong Wu[1]; Zhengmi He[2]; Ping Zhang[2]; Haijiao Li[3]; Chengye Sun[3]; Zuohogn Chen[2]; Jianwei Xie[1]; *[1]Academy of Military Medical Sciences, Beijing, China; [2]College of Life Science, Hunan Normal University, ChangSha, China; [3]Chinese Center for Disease Control and Prevention, Beijing, China*

MP 272 **Evaluation of High Throughput, No Methylene Chloride, Low Cost Sample Clean Up for POPs Analysis**; Rudolf Addink[1]; Tom Hall[1]; *[1]Toxic Report, Watertown, MA*

MP 273 **Simultaneous Determination of Five Illegal Dyes in Foods by LC-MS/MS**; Ho Soo Lim[1]; Ju Young Hwang[1]; EunA Choi[1]; GunYoung Lee[1]; MeeKyung Kim[1]; *[1]Korea Ministry of Food and Drug Safety, Cheongju, South Korea*

MP 274 **Analysis of Pesticide Residues in Fruits and Vegetables by Modified QuEChERS Combined with Liquid Chromatography-Tandem Mass Spectrometry**; Wen-Sin Wang[1]; Chung-Yu Chen[1]; Maw-Rong Lee[2]; *[1]National Chung Hsing University, Taichung, Taiwan; [2]National Chung-Hsing University, Taichung, Taiwan*

MP 275 **Rapid Screening Method for the Detection of Phenols in Fish Sauce Using Gas Chromatography-Mass Spectrometry**; Mantai Z. Mesmer; *US FDA, Cincinnati, OH*

MP 276 **Pesticide in Organic Foods? The Organic Carrots Case**; Marilda Chiarello[1]; Rafael Ortiz[2]; Wanderson Romão[3]; Sidnei Moura[1]; *[1]Caxias do Sul University, Caxias Do Sul, Brazil; [2]Rio Grande do Sul Technical and Scientifical Division, Brazilian Federal Police, Porto alegre, Brazil; [3]Federal University of Espirito Santo, Vitória, Brazil*

MP 277 **Determination of Additives and Metabolites in Wheat Flour by Modified QuPPe Coupled to Liquid Chromatography - Tandem Mass Spectrometry**; Yi-Ching Lo[1]; Chung-Yu Chen[1]; Maw-Rong Lee[2]; *[1]National Chung Hsing University, Taichung, Taiwan; [2]National Chung-Hsing University, Taichung, Taiwan*

MP 278 **Identification of Degradation Products of Herbicides in Soybean Oil After Frying Process by Using LLE-LC-MS/MS and HS-SPME-GC-MS**; Jia-Hao Wu[1]; Hsin-Ju Ke[1]; He-Hsuan Hsiao[1]; Maw-Rong Lee[2]; *[1]National Chung Hsing University, Taichung, Taiwan; [2]National Chung-Hsing University, Taichung, Taiwan*

MP 279 **Glyphosate and Aminomethylphosphonic Acid (AMPA) Analysis in Plants Using LC-MS/MS**; Evelyn H. Wang[1]; Jerry Byrne II[1]; Katie Pryor[1]; Christopher Gilles[1]; *[1]Shimadzu Scientific Instrument, Columbia, MD*

MP 280 **Fragmentation Pathway of Harmful Chemicals in Soft Ionization Mode and Its Application in Novel Analogue Screening**; Feng Zhang[1]; Tong Liu[2]; *[1]Institute of Food Safety, Chinese Academy of Inspection and Quarantine, Beijing, China; [2]Chinese Academy of Inspection and Quarantine, Beijing, China*

MP 281 **Cannabis Sativa Pesticides, Aflatoxins, and Potency by LC/MS/MS: One Extraction, One Analysis**; Tarun Anumol[1]; Agustin Pierri[2]; Jerry Zweigenbaum[1]; *[1]Agilent Technologies, Wilmington, DE; [2]Weck Laboratories, Industry, CA*

MP 282 **Stable Isotope Dilution Quantitation of Heterocycloc Amines in Meat Floss and Meat Jerky by QuEChERS Combined with LC-MS/MS**; Hsin-Chang Chen[1]; Yu-Hsuan Chen[1]; *[1]National Taiwan University, Taipei, Taiwan*

MP 283 **Evaluation of LDTD-MS/MS Technology for Quantification of Mycotoxin (DON and Zearelenone) in Animal Feed**; Katarzyna Krupczynska-Stopa[1]; Maciej

Stopa[1]; Serge Auger[2]; Jean Lacoursière[2]; Pierre Picard[2]; *[1]BioAnalytic, Gdansk, Poland; [2]Phytronix Technologies Inc., Québec, QC, Canada*

MP 284 **creening of Contaminants in Food and Natural Products by GC/Q-TOF with an Accurate Mass Pesticides and Environmental Pollutants Library**; Kai Chen[1]; Courtney Milner[1]; *[1]Agilent Technologies, Inc., Santa Clara, CA*

MP 285 **An APGC-MS MRM Method for the Quantitation of Common Glycols in Food and Beverage Packaging Migration Samples**; Vincent Pagnotti; *PPG Industries, Allison Park, PA*

MP 286 **Simultaneous Screening of 6 Different Antibiotic Families in Meat Using LDTD-MS/MS Quantitation at 9 Seconds per Sample**; Pierre Picard[1]; Jean Lacoursière[1]; Jonathan Rochon[2]; Serge Auger[1]; *[1]Phytronix Technologies, Inc., Quebec, QC, Canada; [2]Universite Laval, Quebec, QC, Canada*

MP 287 **Screening and Quantitation in Food Matrices Using Combined Swath + IDA Acquisition**; David Cox[1]; Jeffery Rivera[1]; Holly Lee[1]; Janna Anichina[1]; Jianru Stahl-Zeng[2]; Julia Jasak[2]; Vanaja Raguvaran[1]; *[1]SCIEX, Concord, ON, Canada; [2]SCIEX, Darmstadt, Germany*

MP 288 **Quantitative Evaluation of DART-QSight for Accurate and High Throughout Analysis of Organic Metallic Species and Pesticide Residues in Agriculture Products**; Xia Geng[1]; Yongming Xie[1]; Xiangdong Zhou[1]; Chengyuan Cai[1]; Feng Qin[2]; Charles C. Liu[3]; Jingcun Wu[2]; *[1]Perkinelmer Management (Shanghai) Co., Ltd., Shanghai, China; [2]PerkinElmer Inc., Woodbridge, ON, Canada; [3]ASPEC Technologies Limited, Beijing, China*

MP 289 **Multi-residue Pesticides Analysis Using Scheduled MRM on SCIEX Triple Quad™ 3500 in Mango and Onion**; Anoop Kumar; *Sciex India Pvt Ltd, Haryana, India*

MP 290 **A Rapid Screening Method of Mycotoxins in Grains by Liquid Chromatograph Tandem Mass Spectrometry**; Manami Kobayashi[1]; Eishi Imoto[2]; Jun Watanabe[2]; Satoshi Yamaki[3]; Junichi Masuda[1]; *[1]Shimadzu Corporation, Kanagawa, Japan; [2]Shimadzu Corporation, MS Business Unit, Kyoto, Japan; [3]Shimadzu Corporation, Beijing, China*

MP 291 **Determination of Heavy Metals in Beverages Using Inductively-Coupled-Plasma-Mass Spectrometry**; Sampada Khopkar[1]; Mangesh Pawar[2]; Amol Shinde[2]; Ajit Datar[2]; Jitendra Kelkar[2]; Pratap Rasam[2]; *[1]Shimadzu Analytical (India) PVT LTD, Mumbai, India; [2]Shimadzu Analytical (India) PVT LTD, Mumbai, India*

MP 292 **Multiclass Veterinary Drugs Analysis in Swine Muscle and Hen Eggs Using Ultivo Triple Quadrupole LC/MS System**; Dorothy Yang[1]; Zhiming Zhang[2]; *[1]Agilent Technologies, Santa Clara, CA; [2]Agilent Technologies, Shanghai, China*

MP 293 **Determination of Short and Medium Chained Chlorinated Paraffins in Salmon Samples Using GC Orbitrap-MS**; Kerstin Kratschmer[1]; Cristian Cojocariu[2]; Alexander Schachtele[1]; Paul Silcock[2]; Fausto Pigozzo[3]; Rainer Malisch[1]; *[1]European Union Reference Laboratory for Dioxins and PCBs in Feed and Food, Freiburg, Germany; [2]Thermo Fisher Scientific, Runcorn, UK; [3]Thermo Fisher Scientific, Rodano, Italy*

MP 294 **Ultra-Low Level Quantification of Pesticides in Baby Foods Using an Advanced Triple Quadrupole GC-MS/MS**; Tim Anderson[1]; Richard Law[2]; Aaron Lamb[2]; Cristian Cojocariu[3]; *[1]Thermo Fisher Scientific, Austin, TX; [2]Thermo Fisher Scientific, Runcorn, UK; [3]Thermo Fisher Scientific, Runcorn, UK*

MP 295 **Analysis of Multi-Residue Pesticides in Tea Using GC-MS/MS with Quick-DB: A Comparative Study Between Semi-Quantitative (Screening) and Quantitative Method**; Durvesh Sawant[1]; Prashant Dattatray Hase[1]; Sanket Anand Chiplunkar[1]; Nitish Suryavanshi[1]; Subodh Budakoti[2]; Dheeraj Handique[1]; Jitendra Kelkar[1]; Pratap Rasam[1]; Ajit Datar[1]; *[1]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India; [2]Shimadzu Analytical (India) Pvt. Ltd., Delhi, India*

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MP 296 **Direct Quality Control of Glycoengineered Erythropoietin Variants**; Tomislav Čaval[1]; Weihua Tian[2]; Zhang Yang[2]; Henrik Clausen[2]; Albert J.R. Heck[1]; *[1]Utrecht University, Utrecht, Netherlands; [2]University of Copenhagen, Copenhagen, Denmark*

MP 297 **Characterization of Intact Glycoproteome Subpopulations Obtained with Commonly Used Enrichment Methods**; Gary M Wilson[1]; Nicholas M Riley[1]; Alexander S. Hebert[2]; Michael S Westphall[2]; Joshua J Coon[2, 3, 4, 5]; *[1]UW-Madison Chemistry, Madison, WI; [2]Genome Center of Wisconsin, Madison, WI; [3]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [4]Morgridge Institute for Research, Madison, WI; [5]Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI*

MP 298 **In-Depth Site-Specific Analysis of Glycoproteome in Human Cerebrospinal Fluid (CSF) and Glycosylation Alterations in Alzheimer's Disease (AD)**; Zhengwei Chen[1]; Qing Yu[1]; Jillian Johnson[1]; Richard Shipman[2]; Xiaofang Zhong[1]; Junfeng Huang[1]; Sanjay Asthana[1]; Cynthia Carlsson[1]; Ozioma Okonkwo[1]; Lingjun Li[1]; *[1]University of Wisconsin-Madison, Madison, Wisconsin; [2]University of Wisconsin-Stout, Menomonie, WI*

MP 299 **Study on Glycosylation of Serum Protein Alpha-1-Antitrypsin**; Haidi Yin[1]; David M. Lubman[2]; Zhongping Yao[1]; *[1]The Hong Kong Polytechnic University, Hong Kong, China; [2]University of Michigan, Ann Arbor, MI*

MP 300 **LC-MS Glycan Analysis of Fusion Proteins Facilitated by Rapid Glycosylamine Labeling and Site-specific Profiling**; William Alley[1]; Matthew A Lauber[1]; Ying Qing Yu[1]; *[1]Waters Corporation, Milford, MA*

MP 301 **Development and Optimization of Analytical Methods for the Detection of O-GlcNAc-Modified Proteins**; Sarath B Jayasinghe[1]; Neil E Olszewski[1]; *[1]Department of Plant Biology, University of Minnesota, St. Paul, MN*

MP 302 **Glycoproteome Analysis Using Nanolc Coupled Ion-Mobility Mass Spectrometry**; Hiroyuki Katayama[1]; Chuan-Yih Yu[1]; Juan Chen[1]; Xiaoqian Liu[1]; Michela Capello[1]; Hong Wang[1]; Sam Hanash[1]; *[1]MD Anderson Cancer Center, Houston, TX*

MP 303 **Structural Characterization of HIV Env Glycoprotein**; Vera B. Ivleva[1]; Nicole A. Schneck[1]; Frank Arnold[1]; Jonathan W. Cooper[1]; Q. Paula Lei[1]; *[1]NIH/NIAID/VPPL, Gaithersburg, MD*

MP 304 **Impact of Fc N-Glycan Sialylation on IgG Structure**; Bhavana Shah[1]; Jason L. Richardson[2]; Zhongqi Zhang[3]; *[1]Amgen Inc., Thousand Oaks, CA; [2]Amgen Inc., Thousand Oaks, CA; [3]Amgen, Thousand Oaks, CA*

MP 305 **mOGP 1.0-Making O-glycoproteomics more Convenient and Meaningful**; Weiqian Cao[1]; Jiangming Huang[1]; Mengxi Wu[2]; Mingqi Liu[2]; Yang Zhang[2]; Pengyang Yang[2]; *[1]Fudan University, Shanghai, China; [2]Fudan Universiry, Shanghai, China*

MP 306 **Development of Glycoproteomic Workflows for the Site-Specific Characterization of Intact N- and O-Linked Glycopeptides**; Matthew Glover[1]; Raghothama Chaerkady[1]; Kristen Lekstrom[1]; Sonja Hess[1]; *[1]MedImmune, Gaithersburg, MD*

MP 307 **Retention Time Prediction for Glycopeptides in Complex Samplesfor Reversed Phase Chromatography**; Evelyn Ang[1]; Victor Spicer[2]; Hélène Perreault[1]; Oleg V. Krokhin[2]; *[1]University of Manitoba, Winnipeg, MB; [2]Manitoba Centre for Proteomics and Systems Biology, Winnipeg, MB*

MP 308 **Why Do I Need a Flu Shot Every Year? Quantitative Comparison of Glycosylation Similarity Across Influenza A Mutants**; Deborah Chang[1]; Joshua A. Klein[2];

Jacquelyn Turcinovic[3]; Kshitij Khatri[1]; Joseph Zaia[1,2]; *[1]Center for Biomedical Mass Spectrometry, Boston University School of Medicine, Boston, MA; [2]Bioinformatics Program, Boston University, Boston, MA; [3]Department of Biological Sciences, St. Edward's University, Austin, TX*

MP 309 **Middle-down Glycoproteomic Approach to Assess Biosimilarity of a Therapeutic Glycoprotein Bearing Multiple Glycosylation Sites**; Youngsuk Seo[1]; Hyun Joo An[1]; *[1]AGRS, Chungnam National University, Daejeon, South Korea*

MP 310 **Extreme Glycosylation Complexity: Characterization of the 2.5 Megadalton Aggrecan Proteoglycan**; Joshua A. Klein[1]; Le Meng[2]; Joseph Zaia[1]; *[1]Boston University, Boston, MA; [2]Boston University School of Medicine, Boston, MA*

MP 311 **Development of Universal Glycoproteomics Tools for the Discovery-Driven Large-Scale Analysis of Diverse Glycosylation Pathways**; Stefan Schulze[1]; Christian Fufezan[2]; Julia Krägenbring[3]; Anne Oltmanns[2]; Anjana Sundarrajan[1]; Michael Hippler[2]; Mecky Pohlschröder[1]; *[1]University of Pennsylvania, Department of Biology, Philadelphia, PA; [2]University of Münster, Institute of Plant Biology and Biotechnology, Münster, Germany; [3]University of Münster, Institute for Hygiene, Biomedical Mass Spectrometry, Münster, Germany*

MP 312 **A Mass Spectrometry Based Glycomics Platform for Analysis of Influenza Vaccines**; John F Cipollo[1]; Yanming An An[2]; Shuang Yang[3]; Sitara Chauhan[3]; Ewa Jankowska[3]; Lisa M Parsons[3]; *[1]Food and Drug Administration/ CBER, Silver Spring, MD; [2]Food and Drug Administration Center for Drug Evaluation, Silver Spring, MD; [3]Center for Biologics Evaluation and Research Food and Drug Administration, Silver Springs, MD*

MP 313 **Molecular Visualization of Plant N-Glycans Using MALDI-MS Imaging**; Dusan Velickovic[1]; Peggi M Angel[2]; Anand S Mehta[2]; Harmin Herrera[2]; Beverly J Agtuca[3]; Gary Stacey[3]; Richard R Drake[2]; Christopher R Anderton[1]; *[1]PNNL, Richland, WA; [2]MUSC Proteomics Center, Medical University of South Carolina, Charleston, SC; [3]University of Missouri, Columbia, MO*

MP 314 **Comparative Glycosylation Mapping of Recombinant and Plasma-Derived Human Factor VIII Reveals Key Biological Differences**; Cheng Ma[1]; Peng George Wang[1]; Weidong Xiao[2]; *[1]Georgia State University, Atlanta, GA; [2]Temple University, Philadelphia, PA*

MP 315 **Linkage Specific Glycosylation Analysis Related to Liver Disease Progression Using Ion Mobility**; Miloslav Sanda[1]; Lindsay Morrison[2]; Fred Glisson[3]; *[1]Georgetown University, Lombardi Cancer Center, Washington, DC; [2]Waters Corporation, Beverly, MA; [3]Waters Corporation, Milford, MA*

MP 316 **Glycopeptide Analyses of Apolipoprotein E from Cerebrospinal Fluid and Plasma Reveals Marked O-Glycosylation Differences in the Lipid-Binding Domain**; Sarah A. Flowers[1]; Oliver C. Grant[2]; Robert J. Woods[2]; G. William Rebeck[1]; *[1]Georgetown University, Washington, DC; [2]Complex Carbohydrate Research Center, University of Georgia, Athens, GA*

MP 317 **Ion Mobility Spectrometry-Mass Spectrometry Reveals the Effect of Glycosylation on the Thermal Stabilities of Proteins and Protein Complexes**; Shannon A. Raab[1]; Tarick J. El-Baba[1]; Daniel W. Woodall[1]; David E Clemmer[1]; *[1]Indiana University, Bloomington, IN*

MP 318 **Quantitative Site, Linkage and Structure Specific Fucosylation Changes in Liver Disease Progression**; Miloslav Sanda[1]; Petr Kozlik[2]; Radoslav Goldmnan[1]; *[1]Georgetown University, Lombardi Cancer Center, Washington, DC; [2]Faculty of Science, Charles University, Prague 2, Czech Republic*

MP 319 **Native Mass Spectrometry Validates In-Solution Single-Molecule Mass Measurements of Glycoproteins Interactions**; Fabian Soltermann; Gavin Young; Weston Struwe; Carol V. Robinson; *University of Oxford, Oxford, UK*

MP 320 **Characterization of Protein/PTM Changes by Chip Capillary Electrophoresis Mass Spectrometry**; Mark E. McComb[1]; Deborah Chang[1]; Deborah R Leon[1]; Christian F Heckendorf[1]; Joseph Zaia[1]; Catherine E. Costello[1]; *[1]Boston University School of Medicine, Boston, MA*

MP 321 **Characterizing Binding of the Glycoprotein CD16a with IgG1 using HDX-MS**; Nicole D. Wagner[1]; Liuqing Shi[1]; Yining Huang[2]; Tun Liu[3]; Michael R. De Felippis[2]; Michael L. Gross[1]; *[1]Washington University in St. Louis, Saint Louis, MO; [2]Eli Lilly & Company, Indianapolis, IN; [3]Janssen Research & Development, Spring House, PA*

MP 322 **High Throughput Cloud Computing System for Identification and Quantification of Site-Specific N- and O-glycoproteins with Mass Spectrometry**; Young-Mook Kang[1]; Gun Wook Park[1]; Hyun Kyoung Lee[1,2]; Ju Yeon Lee[1]; Jin Young Kim[1]; Jong Shin Yoo[1,2]; *[1]Korea Basic Science Institute, Cheongju, South Korea; [2]Chungnam National University, Daejeon, South Korea*

MP 323 **Identifying the *in vivo* Arginine-GlcNAcylation Targets of the NleB/SseK Family of Effectors**; Nichollas E Scott[1]; Joshua Newson[1]; Cristina Giogha[2]; Jaclyn Pearson[2]; Elizabeth Hartland[2]; *[1]University of Melbourne, Parkville, Australia; [2]Hudson Institute of Medical Research, Clayton, Australia*

MP 324 **Comprehensive Glycosylation Profiling of Monoclonal Antibodies at Four Levels using a LC/Q-TOF MS Instrument**; David L. Wong[1]; Oscar G Potter[1]; Jordy J. Hsiao[1]; Te-Wei Chu[1]; *[1]Agilent Technologies, Inc., Santa Clara, CA*

MP 325 **Site-specific Identification and Characterization of Protein Glycosylation by Mass Spectrometry**; Yong Zhang[1]; Xinyuan Zhao[1]; Wantao Ying[1]; Weijie Qin[1]; Xiaohong Qian[1]; *[1]Beijing Proteome Research Center, Beijing, China*

IMAGING MS: INSTRUMENTATION
326-340

MP 326 **Structure of Gangliosides Revealed Using the AP MALDI source and High-Resolution Mass Spectrometer**; Eugene Moskovets[1]; Shelley Jackson[2]; Luidovic Muller[2]; Vladimir Doroshenko[1]; Amina S. Woods[2]; *[1]MassTech Inc, Columbia, MD; [2]NIDA-IRP, NIH, Baltimore, MD*

MP 327 **An Imaging FT-ICR Platform Utilizing Gallium Ablation for Biomolecule Analysis**; Matthew R Brantley[1]; Ian G M Anthony[1]; Raul A Villacob[1]; Shihao Zhou[1]; Touradj Solouki[1]; *[1]Baylor University, Waco, TX*

MP 328 **Infrared Laser Ablation Mass Spectrometry with a Schwarzschild Reflective Objective**; Chao Dong[1]; Fabrizio Donnarumma[1]; Kelin Wang[1]; Carson W. Szot[1]; Kermit K. Murray[1]; *[1]Louisiana State University, Baton Rouge, LA*

MP 329 **Transmission Geometry Instrument Modifications and Laser Energy Deposition Characterization for High Spatial Resolution MALDI Imaging Mass Spectrometry**; Josiah C McMillen[1]; Boone M Prentice[1]; Eric C Spivey[1]; Andre Zavalin[1]; Richard M. Caprioli[1,2]; *[1]Vanderbilt University, Nashville, TN; [2]Vanderbilt Mass Spectrometry Research Center and Department of Biochemistry, Vanderbilt University School of Medicine, Nashville, TN*

MP 330 **Hybrid SIMS: A New SIMS Instrument for High Resolution Organic Imaging with Highest Mass-Resolving Power and MS/MS**; Alexander Pirkl[1]; Rudolf Moellers[1]; Henrik Arlinghaus[1]; David Scurr[2]; Nicola Starr[2]; Ewald Niehius[1]; *[1]IONTOF GmbH, Muenster, Germany; [2]The University of Nottingham, Nottingham, UK*

MP 331 **Spatially Resolved Capillary Electrophoresis Mass Spectrometry of Endogenous Biomolecules Directly from Tissue Sections**; Kyle Duncan[1]; Ingela Lanekoff[1];

[1]Department of Chemistry - BMC, Uppsala University, Uppsala, Sweden

MP 332 **Development of MULTUM-PALM; a Stigmatic Imaging Mass Spectrometer integrated with Super-resolution Microscope**; Jun Aoki[1]; Yukihiro Miyanaga[1]; Masahiro Ueda[1]; Michisato Toyoda[1]; [1]Osaka University, Toyonaka-Shi, Japan

MP 333 **A Novel Prototype Source on a oA-TOF Mass Spectrometer Combined with Ion Mobility Separation**; Mark Towers[1]; Paul Murray[1]; Nichole Lareau[2]; Sheba Jarvis[3]; Richard M. Caprioli[2]; Emmanuelle Claude[1]; [1]Waters Corporation, Wilmslow, UK; [2]Vanderbilt Mass Spectrometry Research Center and Department of Biochemistry, Vanderbilt University School of Medicine, Nashville, TN; [3]Surgery and Cancer, Imperial College London, London, UK

MP 334 **High-Resolution AP MALDI MS Imaging of Proteins and Metabolites on an Ion Funnel Orbitrap Mass Spectrometer**; Bernhard Spengler[1]; Mario Kompauer[1]; Max A. Müller[1]; Kerstin Strupat[2]; Sven Heiles[1]; [1]Justus Liebig University Giessen, Giessen, Germany; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany

MP 335 **Enhanced Ion Funnel Transmission Efficiency up to m/z 24,000 for MALDI FT-ICR Protein Imaging Mass Spectrometry**; Boone M Prentice[1]; Daniel Ryan[1]; Raf Van de Plas[2]; Jeffrey M. Spraggins[1]; Richard M. Caprioli[1]; [1]Vanderbilt University, Nashville, TN; [2]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands

MP 336 **Ambient Submicron Sampling of Biological Samples by Combining AFM with MS**; Jonathan Brauer; Anasys Instruments, Santa Barbara, CA

MP 337 **Simultaneous, High-Resolution Elemental and Molecular Chemical Imaging with Tandem Laser-Ablation Mass Spectrometry and Laser-Induced Breakdown Spectroscopy**; Jake Shelley[1]; Sunil P Badal[1]; Montwaun D Young[1]; Jessica R Hellinger[1]; [1]Rensselaer Polytechnic Institute, Troy, NY

MP 338 **Novel Interface for Combined Matrix-Assisted Laser Desorption Ionization at Elevated Pressure and Electrospray Ionization with Orbitrap Mass Spectrometry**; Mikhail Belov[1, 2]; Gordon A. Anderson[1, 3]; Shane R Ellis[4]; Ron M.A. Heeren[4]; Jens Soltwisch[5]; Klaus Dreisewerd[5]; Marialaura Dilillo[6]; Liam A. McDonnell[6]; Asaph Aharoni[7]; [1]Spectroglyph, LLC, Kennewick, WA; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [3]GAA Custom Engineering, LLC, Benton, WA; [4]M4i Maastricht Multimodal Molecular Imaging Institute, Maastricht, Netherlands; [5]Institute for Hygiene, University of Muenster, Muenster, Germany; [6]Fondazione Pisana per la Scienza - ONLUS, Pisa, Italy; [7]Weizmann Institute of Science, Rehovot, Israel

MP 339 **Protein Imaging Mass Spectrometry**; Jerome F Moore[1]; Ernest K Lewis2; Alexander Zinovev3; Yang Cui (崔) 4; 1Robot Nose, Lemont, IL; 2NASA Postdoctoral Program, Houston, TX; 3Argonne National Laboratory, Lemont, IL; 4Independent Consultant, San Jose, CA

MP 340 **Implementation of an Imaging Optical System for Miniaturized Time of Flight Mass Spectrometers**; Linxia Song[1]; Theresa Evans-Nguyen[1]; [1]Department of Chemistry, University of South Florida, Tampa, FL

IMAGING MS: SAMPLE PREPARATION
341-350

MP 341 **A New Imaging Mass Spectrometry Technique for Visualizing Small Molecules in Co-Cultures of Mammalian Cells and *ex vivo* Tissues**; Katherine Zink[1]; Matthew Dean[1]; Joanna Burdette[1]; Laura Sanchez[1]; [1]University of Illinois at Chicago, Chicago, IL

MP 342 **Increasing Ionization and Desorption Efficiency of Neutral Lipids from Thin Tissue Sections for MALDI IMS**; Martin Dufresne[1]; Richard M. Caprioli[1]; [1]Vanderbilt University, Nashville, TN

MP 343 **Improved Sample Preparation for Comparative MALDI-MS Imaging of Neuropeptides in the Crustacean Brain under Hypoxia and Hypercapnia Stress**; Amanda Buchberger[1]; Nhu Vu[1]; Lingjun Li[1]; [1]University of Wisconsin-Madison, Madison, WI

MP 344 **Lipidomics of the Drosophila Malpighian Tubule by Imaging Mass Spectrometry**; Ethan Yang[1]; Pierre Chaurand[1]; Chiara Gamberi[1, 2]; [1]Université de Montréal, Montréal, QC, Canada; [2]Concordia University, Montreal, Qc

MP 345 **A Nanoparticle Co-Matrix for Matrix-Assisted Ionization of Tissue**; Bijay Banstola[1]; Fabrizio Donnarumma[1]; Kermit K. Murray[1]; [1]Louisiana State University, Baton Rouge, LA

MP 346 **Probing Subcellular Chemical Heterogeneity with Speckle MALDI-MS**; Stanislav Rubakhin[1]; Jonathan V Sweedler[1, 2]; [1]Beckman Institute University of Illinois at Urbana-Champaign, Urbana, IL; [2]Department of Chemistry University of Illinois at Urbana-Champaign, Urbana, IL

MP 347 **Microscopic MALDI- Imaging Mass Spectrometry Inside Horse Hairs to Detect Drug Administration History**; Shuichi Shimma[1]; Masaru Sese[2]; [1]Osaka Univerisity, Suita, Osaka, Japan; [2]Equine Racing Co., Ltd, 479-2, Mukawa-cho Yonehara, Yufutsu-gun, Japan

MP 348 **Radiative-Heating Thermal Decomposition/Digestion for Single-Step On-Tissue Digestion of Proteins for Imaging -MALDI-MS**; Andrew K. Goodenough[1]; Franco Basile[1]; [1]University of Wyoming, Laramie, WY

MP 349 **Metabolomic tracing of immune cells on whole mount adult mouse section with Imaging Mass Microscope**; Yudai Tsuji[1]; Takushi Yamamoto[2]; Hideshi Fujiwake[2]; Nobuto Kakuda[1]; Tomoyuki Nakamura[3]; Masaya Ikegawa[1]; [1]Doshisha university, Kyotanabe City, Japan; [2]Shimadzu Corporation, Kyoto, Japan; [3]Kansai Medical University, Hirakata, Japan

MP 350 **The Detection of Fentanyl & Analogues in Oral Fluid Samples by LC-MS/MS**; Lisa Wanders[1]; Jill Yeakel[2]; Stevi Hooper[2]; [1]Thomson Instrument Co, Oceanside, CA; [2]Lehigh Valley Toxicology, Bethlehem, PA

INFORMATICS: GENERAL, SRM, AND DIA
351-362

MP 351 **A Complex, MS1-MS2 Linked, Fully Annotated Profile Proteomics Benchmark Dataset for Quantitative Evaluation of Mass Spectrometry Data Processing Algorithms**; Amber Yascavage[1]; Rob Smith[1]; [1]University of Montana, Missoula, MT

MP 352 **Rapid Assessment of Contaminants and Interferences in Mass Spectrometry Data Using Skyline**; Matthew Rardin; Amgen, South San Francisco, CA

MP 353 **Extraction Of Maximum Information From DIA(SWATH-MS) In A Spectral Library Free Manner**; Jamie Sherman[1]; Adam Lau[1]; Stephen A Tate[1]; [1]SCIEX, Concord, ON, Canada

MP 354 **Scanning SWATH Acquisition Method for Improved Compound Screening**; David Cox[1]; Gordana Ivosev[1]; Nic Bloomfield[1]; Yves J.C. LeBlanc[1]; [1]SCIEX, Concord, ON, Canada

MP 355 **RawBeans: a Tool for Identification-Independent Quality Control of Raw Mass Spectrometric Data**; David Morgenstern[1]; Rotem Barzilay[1]; Yishai Levin[1]; [1]Weizmann Institute, Rehovot, Israel

MP 356 **ProteomicsDB: A Source for High-Quality Spectral Libraries and an Auxiliary Tool for the Development of Targeted Assays**; Tobias Schmidt[1]; Siegfried Gessulat[1, 2]; Patroklos Samaras[1]; Daniel P Zolg[1]; Martin Frejno[1]; Karsten Schnatbaum[3]; Johannes Zerweck[3]; Tobias Knaute[3]; Ulf Reimer[3]; Hans-Christian Ehrlich[2]; Stephan Aiche[2]; Pedro Navarro[4]; Bernard Delanghe[4]; Andreas Huhmer[5]; Maximilian

Barnert[6]; Harald Kienegger[6]; Helmut Krcmar[6]; Bernhard Kuster[1, 7, 8]; Mathias Wilhelm[1]; *[1]Chair of Proteomics and Bioanalytics, Technical University of Munich (TUM), Freising, Germany; [2]SAP SE, Potsdam, Germany; [3]JPT Peptide Technologies GmbH, Berlin, Germany; [4]Thermo Fisher Scientific, Bremen, Germany; [5]Thermo Fisher Scientific, San Jose, CA; [6]Chair for Information Systems, Technical University of Munich (TUM), Munich, Germany; [7]Center for Integrated Protein Science (CIPSM), Munich, Germany; [8]Bavarian Center for Biomolecular Mass Spectrometry, Freising, Germany*

MP 357 **Avant-garde DIA: Data-Driven DIA Signal-Refinement Tool That Reaches the Same Levels of Selectivity, Accuracy and Reproducibility as Manual Validation**; Alvaro Sebastian Vaca Jacome[1]; Jarrett D Egertson[2]; Karsten Krug[1]; Ryan N Peckner[1]; Adam Officer[1]; Katherine C DeRuff[1]; Michael J MacCoss[2]; Steven A Carr[1]; Jacob D Jaffe[1]; *[1]Broad Institute of MIT and Harvard, Cambridge; [2]University of Washington Genome Sciences, Seattle, WA*

MP 358 **Detecting Genetic Variation in Amyloid Fibrils Using DIA**; Brian C. Searle[1, 2]; Han-Yin Yang[2]; Kelly D. Smith[3]; Andrew N. Hoofnagle[4]; Michael J. MacCoss[2]; *[1]Proteome Software Inc., Portland, OR; [2]University of Washington Genome Sciences, Seattle, WA; [3]University of Washington Pathology, Seattle, WA; [4]University of Washington Clinical Chemistry, Seattle, WA*

MP 359 **BUPID-PALM: Glycopeptide Identification by All-ion Fragmentation(AIF) Ion Mobility MS/MS**; Christian Heckendorf[1]; Joshua A. Klein[1]; James A. Hill[1]; Catherine E. Costello[1]; Mark E. McComb[1]; *[1]Boston University School of Medicine, Boston, MA*

MP 360 **A MS/MS Spectral Library Dedicated to Structure Elucidation of Natural Products**; Sangwon Lee[1, 2]; Ki Beom Shin[3]; Kyoung Tai No[2, 3]; *[1]Yonsei University, Seoul, South Korea; [2]Bioinformatics and molecular design research center, seodaemun-gu, South Korea; [3]Yonsei university, Seoul, South Korea*

MP 361 **LibMatic: DIA- Umpire Based Pipeline for Generation of Spectral Libraries for Targeted Analysis of DIA Data**; Guo Ci Teo[1]; Dattatreya Mellacheruvu[1]; Felipe da Veiga Leprevost[1]; Venkatesha Basrur[1]; Alexey I. Nesvizhskii[1]; *[1]University of Michigan, Ann Arbor, MI*

MP 362 **Software Development in Support of Affinity-Selection LCMS High-Throughput Screening**; Mark F Bean[1]; Adrian Dunn[2]; Neil R Carlson[3]; *[1]GlaxoSmithKline, Collegeville, PA; [2]New Chemical Entity (NCE) Molecular Discovery, GlaxoSmithKline, Stevenage, UK; [3]New Chemical Entity (NCE) Molecular Discovery, GlaxoSmithKline, Cambrdge, MA*

INSTRUMENTATION: GENERAL
363-388

MP 363 **Detection of Limited Protein Digests from Neuron Cultures by Reversed-Phase Fractionation with Capillary Electrophoresis nanoESI MS**; Sam Choi[1]; Camille Lombard-Banek[1]; Pablo Munoz-LLancao[2]; M. Chiara Manzini[2]; Peter Nemes[1]; *[1]University of Maryland, College Park, MD; [2]The George Washington University, Washington, DC*

MP 364 **Field Optimization of Toroidal Ion Trap Mass Analyzers using Toroidal Multipoles**; Jessica Higgs[1]; Karl Warnick[1]; Daniel Austin[1]; *[1]Brigham Young University, Provo, UT*

MP 365 **Efficient Ion Fragmentation in Structures for Lossless Ion Manipulations**; Ian K. Webb[1]; Sandilya Garimella[1]; Isaac K. Attah[1]; Aneesh Prabhakaran[1]; ERIN S. BAKER[1]; Yehia M. Ibrahim[1]; Richard D. Smith[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

MP 366 **Orbitrap Mass Spectrometry at Resolving Power 2,000,000**; Eduard Denisov[1]; Eugen Damoc[1]; Alexander Makarov[1]; *[1]Thermo Fisher Scientific, Bremen, Germany*

MP 367 **High Resolution Time-of-Flight Mass Spectrometry as Versatile and Investigative Tool for the Hyphenation with Different Sample Introduction and Ionization Techniques**; Uwe Kaefer[1]; Maximilian Jennerwein[2]; Mohammad Reza Saraji-Bozorgzad[3]; Jürgen Wendt[4]; Thomas Wilharm[2]; Thomas Gröger[1]; Ralf Zimmermann[1, 5]; *[1]Helmholtz-Zentrum München (CMA), Munich, Germany; [2]Analytik Service GmbH (ASG), Neusäss, Germany; [3]Photonion GmbH, Schwerin, Germany; [4]LECO Germany, Berlin, Germany; [5]University of Rostock, Rostock, Germany*

MP 368 **DRy Ion Localization and Locomotion (DRILL) MS Interface for Sensitivity Enhancement via Desolvation and Hydrodynamic Focusing**; Jung Y. Lee[1]; Peter A. Kottke[1]; Crystal L. Gunther[2]; David C Muddiman[2]; Alex P. Jonke[1]; Matthew P. Torres[1]; Andrei G. Fedorov[1]; *[1]Georgia Institute of Technology, Atlanta, GA; [2]North Carolina State University, Raleigh, NC*

MP 369 **Development of Ion Carpet-Surface Induced Dissociation (SID) Devices for Simplified Tuning**; Alyssa Q. Stiving[1]; Joshua D. Gilbert[1]; Vicki H. Wysocki[1]; *[1]The Ohio State University, Columbus, OH*

MP 370 **A Rectilinear Pulsed-Extraction Ion Trap with Auxiliary Axial DC Trapping Electrodes**; Hamish Stewart[1]; Christian Hock[1]; Anastassios Giannakopulos[1]; Dmitry Grinfeld[1]; Richard Heming[1, 2]; Alexander Makarov[1]; *[1]Thermo Fisher Scientific, Bremen, Germany; [2]University of Münster, Münster, Germany*

MP 371 **A Novel Cell Culture Media Analysis Platform for Culture Process Development**; Takashi Suzuki[1]; Kohei Yamamoto[1]; Tomonori Nozawa[1]; Tatsuya Nishio[1]; Kenichi Toyoda[1]; Yasuhiro Mito[1]; Hajime Bungo[1]; Masatoshi Takahashi[1]; *[1]Shimadzu corp., Kyoto, Japan*

MP 372 **Design and Performance of a Novel FAIMS System Mounted on High Conductance Sampling Mass Spectrometers**; Michael Belford[1]; Satendra Prasad[1]; Susan E. Abbatiello[2]; Romain Huguet[3]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Cambridge, MA; [3]ThermoFisher, San Jose, CA*

MP 373 **Simulation Study of Ion Stability of In-Situ Generated Ions in a 3D Ion Trap Under Different Gas Load Conditions**; Alexander Laue[1]; Michel Aliman[1]; Hin Yiu Chung[1]; Valerie Derpmann[1]; Ruediger Reuter[1]; *[1]Carl Zeiss SMT GmbH, Oberkochen, Germany*

MP 374 **Custom Mass Spectrometry Instrumentation: Best Practices**; Matthew R Brantley[1]; Shihao Zhou[1]; Ian G M Anthony[1]; Raul A Villacob[1]; Touradj Solouki[1]; *[1]Baylor University, Waco, TX*

MP 375 **A Segmented PCB Octapole Ion Trap Coupled to an oTOF Platform for Two-Step Laser Ionization and Photo-Dissociation Mass Spectrometry**; Alexander Lekkas[1]; Diamantis Kounadis[1]; Andreas Bozatzidis[1]; Ioannis Orfanopoulos[1]; Dimitris Papanastasiou[1]; Marin Vojkovic[2]; Yvain Carpentier[2]; Cristian Focsa[2]; Dumitru Duca[2]; *[1]Fasmatech, Athens, Greece; [2]Laboratory of Physics of Lasers, Atoms and Molecules, University of Lille, Lille, France*

MP 376 **Evaluation of kinetic energy distributions in atmospheric pressure ionization mass spectrometers (API-MS)**; Marco Thinius[1]; Nils Rutenbach[1]; Walter Wissdorf[1]; Hendrik Kersten[1]; Thorsten Benter[1]; *[1]University of Wuppertal, Wuppertal, Germany*

MP 377 **Numerical Simulation of Flow Field and Ion Transport in the Fore-End of the First Vacuum Region of a MS**; Wei Wang[1]; Steve Bajic[1]; Benzi John[2]; David R. Emerson[2]; *[1]Waters Corporation, Wilmslow, UK; [2]STFC Daresbury Laboratory, Warrington, UK*

MP 378 **Monitoring in Real Time the Products of Plasma Chemistry in Air and on Surfaces**; Joel Lemaire[1]; Michel Héninger[1]; Essyllt Louarn[1]; Sebastien Thomas[1, 2]; Helene Mestdagh[1]; Gérard Bauville[2]; Nicole Blin Simiand[2]; Blandine

Bournonville[2]; Michel Fleury[2]; Stephane Pasquiers[2]; Joao Santos Sousa[2]; Elsa Bauchard[3]; Julien Leprovost[3]; *[1]LCP CNRS - Université Paris Sud, Orsay, France; [2]LPGP CNRS - Université Paris Sud, Orsay, France; [3]AlyXan, Juvisy sur Orge, France*

MP 379 **A novel PTR-ToF Reaction Cell Superposing DC and RF fields**; Luca Cappellin[1]; Felipe Lopez[1]; Manuel Hutterli[1]; Jordan E. Krechmer[2]; Sonja Klee[1]; Benoit Plet[1]; *[1]Tofwerk AG, Thun, Switzerland; [2]Aerodyne Research Inc., Billerica, MA*

MP 380 **Study of Ion Confinement, Transport and Heating Effects in Traveling Wave IMS Devices**; Sandilya Garimella[1]; Yehia M. Ibrahim[1]; Roza Wojcik[1]; Ian K Webb[1]; Richard D. Smith[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

MP 381 **Negative Electron Transfer Dissociation on an Orbitrap Fusion Lumos**; Nicholas M Riley[1, 2]; Christopher Mullen[3]; Michael S Westphall[1, 2]; John E. P. Syka[3]; Joshua J Coon[1, 2, 4]; *[1]University of Wisconsin-Madison, Madison, WI; [2]Genome Center of Wisconsin, Madison, WI; [3]ThermoFisher, San Jose, CA; [4]Morgridge Institute for Research, Madison, WI*

MP 382 **Simulation of Ion Trajectories in an Electrostatic Bessel-Box Type Energy Filter**; Hendrik Kersten[1]; Chris Heintz[1]; Walter Wissdorf[1]; Thorsten Benter[1]; *[1]University of Wuppertal, Wuppertal, Germany*

MP 383 **Optimization of MALDI-TOF Instrumental Parameters by Solution of Polynomial Functions and Calculation Their Maxima**; Roman Brukh; *Rutgers University, Newark, NJ*

MP 384 **A Custom NanoFlow HPLC Ion Source for An Agilent 6530 QTOF Mass Spectrometer**; Vincent Chen[1]; Nguyen Phuc Nguyen[1]; *[1]Brandon University, Brandon, MB*

MP 385 **Monitoring Synthetic Reactions Using an (inert) Atmospheric Solids Analysis Probe-Mass Spectrometry (iASAP-MS)**; Jennifer Sanderson[1]; Todd Colin[1]; *[1]Advion Inc., Ithaca, NY*

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MP 391 **Integration of Multiple Capabilities in Structures for Lossless Ion Manipulations for Achieving Ultra-High-Resolution Ion Mobility - MS with Complex Samples**; Liulin Deng[1]; Sandilya Garimella[2]; IAN K. WEBB[2]; Ahmed M. Hamid[1]; Spencer A. Prost[2]; Randolph V. Norheim[2]; Yehia M. Ibrahim[2]; Richard D. Smith[2]; *[1]MOBILion Systems Inc., Exton, PA; [2]Pacific Northwest National Laboratory, Richland, WA*

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MP 397 **Development of a High Performance, Modular Ion Mobility Spectrometer using Printed Circuit Boards**; Tobias Reinecke[1]; Brian H Clowers[1]; *[1]Washington State University, Pullman, WA*

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MP 399 **Increased Performance Portable Periodic Focusing Differential Mobility Analyzer (PFDMA)**; Kent Gillig[1]; Guan-Bo Liao[1]; Chung-Hsuan Chen[1]; *[1]Academia Sinica, Taipei, Taiwan*

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MP 401 **Interpreting the Global Shape of Ions by Geometric Analysis Using Ion Mobility-Mass Spectrometry and Data Fitting**; Jean R. N. Haler[1]; Johann Far[1]; Victor R. de la Rosa[2]; Richard Hoogenboom[2]; Eric Béchet[3]; Edwin De Pauw[1]; *[1]Mass Spectrometry Laboratory, University of Liège, Liège, Belgium; [2]Supramolecular Chemistry Group, Ghent University, Ghent, Belgium; [3]Aerospace & Mechanical Engineering Department, Computer-aided Geometric Design, University of Liege, Liege, Belgium*

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MP 443 **Side Effect-Free Protein Sample Preparation for Peptide Mapping Analysis**; Sergei Saveliev[1]; Lyndsey Jager[1]; Chris Hosfield[1]; Mike Rosenblatt[1]; Marjeta Urh[1]; *[1]Promega Corporation, Madison, WI*

MP 444 **Improved Ist Workflows for the Streamlined Analysis of Tissues and High-Throughput Preparation of Samples Using Isobaric Labeling**; Fabian Hosp[1]; Garwin Pichler[1]; Nils Kulak[1]; *[1]PreOmics GmbH, Planegg/Martinsried, Germany*

MP 445 **Evaluation of Matrix Component Removal Using a Novel Flow-Through Scavenging Plate for Drugs of Abuse Testing in Urine**; Rhys Jones[1]; Lee Williams[1]; Helen Lodder[1]; Adam Senior[1]; Geoff Davies[1]; Katie-Jo Teehan[1]; Alan Edgington[1]; Steve Jordan[1]; Claire Desbrow[1]; Paul Roberts[1]; Stephanie Marin[2]; Dan Menasco[2]; Candice Summitt[2]; Elena Gairloch[2]; *[1]Biotage GB Limited, Cardiff, UK; [2]Biotage LLC, Charlotte, NC*

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MP 448 **Gold-Polypyrrole Nanocomposite Sorbent Material for Solid-Phase Extraction, Quantification and Selective Determination of Microcystins in Water**; Amila M Devasurendra[1]; Dilrukshika S W Palagama[1]; Ahmad Rohanifar[1]; Jared L Anderson[2]; Dragan Isailovic[1]; Jon R Kirchhoff[1]; *[1]The University of Toledo, Toledo, OH; [2]Iowa State University, Ames, IA*

MP 449 **Evaluation of Endoproteinase Lys-C/Trypsin Sequential Digestion Used in Proteomics Sample Preparation**; Minjia Tan[1]; Linhui Zhai[1]; *[1]Shanghai Institute of Materia Medica, Shanghai, China*

MP 450 **Adaptation of Proteomic Sample Preparation to Use Positive Pressure in Place of Centrifugation or Vacuum**; Yang Liu[1]; Richard Lam[2]; John Laycock[2]; Nathan A Yates[3]; *[1]University of Pittsburgh, Pittsburgh, PA; [2]Tecan, Baldwin Park, CA; [3]University of Pittsburgh School of Medicine, Pittsburgh, PA*

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MP 452 **Optimization of Sample Preparation for LC-MS/MS Based Cellular-Proteomics Application**; A D A Shahinuzzaman[1]; Abu Hena M Kamal[1]; Saiful M. Chowdhury[2]; *[1]University of Texas At Arlington, Arlington, TX; [2]University of Texas Arlington, Arlington, TX*

MP 453 **Liquid Chromatography and Tandem Mass Spectrometry for Quantitation of Unstable Arginine and Ornithine in the Mouse Liver, Plasma and Tumor**; Xinfa Fu[1]; Hongmei Wang[1]; Cheng Chen[1]; Sitan Xie[1]; Yi Tao[1]; Xin Zhang[1]; *[1]Department of DMPK/Non-GLP Bioanalytical Service, WuXi AppTec Co., Shanghai, China*

MP 454 **An Optimized Method for Quick TMT Labeled Sample Preparation**; David W Avila[1, 2]; Peter Jakob[1, 2]; Manuel Tzouros[1, 2]; *[1]Roche Pharma Research and Early Development, Roche Innovation Center Basel, Hoffmann-La Roche Ltd, Grenzacherstrasse 124, 4070, Basel,*

Switzerland; [2]Pharmaceutical Sciences, Basel, Switzerland

MP 455 **Completely Automated Hydrolysis, Extraction and Analysis of Opiates in Urine using a New Robotic Autosampler and LC/MS/MS Platform**; Fred Foster[1]; John R. Stuff[1]; Jacqueline A. Whitecavage[1]; *[1]Gerstel, Inc., Linthicum, MD*

MP 456 **Streamlined Drug-to-Antibody Ratio Determination for Intact and Deglycosylated Antibody-Drug-Conjugates Using Automated Sample Preparation and an LC/Q-TOF Designed for Biomolecule Analysis**; Jerry Han[1]; Steve Murphy[1]; *[1]Agilent Technologies, Inc., Santa Clara, CA*

MP 457 **A Fully Automated and Modular Multi-Dimensional HPLC/MS System for Expedited Characterization of Monoclonal Antibodies**; Tobias Graf[1]; Christoph Gstöttner[2, 3]; Katrin Heinrich[1]; Denis Klemm[3]; Ingrid Schmid[1]; Michael Leiss[1]; Robert Kopf[3]; *[1]Roche Diagnostics GmbH, Penzberg, Germany; [2]Center for Proteomics and Metabolomics, Leiden University Medical Center, Leiden, Netherlands; [3]Pharma Technical Development Analytics, F. Hoffmann-La Roche AG, Basel, Switzerland*

MP 458 **Towards Establishing Current Best Practices for Peptide-Level Analysis of Biotherapeutics: a Synthesis of Proteomic and Biopharma Methodologies**; Jon M Reed[1]; Ye Gu[1]; Kristina Gueneva-Boucheva[1]; Yining Huang[1]; Paul Mawson[1]; Lee Frego[1]; *[1]Boehringer Ingelheim, Ridgefield, CT*

MP 459 **Complete Integration of a Fully Automated Flash Hydrolysis Protocol of Glucuronides in Urine with LC-MS/MS Quantification**; Joshua F. Emory[1]; Brian Feild[2]; Yves-Vincent Duperron[3]; Camila Berner[3]; *[1]Shimadzu Scientific Instruments, Inc, Columbia, MD; [2]Shimadzu Scientific Instruments, Inc, Columbia, MD; [3]Kura Biotec, Puerto Varas, Chile*

MP 460 **Protein In-Gel Digestion Using Pressure Cycling Technology for identification by LCMSMS**; Tatiana N. Boronina[1]; Lauren Devine[1]; Robert N. Cole[1]; *[1]Johns Hopkins School of Medicine, Baltimore, MD*

MP 461 **Evaluation of Sample Preparation Options for the Simultaneous Extraction of Angiotensin and Aldosterone Prior to LC-MS/MS Analysis**; Katie-Jo Teehan[1]; Alan Edgington[1]; Lee Williams[1]; Adam Senior[1]; Rhys Jones[1]; Helen Lodder[1]; Geoff Davies[1]; Steve Jordan[1]; Claire Desbrow[1]; Paul Roberts[1]; Stephanie Marin[2]; Dan Menasco[2]; Candice Summitt[2]; Elena Gairloch[2]; *[1]Biotage GB Limited, Cardiff, UK; [2]Biotage LLC, Charlotte, NC*

MP 462 **Lossless Reproducible Sample Preparation for Simultaneous Metabolomics and Proteomics with Universal S-Trap Sample Processing**; John P. Wilson[1]; Keith D. Rivera[2]; Alexandre Zougman[3]; Darry J. Pappin[2]; *[1]Cold Spring Harbor Laboratory, Cold Spring Harbor, NY; [2]Cold Spring Harbor laboratory, Cold Spring Harbor, NY; [3]University of Leeds, Leeds, UK*

MP 463 **SPME Surface-Based Open-Port Sampling Interface for LC-MS/MS Analysis**; Craig Aurand[1]; John Janiszewski[2]; Brendon Kapinos[3]; Olga Shimelis[1]; Dave Bell[1]; Vassilios Bletsos[4]; Scott Frederick[4]; Ryan Horgan[4]; Gary J. Van Berkel[5]; Wayne Lootsma[6]; *[1]Millipore Sigma, Bellefonte, PA; [2]Pfizer Inc., Groton, CT; [3]Pfizer Worldwide Research, Groton, CT; [4]DeTech, Palmer, MA; [5]Oak Ridge National Laboratory, Oak Ridge, TN; [6]Sound Analytics, Niantic, CT*

MP 464 **Quantitative UPLC-MSE Analysis of Disulfide Bonds and Free Sulfhydryls in Monoclonal Antibodies Using IgdE Protease Assisted Digestion**; Jeroen de Keijzer[1]; Peter van Maurik[1]; Anja Boumeester[1]; Emile van Corven[1]; Gideon Oudgenoeg[1]; *[1]Bioceros, Utrecht, Netherlands*

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MP 466 **Qualitative and Quantitative Analysis of Unsaturated Lipids by Epoxidation and Tandem Mass Spectrometry**; Xu Zhao[1]; Wenbo Cao[2]; Yaoyao Zhao[1]; Sichun Zhang[1]; Zheng Ouyang[2]; Xinrong Zhang[1]; Xiaoxiao Ma[2]; *[1]Department of Chemistry, Tsinghua University, Beijing, China; [2]State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instrument, Tsinghua University, Beijing, China*

MP 467 **Identification and Structural Characterization of Glycosphingolipids Extracted from an Ovarian Cancer Cell Line UsingMALDI- and ESI-MS/MS**; Krishani K. Rajanayake[1]; William R. Taylor[1]; Deborah N. Chadee[1]; Dragan Isailovic[1]; *[1]The University of Toledo, Toledo, OH*

MP 468 **Coupling Headgroup and C=C Specific Solution Modifications with Gas-Phase Ion-Ion Reactions for Sensitive Phospholipid Identification and Characterization**; Elissia Franklin[1]; Samuel W. J. Shields[2]; Jeffrey C. Smith[2]; Yu Xia[1, 3]; Scott A McLuckey[1]; *[1]Purdue University, West Lafayette, IN; [2]Carleton University, Ottawa, ON, Canada; [3]Tsinghua University, Beijing, China*

MP 469 **Proposal for a Common Nomenclature for Fragment Ions in Mass Spectra of Lipids**; Josch K Pauling[1]; Martin Hermansson[1]; Peter Husen[1]; Jürgen Hartler[2]; Sandra F. Gallego[1]; Bing Peng[3]; Robert Ahrends[3]; Christer Ejsing[1, 4]; *[1]University of Southern Denmark, Odense, Denmark; [2]Graz University of Technology, Graz, Austria; [3]ISAS, Dortmund, Germany; [4]EMBL, Heidelberg, Heidelberg, Germany*

MP 470 **LC-MSn Method for Comprehensive Analysis of Ox-Lipidomes: Optimization of MS Parameter in Order to Maximize Lipids Detection and Characterization.**; Angela Criscuolo[1, 2, 3]; Martin Zeller[2]; Ken Cook[4]; Maria Fedorova[1, 3]; *[1]Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, Universität Leipzig, Leipzig, Germany; [2]Thermo Fisher Scientific, Bremen, Germany; [3]Center for Biotechnology and Biomedicine, Universität Leipzig, Leipzig, Germany; [4]Thermo Fisher Scientific, Hemel Hempstead, UK*

MP 471 **Structural Characterization of Phosphatidylcholines at the Level of sn-Position and C=C Location**; Xue Zhao[1]; Xinwei Liu[2]; Wenbo Cao[2]; Wenpeng Zhang[3]; Xiaobo Xie[1]; Zheng Ouyang[2, 3]; Yu Xia[4, 5, 6]; *[1]Department of Chemistry,Tsinghua University, Beijing, China; [2]Department of Precision Instrument, Tsinghua University, Beijing, China; [3]Weldon School of Biomedical Engineering, Purdue University, West Lafayette, IN; [4]Department of Chemistry , Tsinghua University, Beijing, China; [5]Department of Chemistry,Purdue University, West Lafayette, IN; [6]Department of Chemistry,Tsinghua University, Beijing, Beijing, China, Beijing, China*

MP 472 **Identification of Conjugated Linoleic Acid Isomers via Coupling the Paternò-Büchi Reaction with Tandem Mass Spectrometry**; Xiaobo Xie[1]; Yu Xia[1]; *[1]Department of Chemistry, Tsinghua University, Beijing, China*

MP 473 **Characterization of Fragmentation Pathways of Lipids During Prompt Ionization in MALDI-Imaging Experiments**; Roberto Fernandez[1]; Jone Garate[1]; Sergio Lage[1]; Lucia Martin[1]; Maria Dolores Boyano[1]; Jose Andres Fernandez[1]; *[1]University of Basque Country, Universidad del País Vasco (UPV/EHU), Leioa, Spain*

MP 474 **Lipid Aggregations Studied Using Electrospray Ionization and Ion Mobility**; Peter S. Backlund[1]; Paul S. Blank[1]; Jens R. Coorssen[2]; Stephanie M. Cologna[3]; Christian Klein[4]; Alfred L. Yergey[1]; *[1]National Institutes of Health, Bethesda, MD; [2]Brock University, St. Catherines,*

ON, Canada; [3]University of Illinois at Chicago, Chicago, IL; [4]Agilent Technologies, Santa Clara, CA

MP 475 **Structural Analysis of Plasmalogens by Coupling the Paternò–Büchi Reactions with Tandem Mass Spectrometry**; Qiaohong Lin[1]; Yu Xia[2]; *[1]Tsinghua University, Beijing, China; [2]Tsinghua University, Beijing, China*

MP 476 **Structural Characterization of N-Acyl Phosphatidylethanolamines (NAPEs) via 193 nm Ultraviolet Photodissociation (UVPD)**; Molly S. Blevins[1]; Emily Grantham[1]; R. Adron Harris[1]; Bryan W. Davies[1]; Jennifer S. Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX*

MP 477 **Structural Characterization of Complex Lipids by Ozone-Induced Dissociation and Ultraviolet Photodissociation on High-Resolution Mass Spectrometers**; Angela Criscuolo[1, 2, 3]; David L. Marshall[4]; Martin Zeller[2]; Vanessa Linke[5]; Berwyck L. J. Poad[4]; Jan-Peter Hauschild[2]; Todd W. Mitchell[6]; Gavin E Reid[7]; Stephen J Blanksby[4]; *[1]Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, Universität Leipzig, Leipzig, Germany; [2]Thermo Fisher Scientific, Bremen, Germany; [3]Center for Biotechnology and Biomedicine, Universität Leipzig, Leipzig, Germany; [4]Central Analytical Research Facility, Institute for Future Environments, Queensland University of Technology, Brisbane, Australia; [5]Department of Chemistry, University of Wisconsin–Madison, Madison, WI; [6]School of Medicine, Illawarra Health and Medical Research Institute, University of Wollongong, Wollongong, Australia; [7]School of Chemistry, Department of Biochemistry and Molecular Biology, Bio21 Molecular Science and Biotechnology Institute. The University of Melbourne, Parkville, Australia*

MP 478 **Liquid Chromatography Mass Spectrometry-based Lipidomics and Imaging of Lipid Double Bond Positional Isomers Using mCPBA Epoxidation**; Ting-Hao Kuo[1]; Hsin-Hsiang Chung[1]; Li-Hua Li[2]; Chiao-Wei Lin[3]; Hsin-Yuan Chang[1]; Chiao-Hui Hsieh[4]; Hsueh-Fen Juan[4, 5, 6]; Tang-Long Shen[3]; Cheng-Chih Hsu[1]; *[1]Department of Chemistry, National Taiwan University, Taipei, Taiwan; [2]Department of Pathology and Laboratory Medicine, Taipei Veterans General Hospital, Taipei, Taiwan; [3]Department of Plant Pathology and Microbiology, National Taiwan University, Taipei, Taiwan; [4]Institute of Molecular and Cellular Biology, National Taiwan University, Taipei, Taiwan; [5]Department of Life Science, National Taiwan University, Taipei, Taiwan; [6]Graduate Institute of Biomedical Electronics and Bioinformatics, National Taiwan University, Taipei, Taiwan*

MP 479 **Visualization and Identification of Cardiolipins by Means of LC-HRMS and Kendrick Mass Plots**; Patrick Olaf Helmer[1]; Ansgar Korf[1]; Heiko Hayen[1]; *[1]Institute of Inorganic and Analytical Chemistry, University of Muenster, Muenster, Germany*

MP 480 **SimLipid: Informatics Support for Profiling Glycerolipid, Diacyl-, Monoacyl- Glycerophospholipids with Details of the Fatty Acyl Composition Using Tandem Mass Spectrometry**; Ningombam Sanjib Meitei[1]; Rajesh Pujari[1]; Himani Gupta[1]; Arun Apte[2]; Ulrike Schweiger Hufnagel[3]; Sebastian Goetz[3]; Sven Meyer[3]; Aiko Barsch[3]; *[1]Premier Biosoft, Indore, India; [2]Premier Biosoft, Palo Alto, CA; [3]Bruker Daltonik GmbH, Bremen, Germany, Bremen, Germany*

MP 481 **Software Utilizing Positive and Negative Ion MS2/MS3HCD and CID Spectra for Improved MSn**; David A Peake[1]; Reiko Kiyonami[1]; Gavin E Reid[2]; Yasuto Yokoi[3]; Andreas Huhmer[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]University of Melbourne, Parkville, Australia; [3]Mitsui Knowledge Industry, Atago, Tokyo, Japan*

MP 482 **Localization of Double Bond Positions in Lipids by Post-Column Derivatization and LC-MS/MS**; Viola Jeck[1]; Heiko Hayen[1]; *[1]Institute of Inorganic and Analytical Chemistry, University of Münster, Münster, Germany*

MP 483 **Role of Ion-Neutral Intermediates on Specific H+/Na+ Exchanges During Sodiated Glycerophospholipid Dissociations Under Resonant and Non-Resonant Excitation Conditions**; Jean-Claude Tabet[1]; Benoit Colsch[2]; François Fenaille[2]; Anna Warnet[2]; Christophe Junot[2]; *[1]UPMC-CEA, PARIS, France; [2]CEA Saclay, DRF, Institut Joliot, Service de Pharmacologie et d'Immunoanalyse- CEA-INRA UMR 0496, Laboratoire d'Etude du Métabolisme des Médicament, Gif-sur-Yvette, France*

MP 484 **Characterization of Phosphoinositides by Negative Ion Electron Capture Dissociation**; Hye Kyong Kweon[1]; Kristina Hakansson[1]; *[1]University of Michigan, Ann Arbor, MI*

MP 485 **Conformational Analysis of Lipids and Fatty Acids by Uniform Field Ion Mobility-Mass Spectrometry**; Katrina L. Leaptrot[1]; Jody C. May[1]; James N. Dodds[1]; John A. McLean[1]; *[1]Vanderbilt University, Nashville, TN*

MP 486 **Informatics Solutions for Improved Identifications in 2D-LC/MS and IM-MS Lipidomics Workflows**; Sarah M. Stow[1]; Jeremy P. Koelmel[2]; Sonia Liggi[3]; Christine Hinz[3]; Julian L. Griffin[3]; Xiangdong Li[1]; Alex Apffel[1]; Mark Sartain[1]; Norton Kitagawa[1]; John C. Fjeldsted[1]; *[1]Agilent Technologies Inc, Santa Clara, CA; [2]Department of Pathology, Immunology, and Laboratory Medicine, University of Florida, Gainesville, FL; [3]Department of Biochemistry and Cambridge Systems Biology Centre, University of Cambridge, UK*

MP 487 **Top Down Tandem Mass Spectrometric Analysis of Lipopolysaccharides from Colistin Resistant Gram Negative Bacteria**; Benjamin L. Oyler[1]; Donald F Smith[2]; Belita N Opene[3]; Courtney E Chandler[3]; Robert K Ernst[3]; David R Goodlett[3]; *[1]University of Maryland, Baltimore, Baltimore, MD; [2]National High Magnetic Field Laboratory, Tallahassee, FL; [3]University of Maryland, Baltimore, MD*

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MP 488 **Isobaric Labeling of Intact Gangliosides Towards Multiplexed LC-MS/MS Based Quantitative Analysis**; Rodell Barrientos[1, 2]; Qibin Zhang[1, 2]; *[1]Department of Chemistry and Biochemistry, The University of North Carolina at Greensboro, Greensboro, NC; [2]UNCG Center for Translational Biomedical Research, NC Research Campus, Kannapolis, NC*

MP 489 **Separation, Characterization and Quantification of Fatty Acid Isomers with Epoxidation and Isobaric Multiplex Reagents for Carbonyl Containing Compound (SUGAR) Labeling**; Zichuan Tian[1]; Yu Feng[2]; Miyang Li[1]; Lingjun li[1, 2]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [2]School of Pharmacy, University of Wisconsin-Madison, Madison, WI*

MP 490 **Targeting Modified Lipids by Hydrophilic Interaction and Reverse Phase Liquid Chromatography Coupled to High Resolution Tandem Mass Spectrometry**; Thu Huong (Nicole) Pham[1]; Ryley P Pumphrey[1]; Muhammad M Zaeem[1]; Muhammad Nadeem[1]; Natalia P Vidal[1]; Raymond H Thomas[1]; *[1]Memorial University of Newfoundland, Corner Brook, NL*

MP 491 **Intensity Independent Filtering of FT MS and FT MS/MS Spectra for Shotgun Lipidomics**; Kai Schuhmann[1]; Jacobo Miranda Ackerman[1]; Henrik Thomas[1]; Konstantin Nagornov[2]; Yury Tsybin[2]; Andrej Shevchenko[1]; *[1]MPI-CBG, Dresden, Germany; [2]Spectroswiss Sàrl, Lausanne, Switzerland*

MP 492 **Relative Quantification of Potential Lipid Biomarkers for Treated Patients with Bipolar Disorder**; Henrique Caracho Ribeiro[1]; Aline Klassen[2]; Célio Fernando Figueiredo Angolini[3]; Luiz Fernando de A. Lima e Silva[4];

Clarissa R Dantas[4]; Cláudio E.M. Banzato[4]; Marcos Nogueira Eberlin[3]; Alessandra Sussulini[1]; *[1]Laboratory of Bioanalytics and Integrated Omics (LaBIOmics), Institute of Chemistry, University of Campinas (UNICAMP), Campinas, Brazil; [2]Department of Chemistry, Federal University of São Paulo (UNIFESP), Diadema, Brazil; [3]ThoMSon Mass Spectrometry Laboratory, University of Campinas, Campinas, Brazil; [4]Department of Psychiatry, University of Campinas (UNICAMP), Campinas, Brazil*

MP 493 **Lipid Omega Analyzer – *in silico* Program Designed for Unsaturated Lipid Analysis**; Donghui Zhang[1]; Wenpeng Zhang[1, 2]; Yu Xia[3, 4]; Zheng Ouyang[1, 2]; Xiaoyu Zhou[1]; *[1]State Key Laboratory of Precision Measurement Technology and Instrument, Department of Precision Instruments, Tsinghua University, Beijing, China; [2]Weldon School of Biomedical Engineering, Purdue University, West Lafayette, IN 47907; [3]Department of Chemistry, Tsinghua University, Beijing, China; [4]Department of Chemistry Purdue University, West Lafayette, China*

MP 494 **Ultrahigh-Performance Supercritical Fluid Chromatography Hyphenated with Mass Spectrometry: Clinical Monitoring of Wide Range of Lipid Species**; Denise Wolrab[1]; Ondřej Peterka[1]; Roman Hrstka[2]; Michal Holčapek[1]; *[1]University of Pardubice, Department of Analytical Chemistry, Pardubice, Czech Republic; [2]Masaryk Memorial Cancer Institute, Regional Centre for Applied Molecular Oncology, Brno, Czech Republic*

MP 495 **UHPLC/MS Determination of Oxylipins in Clinical Samples**; Michaela Chocholoušková[1]; Robert Jirásko[2]; Michal Holčapek[2]; *[1]University of Pardubice, Pardubice, Czech Republic; [2]University of Pardubice, Department of Analytical Chemistry, Pardubice, Czech Republic*

MP 496 **LC-MS Analysis of Oxidized Phosphatidylethanolamine in Ferroptosis-Sensitive PLA2G6 Mutant Human Fibroblast**; Hsiu-Chi Ting[1]; Yujia Zhai[2]; Yulia Y. Tyurina[1]; Oleksandr O. Kapralov[1]; Hülya Bayir[1]; Rong-Rong He[2]; Valerian E. Kagan[1]; *[1]University of Pittsburgh, Pittsburgh, PA; [2]Jinan University, Guangzhou, China*

MP 497 **A Simple High –Throughput Method for the Analysis of Sphingolipids, Ceramides and Other Lipids in Serum by LC-MS/MS**; Rory M Doyle[1]; Adrian Sanchez-Woehler[2]; *[1]Thermo Scientific, Somerset, NJ; [2]Thermo Fisher Scientific, West Palm Beach, Fl*

MP 498 **Metabolic Partial Heavy Water (2H2O) Labeling for Relative Quantification of Lipid on a Global Scale**; Jonghyun Kim[1]; Tae-Young Kim[1]; *[1]School of Earth Sciences and Environmental Engineering, Gwangju Institute of Science and Technology, Gwangju, South Korea*

MP 499 **Absolute Quantification of Neuronal Lipids Using Deuterated Standards and Short Acyl Chain Analogues**; Tommy Hofmann[1]; Carla Schmidt[1]; *[1]Martin-Luther University Halle-Wittenberg, Halle (saale), Germany*

MP 500 **Lipidomics to Study Health Disparities in Alzheimer's Disease**; Mostafa J. Khan[1]; Renã A. S. Robinson[1]; Simona G Codreanu[1, 2]; Stacy D. Sherrod[1, 2]; John A McLean[1, 2]; *[1]Department of Chemistry, Vanderbilt University, Nashville, TN; [2]Center for Innovative Technology, Vanderbilt University, Nashville, TN*

MP 501 **Lipid Metabolites in Mouse Brain After Repeated Closed Head Concussive Injury Analyzed by Liquid Chromatography/High Resolution Tandem Mass Spectrometry**; Karl R Kevala[1]; Huazhen Chen[1]; Abhishek Desai[1]; Hee-Yong Kim[1]; *[1]National Institutes of Health, Rockville, MD*

MP 502 **Development of a Second-Tier Newborn Screening Assay for Cerebrotendinous Xanthomatosis and X-Linked Adrenoleukodystrophy Through LC-ESI-MS/MS Quantitation of Ketosterols and Lysophosphatidylcholines**; Christopher Haynes[1]; Konstantinos Petritis[1]; *[1]CDC, Atlanta, GA*

MP 503 **Results of an International Ring Trial for the Biocrates AbsoluteIDQ p400HR Targeted Metabolomics Kit**; Lisa St. John-Williams[1]; Tuan Hai Pham[2]; Therese Koal[2]; Anastasia Kalli[3]; Andreas FR Huhmer[3]; John A. Bowden[4]; Stormy Koeniger[5]; Florence I Raynaud[6]; Akos Pal[6]; Yasmin Asad[6]; Catherine L. Winder[7]; Andrew Southam[7]; Mark Viant[7]; Warwick Dunn[7]; Donna O'Neill[7]; Jerzy Adamski[8]; Tong Shen[9]; Luiz Valdiviez[9]; Oliver Fiehn[10]; Gregory Byram[10]; Rupasri Mandal[11]; Danuta Chamot[11]; David Wishart[11]; Facundo M. Fernandez[12]; David A. Gaul[12]; Catherine G. Vasilopoulou[13]; Florian Meier[13]; Matthias Mann[14]; Fuad J Naser[15]; Gary J Patti[15]; Viet D Dang[16]; David J. Borts[16]; Joseph E. Lucas[17]; M. Arthur Moseley[1]; J. Will Thompson[1]; *[1]Duke University School of Medicine, Durham, NC; [2]BIOCRATES Life Sciences AG, Innsbruck, Austria; [3]Thermo Scientific, San Jose, CA; [4]National Institute of Standards and Technology, Charleston, SC; [5]AbbVie, North Chicago, IL; [6]Cancer Research UK Cambridge Institute, University of cambridge, Cambridge, UK; [7]University of Birmingham, Birmingham, UK; [8]Helmholtz-Zentrum München (CMA), Munich, Germany; [9]University of California Davis, CA; [10]University of California Davis, Davis, CA; [11]University of Alberta, Edmonton, AB, Canada; [12]Georgia Institute of Technology, Atlanta, GA; [13]Max Planck Institute of Biochemistry, Martinsried, Germany; [14]Max Planck Institute of Biochemistry, Planegg-Martinsried, Germany; [15]Washington University, St. Louis, St. Louis, MO; [16]Iowa State University, Ames, IA; [17]Duke University School of Medicine, Deparments of Cell Biology and Neurobiology, Durham, NC*

MP 504 **Can SFC-MS/MS Be an Alternative Method for Analyzing Thyroid Hormones?** Neil de Kock[1]; Daan Cramer Bornemann[1]; Jonas Bergquist[1]; Kumari Ubhayasekera[1]; *[1]Uppsala University, Uppsala, Sweden*

MP 505 **Optimization of UHPSFC/ESI-MS Determination of Polar and Nonpolar Lipids in Biological Samples**; Ondrej Peterka[1]; Denise Wolrab[1]; Michal Holčapek[1]; *[1]University of Pardubice, Department of Analytical Chemistry, Pardubice, Czech Republic*

MALDI: APPLICATIONS
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MP 506 **Quantitative Platform for the Analysis of Estron in Human Breast Cancer Cell Based Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry**; Da-Hee Ahn[1]; Yun-Gon Kim[1]; Han-Gyu Park[1]; Won-Suk Song[2]; Yung-Hun Yang[3]; *[1]Soongsil university, seoul, South Korea; [2]Seoul national university, seoul, South Korea; [3]Konkuk University, Seoul, South Korea*

MP 507 **Chemical structure and Pathogenicity of Lipid A Component of Psedumonas sp. From Thawing Permafrost**; Han-Gyu Park[1]; Da-Hee Ahn[1]; Won-Suk Song[2]; Yun-Gon Kim[1]; Yung-Hun Yang[3]; *[1]Soongsil university, seoul, South Korea, Seoul, South Korea; [2]Seoul National University, Seoul, South Korea, Seoul, South Korea; [3]Department of Biological Engineering, Konkuk University, Seoul 05029, Korea, Seoul, South Korea*

MP 508 **Investigating Chemical Evolution by MALDI-TOF Mass Spectrometry: Characterization of Model Prebiotic Peptides**; Sloane L. English[1]; Rachel E. Simoneaux[1]; Jay G. Forsythe[1]; *[1]College of Charleston, Charleston, SC*

MP 509 **Metabolomic and Proteomic Analysis of GluN2D-/- and Wild-Type Mouse Brains After Ischemic Stroke Using MALDI-TOF MSI.**; William Andrews[1, 2]; Deborah Donahue[1]; Adam Holmes[1]; Rashna Balsara[1]; Francis J. Castellino[1]; Amanda B. Hummon[2]; *[1]University of Notre Dame, Notre Dame, IN; [2]Ohio State University, Columbus, OH*

MP 510 **MALDI MS Imaging of N-Glycans and Peptides from Human FFPE Aneurysmal and Atherosclerotic Tissue Sections**; Yatao Shi[1]; Zihui Li[2]; Bowen Wang[3];

Xudong Shi[4]; Lian-wang Guo[3]; Lingjun Li[5, 6]; *[1]University of Wisconsin, Madison, WI; [2]Department of chemistry University of Wisconsin Madison, Madison, WI; [3]Davis Heart and Lung Research Institute, The Ohio State University, Columbus, OH; [4]Department of Surgery, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI; [5]School of Pharmacy, University of Wisconsin, Madison, WI; [6]Department of Chemistry, University of Wisconsin–Madison, Madison, WI*

MP 511 **Development of an Automated Immuno-MALDI Mass Spectrometry Assay for Insulin Quantitation in Plasma**; Bjorn Frohlich[1]; Michael X. Chen[2, 3]; Christoph H. Borchers[1, 4, 5, 6]; *[1]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [2]Department of Pathology and Laboratory Medicine, University of British Columbia, Vancouver, British Columbia; [3]Division of Medical Sciences, University of Victoria, Victoria, British Columbia; [4]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada; [5]Jewish General Hospital Proteomics Centre, McGill University, Montreal, QC, Canada; [6]Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC, Canada*

MP 512 **α-CNPV-CH3: A Multi-Purpose Et Matrix for Maldi Analysis of Metal Complexes, Fullerenes, Polymers and Nanoparticles**; Juan Sebastian Ramirez-Pradilla[1]; Cristian Blanco-Tirado[1]; Marianny Y. Combariza[1]; *[1]Universidad Industrial de Santander, Bucaramanga, Colombia*

MP 513 **High-Throughput Detection and Identification Method for Microbial Warfare Agents by Directin-Situ MALDI-TOF MS**; Young-Su Jeong[1]; Eugene Chong[1]; *[1]Agency for Defense Development, Daejeon, South Korea*

MP 514 **Molecular Analysis of Single Neurons from Lymnaea Stagnalis Central Nervous System by MALDI Mass Spectrometry**; Nikkita Khattar[1]; Linwen Zhang[1]; Ildiko Kemenes[2]; Gyorgy Kemenes[2]; Zita Zrinyi[3]; Pirger Zsolt[3]; Akos Vertes[1]; *[1]George Washington University, Washington, DC; [2]Sussex Neuroscience, School of Life Sciences, University of Sussex, Falmer, UK; [3]Balaton Limnological Institute, Tihany, Hungary*

MP 515 **Impact of Hyaluronan on the Ionization Efficiency of Glucose and Phospholipids Using MALDI-MS**; Abby Schnepf[1]; M. C. Yappert[2]; *[1]University of Louisville, Louisville; [2]University of Louisville, Louisville, KY*

MP 516 **MALDI-TOF Mass Spectrometry Method for Differential Diagnosis of Zika, Chikungunya and Dengue Virus Through Protein/Peptide And/Or Lipid Profiles of Serum**; Fábio Neves dos Santos[1]; Aline Maria Araújo Martins[2]; Kelly Grace Magalhães[2]; Marcos Nogueira Eberlin[1]; *[1]ThoMSon Mass Spectrometry Laboratory, University of Campinas, Campinas, Brazil; [2]Laboratory of Immunology and Inflammation, Department of Cell Biology, University of Brasília, Brasilia, Brazil*

MP 517 **Application of MALDI Imaging MS for Relative Quantitation of Post-Translational Modifications of Amyloid-β Peptide**; Stanislav Pekov[1, 2]; Daniil Ivanov[1]; Maria Indeykina[3]; Alexey Kononikhin[1, 3]; Igor Popov[1, 2]; Eugene (Evgeny) Nikolaev[4]; *[1]Moscow Institute of Physics and Technology, Moscow, Russia; [2]Institute for Energy Problems of Chemical Physics of RAS, Moscow, Russia; [3]Institute of Biochemical Physics of RAS, Moscow, Russia; [4]Skolkovo institute of science and technology, Moscow Region, Russian Federation*

MP 518 **Mass Profiling of Intact Immune Cells by MADLI-TOF Towards a Cellular Drug Discovery Assay for Inflammatory Diseases**; Rachel Heap[1]; Shin Hui Lim[1]; Matthias Trost[1]; *[1]University of Newcastle, Newcastle upon Tyne, UK*

MP 519 **MALDI Profiling of Cancerous Vesicles in Culture Media: Application to Liquid Biopsies**; Michael Douglas Nairn[1]; Tom K Abban[1]; Matthew E Openshaw[2]; Robert Mader[3, 4]; Gerald Stübiger[3, 5]; *[1]Shimadzu, Manchester, UK; [2]Shimadzu, Manchester, UK, Manchester, UK; [3]Medical University of Vienna, Vienna, Austria; [4]Comprehensive Cancer Center, Vienna, Austria; [5]CBmed- Center for Biomarker Research in Medicine, Graz, Austria*

MP 520 **A Novel Detection of Sulphated Haemoglobin Using Matrix-Assisted Laser Desorption Ionisation Time-Of-Flight (MALDI-TOF) Mass Spectrometry**; Suzanne Docherty[1]; Ray Iles[2]; Tom Kweku Abban[3]; Raminta Zmuidinaite[2]; Matthew E Openshaw[3]; Martin Besser[4]; *[1]Norfolk and Norwich University Hospital NHS Foundation Trust, Norwich, UK; [2]MAP Sciences, Bedford, UK; [3]Shimadzu, Manchester, UK; [4]Addenbrookes Cambridge University Hospital, Cambridge, UK*

MP 521 **Use of MALDI-TOF Mass Spectrometry and Machine Learning to Detect the Adulteration of Extra Virgin Olive oils**; Simona Salivo[1]; Tom K. Abban[1]; Ismael Duque[2]; Luis Mancera[2]; Matthew E. Openshaw[1]; *[1]Shimadzu, Manchester, UK; [2]Clover Bioanalytical Software, Granada, Spain*

MP 522 **Metabolomics for Allograft Assessment in Liver Transplants using Matrix Assisted Laser Desorption Ionization Mass Spectrometry**; Louis Searcy[1]; John Seal[2]; Timothy J. Garrett[1]; Richard A. Yost[1]; *[1]University of Florida Department of Chemistry, Gainesville, FL; [2]Ochsner Health System, Ochsner, LA*

MP 523 **A Translational Pilot Study of Global Lipid Profile as Risk Marker in Coronary Plaque: Mass Spectrometry Approach on Asymptomatic Patients**; Aline Martins[1]; Mariana Ubaldo Barbosa Paiva[1]; Diego Viana Neves Paiva[1]; Leonardo Jadyr[2]; Henrique Louzan Machado[2]; Helmgton Jose Brito Souza[2]; Fábio Neves dos Santos[3]; Marcos Nogueira Eberlin[3]; Fernando Antibas Atik[1]; *[1]UnB, Brasília-DF, Brazil; [2]University Center of Brasília, Brasília - DF, Brasilia, Brazil; [3]UNICAMP, Campinas, Brazil*

MP 524 **Glucose and Cyclodextrins for Inhibition of Sublimation of 4-Nitroaniline in MALDI-MS Analysis of Phospholipids**; Anthony C Ewurum[1]; M. C. Yappert[1]; *[1]University of Louisville, Louisville, KY*

MP 525 **FTICR and TOF MALDI Analysis for Protein Footprinting**; Jerry Jiang; *Washington University at St. Louis, St. Louis, MO*

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MP 526 **Polymer-based Electrospun Nanofibers for Surface-Assisted Laser Desorption/Ionization Mass Spectrometry: Design of SALDI Substrate and Implication for Desorption Mechanisms**; Juan Bian[1]; Susan Olesik[1]; *[1]Ohio State University, Columbus, OH*

MP 527 **Laser Desorption by Impulsive Vibrational Excitation (DIVE) Mass Spectrometry in Transmission Geometry**; Frederik Busse[1]; Wesley D. Robertson[1]; R. J. Dwayne Miller[1, 2]; *[1]Max-Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany; [2]Department of Chemistry and Physics, University of Toronto, Toronto, ON, Canada*

MP 528 **A Method for Defining Initial Ion Position in a TOFMS by Analysis of the Laser Image on the Sample Surface**; Michelle Piotrowski[1]; Brian Malys[1]; Kevin G. Owens[1]; *[1]Drexel University, Philadelphia, PA*

MP 529 **Investigating Ablation Volumes and Ion Yields in UV-MALDI MSI**; Kenneth N. Robinson[1, 2]; Alan M. Race[3]; Rory T. Steven[1]; Josephine Bunch[1, 4]; *[1]National Physical Laboratory, Teddington, UK; [2]Advanced Materials and Healthcare Technologies Division, University of Nottingham, Nottingham, UK; [3]Universität Bayreuth, Bayreuth, Germany; [4]Imperial College London, London, UK*

MP 530 **Gas-Phase Electron Transfer Reactivity of α-Cyanophenylenevinylenes**; Juan Sebastian Ramirez-Pradilla[1]; Damaris Godoy[1]; Dmytro Nykypanchuk[2]; Cristian

Blanco-Tirado[1]; Marianny Y. Combariza[1]; *[1]Universidad Industrial de Santander, Bucaramanga, Colombia; [2]Brookhaven National Laboratory, Upton, NY*

MP 531 **Using Solid State NMR to Rationalize the Efficiency of 2,X-DHB Isomers for MALDI of Poly(Ethylene Glycol)**; Christophe Chendo[1]; Hélène Pizzala[2]; Laurence Charles[2]; *[1]Aix Marseille Université, CNRS, Fédération des Sciences Chimiques de Marseille (FR 1739), Marseille, France; [2]Aix Marseille Université, CNRS, UMR 7273, Institut de Chimie Radicalaire, Marseille, France*

MALDI: SAMPLE PREPARATION
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MP 532 **Bead Assisted Mass Spectrometry (BAMS): A Multiplexed Affinity Capture Platform for MALDI TOF MS Based Biomarker Screening and Pathway Analysis**; Sergey Mamaev[1]; Jeffrey C. Silva[1]; Camilla Worsfold[1]; Vladislav B Bergo[1]; *[1]Adeptrix Corp., Beverly, MA*

MP 533 **Profiling Low Abundant Species in Sera with Coupled Use of an Innovative Albumin Depletion Sample Preparation and MALDI-MS**; Lyna Sellami[1]; Omar Belgacem[1]; Swapan Roy[2]; Matthew Kuruc[2]; *[1]Ascend Diagnostics, Manchester, UK; [2]Biotech Support Group LLC, New Jersey, NJ*

MP 534 **Graphene Films as Attractive Target Surfaces for Highly Uniform Sample Preparation for Quantitative MALDI Mass Spectrometry**; Sang Yun Han[1]; Yoon Kyung Choi[2]; TaeYoung Kim[2]; Joo Yeon Oh[3]; *[1]Gachon University, Seongnam, South Korea; [2]Gachon University, Seongnam, South Korea; [3]ASTA Corp, Suwon, South Korea*

MP 535 **Development of a Binary MALDI Matrix System to Improve Absolute Peptide Signal and Reproducibility**; Ashley Phetsanthad[1]; Elsa Gorre[1]; Kevin G. Owens[1]; *[1]Drexel University, Philadelphia, PA*

MP 536 **MALDI-TOF-MS and FT-ICR-MS Analysis of Free Fatty Acids within Single Rodent Hippocampal Cells**; Joseph F Ellis[1]; Elizabeth K Neumann[1]; Stanislav S Rubakhin[1]; Jonathan V Sweedler[1]; *[1]Department of Chemistry and the Beckman Institute, University of Illinois at Urbana-Champaign, Urbana, IL*

MP 537 **Carbon Dot@Iron Oxide Nanoparticles as a Co-Matrix Enhancing MALDI-MS Detection of Glycans**; Alireza Banazadeh[1]; Yehia Mechref[1]; *[1]Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX*

MP 538 **Simple Surface Modification for Enhancing Ion Sensitivity in Matrix-Assisted Laser Desorption/ Ionization Time-of-Flight Mass Spectrometry**; Yu-Meng Ou; *Academia Sinica, Taipei City, Taiwan*

MP 539 **Paper Substratum for MALDI-TOF Disposable Targets**; Nadine Perrot[1]; Patrick Broyer[2]; Jerome Blaze[2]; Jean-Marie Baumlin[3]; Jean-Philippe Charrier[4]; *[1]bioMerieux, La Balme Les Grottes, France; [2]bioMerieux, Grenoble, France; [3]Arjowiggins Creative Papers, Boulogne-Billancourt, France; [4]bioMerieux, Marcy L'etoile, France*

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MP 540 **SWATHtoMRM: Development of High-Coverage Targeted Metabolomics Method Using SWATH Technology**; Haihong Zha[1]; Yuping Cai[1]; Yandong Yin[1]; Zhengjiang Zhu[1]; *[1]Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai, China*

MP 541 **Characterization of New NIST Plasma Reference Materials for Metabolomics Quality Control**; Christina M. Jones[1]; Tracey B. Schock[2]; Aaron Urbas[1]; Carolyn Q. Burdette[1]; Federica Nalin[1]; John A. Bowden[2]; Jacolin A. Murray[1]; David A. Sheen[1]; Werickson F. C. Rocha[1]; Katrice A. Lippa[1]; *[1]National Institute of Standards and Technology, Gaithersburg, MD; [2]National Institute of Standards and Technology, Charleston, SC*

MP 542 **Limiting the Manual Verification of Metabolomics Data Processing from DIA Data**; Matthew Huebsch[1]; Adam Lau[1]; Stephen A Tate[1]; *[1]SCIEX, Concord, ON, Canada*

MP 543 **Microflow Metabolomics Differentiates Pre-Classified Healthy and Cancer Samples**; Khatereh Motamedchaboki[1]; Baljit K. Ubhi[1]; Erika Lin[2]; *[1]Sciex, Redwood City, CA; [2]SCIEX, Redwood City, CA*

MP 544 **CESI-MS - A Sensitive and Versatile Approach for Metabolomics**; Esme Candish[1]; Stephen Lock[2]; Yunan Wang[3]; Mei Han[3]; *[1]Sciex, Framingham, MA; [2]SCIEX, Warrington, UK; [3]Amgen, South San Francisco, CA*

MP 545 **Identification of Natural Products in Scab Resistant Pecan Trees**; Zhentian Lei[1]; Clayton D. Kranawetter[1]; Barbara W. Sumner[1]; Santosh Kumar[1]; LLOYD W. SUMNER[1]; *[1]University of Missouri, Columbia, MO*

MP 546 **Strategies for Detection and Quantification of Metabolites in SWATH Analysis**; Pradeep Narayanaswamy[1]; Adam lau[2]; Lyle Burton[2]; Stephen Tate[2]; *[1]SCIEX, Singapore, Singapore; [2]SCIEX, Concord, ontario*

MP 547 **Sub-Microliter Metabolomics with Triboelectric Nanogenerator-Induced (TENGi) Nanospray Mass Spectrometry: a Case Study of Exhaled Breath Condensate from Cystic Fibrosis Patients**; Yafeng Li[1]; Changsheng Wu[2]; Nael A. McCarty[3]; Arlene A. Stecenko[3]; Zhong Lin Wang[2, 4]; Facundo M. Fernandez[1, 5]; *[1]School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA; [2]School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA; [3]Emory+Children's Center for Cystic Fibrosis and Airways Disease Research and Department of Pediatrics, Emory University School of Medicine and Children's Healthcare of Atlanta, Atlanta, GA; [4]Beijing Institute of Nanoenergy and Nanosystems, Chinese Academy of Sciences, Beijing, China; [5]Institute of Bioengineering and Biosciences, Georgia Institute of Technology, Atlanta, GA*

MP 548 **Adduct Formation in ESI-MS with HILIC- Type Chromatography Is Strongly Affected by the Inorganic Ion Concentration of the Samples**; Ida Erngren[1]; Jakob Haglöf[1]; Mikael Engskog[1]; Curt Pettersson[1]; Torbjörn Arvidsson[1]; *[1]Uppsala University, Uppsala, Sweden*

MP 549 **Chiral Metabolomics: Development of Comprehensive and Highly Accurate Analysis for Chiral Metabolites**; Takahiro Takayama[1]; Hajime Mizuno[2]; Toshimasa Toyo'oka[2]; Koichi Inoue[3]; Hiroyasu Akatsu[4, 5]; Kenichiro Todoroki[2]; *[1]Graduate School of Integrated Pharmaceutical and Nutritional Sciences, University of Shizuoka, Shizuoka, Japan; [2]School of Pharmaceutical Sciences, University of Shizuoka, Shizuoka, Japan; [3]College of Pharmaceutical Sciences, Ritsumeikan University, Kusatsu, Japan; [4]Department of Medicine for Aging Place, Community Health Care/Community-Based Medical Education, Nagoya City University Graduate School of Medical Sciences, Nagoya, Japan; [5]Department of Neuropathology, Choju Medical Institute, Fukushimura Hospital, Toyohashi, Japan*

MP 550 **Supercritical Fluid Chromatography - Mass Spectrometry as a Complementary Approach for Qualitative and Quantitative Analysis in Metabolomics**; Laura Akbal[1]; Gérard Hopfgartner[1]; *[1]Life Sciences Mass Spectrometry, University of Geneva, Geneva, Switzerland*

MP 551 **Metabolite Profiling in Fruit Juice Using X500B QTOF System for Determining Its Antioxidant Activity**; Akanksha Singh[1]; Vijayanand B.N. [2]; Dipankar Malakar[1]; Manoj Pillai[1]; *[1]SCIEX, Gurugram, India; [2]ITC Life Sciences and Technology Centre, Bengaluru, India*

MP 552 **Qualitative Flux Analysis of the ENCODE Lymphoblastoid Cell Lines to StudyMetabolome Changes and Cellular Energy Flux Among Passages**; Songjie Chen[1]; Yuqin Dai[2]; Lihua Jiang[1]; Michael Snyder[1]; *[1]Stanford University, Stanford, CA; [2]Agilent Technologies, Inc., Santa Clara, CA*

MP 553 **Efficient Prediction of Metabolite Fragmentation Patterns for Searching Structural Databases**; Bela Paizs[1, 2]; Zoltan Takats[2, 3]; *[1]Bangor University, Bangor, UK; [2]deshape ltd, Bangor, UK; [3]Imperial College, London, UK*

MP 554 **Mass Spectrometric Investigation of Amine Compounds Derivatized with Di-tert-butyl Dicarbonate and Its Metabolomic Application for Rice Crop**; Lei Peng[1]; Jae Kwang Kim[2]; Yongsoo Choi[3]; *[1]UST-KIST, Gangneung, South Korea; [2]Incheon National University, Incheon, South Korea; [3]Korea institute of Science and Technology, Gangneung, South Korea*

MP 555 **Inter-Laboratory Comparison of Metabolite Measurements for Metabolomics Data Integration**; Yoshihiro Izumi[1, 2]; Fumio Matsuda[2, 3]; Akiyoshi Hirayama[2, 4]; Kazutaka Ikeda[2, 5]; Yoshihiro Kita[2, 6]; Kanta Horie Horie[2, 7]; Takeshi Bamba[1, 2]; Yoshiya Oda[2, 7]; *[1]Kyushu University, Higashi-ku, Japan; [2]Japan Metabolome Technical Challenge Consortium (JMTC), Bunkyo-ku, Japan; [3]Osaka University, Suita, Japan; [4]Keio University, Tsuruoka, Japan; [5]RIKEN Center for Integrative Medical Sciences, Yokohama, Japan; [6]The University of Tokyo, Bunkyo, Japan; [7]Eisai Co., Ltd., Tsukuba, Japan*

MP 556 **High Resolution Mass Spectrometry (HRMS) Bioanalysis in Drug Discovery Utilizing Fully Integrated Customized Software**; Mary Piotrowski[1]; Darren Dumlao[2]; John Janiszewski[2]; Larry Elvbak[3]; *[1]Pfizer, Groton, CT; [2]Pfizer, Groton; [3]Gubbs Inc, Alpharetta, GA*

MP 557 **A Routine Targeted Lc-Ms Methodology Uncovers Metabolite Changes in the Frontal Lobe and Striatum of Patients with Huntington's Disease**; Stewart F Graham[1]; Xiaobei Pan[2]; Ali Yilmaz[1]; Shirin Macias[2]; Andrew Robinson[3]; David M Mann[3]; Brian D Green[2]; *[1]Beaumont Health, Royal Oak, MI; [2]Queen's University Belfast, Belfast, UK; [3]University of Manchester, Manchester, UK*

MP 558 **Global Metabolomics Workflows to Understanding Interactions Between Chemotherapy Drugs and Lung Cells**; Timothy Charles Sanchez[1]; Ayesha Arefin[1]; Ricardo Marti-Arbona[1]; Srinivas Iyer[1]; *[1]Los Alamos National Laboratory, Los Alamos, NM*

MP 559 **Exploring the Rumen Fluid Metabolome Using High-Resolution Mass Spectrometry Based Approach and Molecular Networking**; Rafaela Takako Ribeiro Almeida[1]; Rodolpho Martin Prado[1]; Carla Porto[1]; Geraldo Tadeu Santos[2]; Sharon Ann Huws[3]; Eduardo Jorge Pilau[1]; *[1]LaBioMass, Departamento de Química, Universidade Estadual de Maringá, Maringá, Brazil; [2]Departamento de Zootecnia, Universidade Estadual de Maringá, Maringá, Brazil; [3]Medical Biology Centre, School of Biological Sciences, Queen's University Belfast, Belfast, UK*

MP 560 **Bridging Targeted and Untargeted Metabolomics-Development and Application of Time Stagger/Mass Stagger-Global Optimized Targeted Mass Spectrometry**; Fanyi Zhong[1]; Jiangjiang Zhu[1]; *[1]Miami University, Oxford, OH*

MP 561 **Analysis of Catecholamines by Reversed-Phase HPLC Columns Without Ion-Pairing Agents**; KEN TSENG[1]; Toshi Ono[1]; Tsunehisa Hirose[1]; *[1]Nacalai, San Diego, CA*

MP 562 **High-Throughput Comprehensive Coverage of Hydrophilic and Hydrophobic Metabolites in Beer Utilizing a Dual Separation/High Resolution Accurate Mass Spectrometry System**; Ioanna Ntai[1]; Martin Samonig[2]; Stephanie N. Samra[1]; Aran Paulus[1]; Ralf Tautenhahn[1]; Amanda L. Souza[1]; Andreas FR Huhmer[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Germering, Germany*

MP 563 **Immunomodulation by Probiotic Lactobacillus Reuterivia a Novel Branch of the Folate Cycle**; Daniel Roeth[1]; Abby J Chiang[1]; Gabriel B Gugiu[1]; Christina Morra[2, 3]; James Versalovic[3, 4]; Markus Kalkum[1]; *[1]City of Hope, Duarte, CA; [2]Baylor College of Medicine, Houston, Texas; [3]Texas Children's Hospital, Houston, Texas; [4]Baylor College of Medicine, Houston, TX*

MP 564 **An Extensive Comparison of Mass Spectral Libraries of Plant Natural Products Across LTQ, Q Exactive HF, and Q-TOF Mass Spectrometers**; Arpana Vaniya[1]; Sajjan Singh Mehta[1]; Bennett Haffner[1]; Alice Dalo[1]; Ilayda Agar[1]; Oliver Fiehn[1]; *[1]NIH West Coast Metabolomics Center, University of California, Davis, CA, Davis, CA*

MP 565 **Real-Time Monitoring of 12C/13C Carbon Dioxide Production During E.coli Cultivations to Complement Metabolic Flux Analysis (MFA) Experiments by Mass Spectrometry**; Karl Weitz[1]; Eric A. Hill[1]; Nancy J. Isern[1]; Hans C. Bersein[1]; Ronald J. Moore[1]; Mary S. Lipton[1]; Malak Tfaily[1]; Ljiljana Pasa Tolic[1]; Patrick Reardon[2]; *[1]Battelle - PNNL, Richland, Washington; [2]Oregon State University, Corvallis, OR*

MP 566 **Analysis of Underivatized Amino Acids and Metabolites in Cell Culture Media by HILIC-LC/MS**; Anne E Blackwell[1]; Richard Hurteau[1]; Jordy J. Hsiao[2]; Te-Wei Chu[2]; Suma Ramagiri[1]; *[1]Agilent Technologies, Inc., Wilmington, DE; [2]Agilent Technologies, Inc., Santa Clara, CA*

MP 567 **Measuring Oceanic Respiration with a Unique High-Efficiency, Low-Energy Electron Ionization Approach**; Stephan A Baumann[1]; John R Casey[2]; *[1]Agilent Technologies, Inc., Alpharetta, GA; [2]Center for Microbial Oceanography, University of Hawaii at Manoa, Honolulu, HI*

MP 568 **Single-Injection Method for Simultaneous Quantitation of 30 Metabolites by UHPLC-HRMS**; Vanessa Y. Rubio[1]; Clive H. Wasserfall[2]; Chris Beecher[3, 4]; Richard A. Yost[5]; Timothy J. Garrett[2]; Jaime Guevara[6]; *[1]University of Florida, Department of Chemistry, Gainesville, FL; [2]University of Florida, Department of Pathology, Immunology and Laboratory Medicine, Gainesville, FL; [3]IROA Technologies, Bolton, MA; [4]University of Florida, Gainesville, FL; [5]University of Florida Department of Chemistry, Gainesville, FL; [6]Universidad San Francisco de Quito, Quito, Ecuador*

MP 569 **The Impact of Pathogen Inactivation on the Platelet Metabolome During Blood Bank Storage**; Freyr Jóhannsson; *University of Iceland, Reykjavík, Iceland*

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MP 570 **A Novel Calcium (II)-Based Metal-Organic Framework Material for the Dispersive Solid-Phase Extraction Oftryptophan Metabolitesfor Biological Samples with**; Yen-Hsiang Liu[1]; Wei-Ting Jung[1]; Cheng-Yen Tsai[1]; Hui-Ling Lee[1]; *[1]Department of Chemistry, Fu Jen Catholic University, New Taipei City, Taiwan*

MP 571 **Optimizing Quantitative LC-MS of Cancer Metabolites: Addressing Early Eluting Peaks and Split Peaks**; Delaine Zayas-Bazán[1, 2]; Aaron Goldman[1]; Hsin-Yao Tang[1]; Nicole Gorman[1]; David Speicher[1]; *[1]The Wistar Institute, Philadelphia, PA; [2]University of Pennsylvania, PA*

MP 572 **Mass Spectrometric Assessment of Swabs Used for Sample Collection**; Kelly C Weldon[1]; Fernando Vargas[1]; Pieter C. Dorrestein[1]; *[1]Skaggs School of Pharmacy & Pharmaceutical Sciences, University of California – San Diego, San Diego, CA*

MP 573 **Tissue Sample Preparation Method for Simultaneous Isolation of Lipid and Protein Fractions and Untargeted MS and MS/MS Analyses**; Luke Richardson[1]; Michael E. Pettit[1]; Amy N. W. Schnelle[1]; Christina A Gaw[1]; Fabrizio Donnarumma[2]; Kermit K Murray[2]; Sharon DeMorrow[3]; Touradj Solouki[1]; *[1]Baylor University, Waco, TX; [2]Louisiana State University, Baton Rouge, LA; [3]Texas A&M Health Science Center, Temple, TX*

MP 574 **Sequential Extractions Enhances Metabolome Coverage and Data Quality Using Untargeted Metabolomics**; Dmitri Sitnikov[1]; Dajana Vuckovic[2]; *[1]Concordia University, Montreal, Qc; [2]Concordia University, Montreal, QC, Canada*

MP 575 **Formation of Maillard Reaction Products During Sample Preparation for Metabolite Profiling: Sample Dry-Down Generates Artifactual Glycosylated Amino Acids**; Davinder Sandhu[1]; Qiuying Chen[1]; Steven S. Gross[1]; *[1]Weill Cornell Medical College, New York, NY*

MP 576 **Towards Developing an Automated, Phenotype Driven, Multi-Parallel Sampling Device for Mass Spectrometry-Based Metabolomics**; Jaqueline A. Picache[1]; Simona G. Codreanu[1]; Jody C. May[1]; Stacy D. Sherrod[1]; John A. McLean[1]; *[1]Vanderbilt University, Nashville, TN*

MP 577 **Assessment of Solid Phase Microextraction as a Sample Preparation Tool for Metabolomics Analysis of Brain Tissue by Liquid Chromatography-Mass Spectrometry**; Nathaly Reyes Garces[1]; Ezel Boyacı[2]; German Augusto Gomez-Rios[3]; Barbara Bojko[3]; Dajana Vuckovic[4]; Janusz Pawliszyn[3]; *[1]University of Waterloo, Waterloo, ON, Canada; [2]University of Waterloo, Department of Chemistry, Waterloo, ON, Canada; [3]University of Waterloo, Waterloo; [4]Concordia University, Montreal, QC, Canada*

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MP 578 **Measurement of Polar Metabolites by Ion Chromatography-High Resolution Mass Spectrometry**; Lin Tan[1]; Wai Kin Chan[1]; Di Du[1]; John Weinstein[1]; Philip Lorenzi[1]; *[1]MD Anderson Cancer Center, Houston, TX*

MP 579 **Targeted Lipidomics and Amino Acid Profiling of Acute Arsenic Exposure in Mice Using Liquid Chromatography-Mass Spectrometry**; Hui Ling Lee[1]; Cheng Yen Tsai[1]; Wei Ting Jung[1]; Pinpin Lin[2]; *[1]Department of Chemistry, Fu Jen Catholic University, New Taipei City, Taiwan; [2]National Institute of Environmental Health Sciences, National Health Research Institutes,, Zhunan, Miaoli County, Taiwan*

MP 580 **A Coordination-Assisted LC-MS Method for Metabolic Profiling of Isoprenoid Compounds in Mouse Liver**; Jun Han[1]; James Hui[1]; Alexandria Doerfler[2]; Ayrea Hurley[2]; William R. Lagor[2]; Christoph H. Borchers[1, 3, 4, 5]; *[1]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [2]Department of Molecular Physiology and Biophysics, Baylor College of Medicine, Houston, TX; [3]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada; [4]Jewish General Hospital Proteomics Centre, McGill University, Montreal, QC; [5]Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC, Canada*

MP 581 **Screening and Quantitative Analysis of Targeted Metabolites for Model Cancer Cells Metabolisms Utilizing of Both RP and HILIC LC-MS/MS Platforms**; Li Zhang[1]; Daniel Kremer[2]; Peter Sajjakulnukit[2]; Ho Joon Lee[2]; Xiang Xue[3]; Shah Yatrik[3]; Costas Lyssiotis[2]; *[1]The Michigan Regional Comprehensive Metabolomics Research Core, University of Michigan, Ann Arbor, MI; [2]Department of Molecular and Integrative Physiology, University of Michigan, Ann Arbor, MI; [3]Departments of Molecular & Integrative Physiology and Internal Medicine University of Michigan, Ann Arbor, MI*

MP 582 **A Quantitative Comparison of Cellular Redox State as Measured by Metabolomics and Enzymatic Assays**; Lingjue Wang[1]; Yahui Wang[1]; Gary J Patti[1]; *[1]Washington University, St. Louis, St. Louis, MO*

MP 583 **Understanding the Consequences of Radiation Therapy in Humans Through the Acylcarnitine Profile**; Nicholas B. Vera[1, 2]; Stephen L. Coy[2]; Michelle F. Clasquin[1]; Paul Vouros[2]; *[1]Pfizer, Cambridge, MA; [2]Northeastern University, Boston, MA*

MP 584 **Quantitation of Prostaglandin E2 and Related Prostaglandins in Tumors, Tumor Supernatants and Tumor Cell Line Media using LC/MS**; Bethanne M. Warrack[1]; Michael D. Reily[2]; Julie Carman[2]; David Nelson[2]; Joelle Onorato[2]; Mark Selby[3]; Kathryn Vanderlaag[3]; Petia Shipkova[2]; *[1]Bristol-Myers Squibb, Princeton, NJ; [2]Bristol Myers Squibb, Princeton, NJ; [3]Bristol Myers Squibb, Redwood City, CA*

MP 585 **METLIN-MRM and XCMS-MRM: Cloud-Based Tools for Cooperative Targeted Analysis of Small Molecules**; Xavier Domingo-Almenara[1]; J. Rafael Montenegro-Burke[1]; Julijana Ivanisevic[2]; Aurelein Thomas[2, 3]; Jonathan Sibidé[2, 3]; Tony Teav[2]; Carlos Guijas[1]; Duane Rinehart[1]; Aries E Aisporna[1]; Anders Nordström[4]; Maria Gomez-Romero[5]; Luke Whiley[5]; Jeremy K Nicholson[5]; Paul H Benton[1]; Gary Siuzdak[1]; *[1]The Scripps Research Institute, La Jolla, CA; [2]University of Lausanne, Lausanne, Switzerland; [3]Lausanne University Hospital, Lausanne, Switzerland; [4]Umeå University, Umeå, Sweden; [5]Imperial College London, London, UK*

MP 586 **Parallel Reaction Monitoring for Quantification of Phytochemical Constituents in Plant Extracts**; Armando Alcazar Magana[1]; Maya Caruso[2, 2]; Kirsten Wright[2]; Mona Khorani[3]; Amala Soumyanath[2]; Joseph Quinn[2]; Jan Frederik Stevens[3]; Claudia S. Maier[3]; *[1]OSU, Corvallis, OR; [2]Oregon Health & Science University, Portland, OR; [3]Oregon State University, Corvallis, OR*

MP 587 **Quantitation of Multiple Metabolic Markers of NHP Radiation Exposure by SPE-DMS-MS and Inversion to a Human-Relevant Medical Threshold**; Zhidan Chen[1]; Stephen L Coy[1, 2]; Evan Pannkuk[3]; Evagelia C Laiakis[3]; Albert J Fornace[3]; Paul Vouros[1]; *[1]Northeastern University, Boston, MA; [2]LC Research, Wayland, MA; [3]Georgetown University, Washington Dc, DC*

MP 588 **Racial Disparity in Bladder Cancer and Identification of Altered Metabolism in African American Compared to European Bladder Cancer**; Nagireddy Putluri[1]; Vasanta putluri[1]; *[1]Baylor College of Medicine, Houston, TX*

MP 589 **Targeted Profiling with LC-TQ MS for 3-NPH Derivatized Short-Chain Fatty Acids and Organic Acids Produced by Gut Microbiota**; Tsuyoshi Nakanishi[1]; Yuki Sugiura[2]; Yuko Hattori[2]; Makoto Suematsu[2]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]Keio University, Tokyo, Japan*

MP 590 **Quantification of Folate Cycle Metabolites in Cellular Extracts**; Bettina Gürtl[1]; Sara Sdelci[1]; Gerald Hofstaetter[1]; Stefan Kubicek[1]; Kristaps Klavins[1]; *[1]Research Center for Molecular Medicine, Vienna, Austria*

MP 591 **Using LC/MS to Quantify Metabolites in Urine Samples Post Clinical Exposure to Benzoates in Beverages**; Cameron D. Worthington[1]; Aaron H. Robinson[1]; Nicole El-Khoury[1]; Kimberly A. Kew[1]; David N. Collier[1]; Allison S. Danell[1]; *[1]East Carolina University, Greenville, NC*

MP 592 **Merging Bile Acids and Steroids Targeted Analysis using Parallel Reaction Monitoring on a Q Exactive HF Mass Spectrometer**; Tong Shen[1]; Patrick Fitzgerald[1]; Michael Webb[1]; Jacob Folz[1]; Oliver Fiehn[1]; *[1]NIH West Coast Metabolomics Center, University of California, Davis, CA, Davis, CA*

MP 593 **Quantitative Assay for Insecticide Uptake and Metabolism in Aedes Aegypti Resistant to Pyrethroids by Gas Chromatography-Tandem Mass Spectrometry (GC-MS/MS)**; Patricia Penilla[1]; Megan Dunlap[2]; Karolien Denef[2]; Rushika Perera[2]; Karla Saavedra[2]; Américo Rodríguez[1]; William Black[2]; *[1]Instituto Nacional de Salud Pública, Cuernavaca, Mexico; [2]Colorado State University, Fort Collins, CO*

MP 594 **argeted Metabolomics Analysis Using LC-MS for Determining Metabolic Changes in Canines in Response to Two Different Diets**; Robin A.T. Moore; *University of Helsinki, Helsinki, Finland*

MP 595 **A Chemical Derivatization Method for Quantification of Free Fatty Acids by Liquid Chromatography-Mass Spectrometry for Improved Sensitivity**; Beixi Wang[1]; Kai

Wang[1]; Weixuan Chen[1]; Lien Wang[1]; Changlu liu[1]; Kevin Coe[1]; Jiejun Wu[1]; *[1]Janssen Research & Development, LLC, San Diego, CA*

MP 596 **The Targeted Metabolomics with UHPLC/HRMS for the Simultaneous Analysis of Tricarboxylic Acid Cycle in a Range of Biological Matrices**; Yue Song[1]; Shan-An Chan[2]; *[1]Agilent Technologies, Inc, Shanghai, China; [2]Agilent Technologies, Inc, Taipei, Taiwan*

MP 597 **An Extensive Evaluation of Column Chemistries to Retain Biologically Relevant Metabolites for Targeted Metabolomics Analyses**; Si Mou[1]; Lei Xiong[1]; Baljit K. Ubhi[1]; *[1]Sciex, Redwood City, CA*

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MP 598 **Untargeted Metabolomics Identifies Novel Mechanism of Action and Putative Targets of New Antimalarial Drugs in Development, JPC-3210 and TSC-3**; Geoff W Birrell[1]; Ghizal Siddiqui[2]; Amanda De Paoli[2]; David P Jacobus[3]; Chris Parkinson[4]; Nyssa Drinkwater[5]; Sheena McGowan[5]; Mike D Edstein[1]; Darren J Creek[2]; *[1]Australian Defence Force Malaria and Infectious Disease Institute, Brisbane, Australia; [2]Monash Institute of Pharmaceutical Sciences, Monash University, Melbourne, Australia, Melbourne, Australia; [3]Jacobus Pharmaceutical Company, Plainsboro, Australia; [4]School of Biomedical Sciences, Charles Sturt University, Orange, Australia; [5]Monash Biomedicine Discovery Institute and Department of Microbiology, Monash University, Melbourne, Australia*

MP 599 **Investigating the Metabolic Profile of Lipopolysaccharide Induced Neuroinflammation *in vitro* in SIM-A9 Microglial Cells**; Taylor M. Domenick[1]; Emily L. Gill[1]; Timothy J. Garrett[2]; Richard A. Yost[3]; Vinata Vedam-Mai[4]; *[1]University of Florida, Department of Chemistry, Gainesville, FL; [2]University of Florida, Gainesville, FL; [3]University of Florida Department of Chemistry, Gainesville, FL; [4]University of Florida, Department of Neurosurgery, Gainesville, FL*

MP 600 **Optimized Global Metabolomics Pipeline Combining Reverse-Phase and Hydrophilic Interaction Liquid Chromatography-Mass Spectrometry for Multiplexed Profiling of Yeast Metabolites**; Boer Xie; *St.Jude Children's Research Hospital, Memphis, TN*

MP 601 **The Metabolome of Human Mesenchymal Stem Cells Conditioned by Hypoxia and the Pro-Inflammatory Cytokine Interferon-Gamma**; Holly M. Wobma[1]; Shahar Goeta[1]; Chuanning Tang[1]; Lewis Brown[1]; Gordana Vunjak-Novakovic[1]; *[1]Columbia University, New York, NY*

MP 602 **Impact of Clothing on Skin Metabolome and Microbiome**; Alexey V. Melnik[1]; Chris Callewaert[2]; Kathleen Dorrestein[1]; Alexander A. Aksenov[1]; Jeremiah J. Minich[2]; Greg Humphrey[2]; Gail Ackermann[2]; Rob Knight[2, 3, 4]; Pieter C. Dorrestein[1, 2, 4, 5]; *[1]Collaborative Mass Spectrometry Innovation Center, Skaggs School of Pharmacy and Pharmaceutical Sciences, La Jolla, CA; [2]Department of Pediatrics, University of California San Diego, La Jolla, CA; [3]Department of Computer Science and Engineering, University of California, San Diego, La Jolla, CA; [4]Center for Microbiome Innovation, University of California San Diego, La Jolla, CA; [5]Department of Pharmacology, University of California, San Diego, La Jolla, CA*

MP 603 **Smoker's and Non-smoker's Urine Comparison Using Comprehensive Two-Dimensional Gas Chromatography-High Performance Time-of-Flight Mass Spectrometry**; David E Alonso[1]; Joseph E Binkley[2]; Lorne Fell[3]; *[1]Leco Corporation, St. Joseph, MI; [2]LECO Corporation, St. Joseph, MI; [3]LECO Corporation, Saint Joseph, MI*

MP 604 **Rewired Metabolism of T-Cells Upon mTOR Inhibition: Development of an Integrated Omics Pipeline**; Darren Dumlao[1]; Mary A Piotrowski[1]; Shashank Jatav[2]; Shefali Lathwal[2]; Raghav Sehgal[2]; Abhishek Jha[2]; John Janiszewski[1]; *[1]Pfizer, Groton; [2]Elucidata, Cambridge, MA*

MP 605 **Using Multi-Omics Approach to Reveal the Metabolism Change in Pulmonary Arterial Smooth Muscle Cells in Patient with Loss-of-function of ALDH1**; Dan Li[1]; Songjie Chen[1]; Yuqin Dai[2]; Michael Snyder[1]; Marlene Rabinovitch[1]; *[1]Stanford, Stanford, CA; [2]Agilent Technologies, Santa Clara, CA*

MP 606 **Untargeted Metabolomics Profiling of Tumor-Derived Exosomes by NanoUPLC-MS/MS**; Ching Lo[1]; Yu-Ling Tai[2]; Pin-Rui Su[1]; Tang-Long Shen[2]; Cheng-Chih Hsu[1]; *[1]Department of Chemistry, National Taiwan University, Taipei, Taiwan; [2]Department of Plant Pathology and Microbiology, National Taiwan University, Taipei, Taiwan*

MP 607 **Anionic and Cationic Profiling of Metabolites in Frog (Xenopus) Embryonic Cells using CE-ESI-MS**; Erika P Portero[1]; Sally A Moody[2]; Peter Nemes[1]; *[1]University of Maryland, College Park, MD; [2]The George Washington University, Washington, DC*

MP 608 **Integrating MALDI Imaging and ESI Metabolomics for Broadband Identification and Validation**; Corinna Henkel[1]; Matthias Witt[1]; Shannon Cornett[2]; Nikolas Kessler[1]; Heiko Neuweger[1]; Aiko Barsch[1]; Dennis Trede[1]; Matthias Szesny[1]; Jens Fuchser[1]; Jochen Friedrich[1]; *[1]Bruker Daltonik GmbH, Bremen, Germany; [2]Bruker Daltonics Inc., Billerica, MA*

MP 609 **Chemical and Correlation Similarity Enrichment Analysis for Interpreting Untargeted Lipidomics Datasets from the Alzheimer's Disease Neuroimaging Initiative Cohort**; Dinesh Barupal[1]; Sili Fan[1]; Benjamin Wancewicz[1]; Tomas Cajka[1]; Michael Sa[1]; Megan Showalter[1]; Rebecca Baillie[2]; Jessica D Tenenbaum[3]; Alzheimer's Disease Metabolomics Consortium[4]; Rima Kaddurah-Daouk[5]; Oliver Fiehn[1]; *[1]Genome Center, University of California Davis, Davis, CA; [2]Rosa & Co LLC, San Carlos, CA; [3]Department of Biostatistics and Bioinformatics, Duke University, Durham, NC; [4]Duke University, Durham, NC; [5]Duke University School of Medicine, Durham, NC*

MP 610 **Trapped Ion Mobility Spectrometry with Parallel Accumulation SErial Fragmentation (TIMS-PASEF) for untargeted Metabolomics**; Catherine G. Vasilopoulou[1]; Karolina Sulek[2]; Andreas-David Brunner[1]; Florian Meier[1]; Ulrike Schweiger-Hufnagel[3]; Aiko Barsch[3]; Matthias Mann[1]; *[1]Max Planck Institute of Biochemistry, Martinsried, Germany; [2]NNF CENTER FOR PROTEIN RESEARCH, Copenhagen, Denmark; [3]Bruker Daltonik GmbH, Bremen, Germany*

MP 611 **Multi-Modal Metabolomic Data Integration for Comprehensive Pathway Analysis and Systems Biology Studies**; Tao Huan[1]; Amelia Palermo[1]; Duane Rinehart[1]; Thiery Phommavongsay[1]; Gary Siuzdak[1]; *[1]The Scripps Research Institute, La Jolla, CA*

MP 612 **Isotopic Ratio Outlier Analysis Improves Metabolomics Prediction of Nitrogen Treatment in Maize**; Jan Hazebroek[1]; Chris Vlahakis[1]; Chris Beecher[2]; Felice A. De Jong[2]; *[1]Dow-DuPont, Johnston, IA; [2]IROA Technologies, Bolton, MA*

MP 613 **Towards Developing a Multi-Omic Approach to Understanding Human X Gut Microbe Interactions**; James Poland[1]; Andrew W Brooks[1]; Stacy D. Sherrod[1]; Seth R Bordenstein[1]; John A McLean[1]; *[1]Vanderbilt University, Nashville, TN*

MP 614 **Development and Application of High-Performance Chemical Isotope Labeling LC-MS for Single-Cell Metabolomics**; Wan Chan[1]; Yiman Wu[1]; Xian Luo[1]; Michael

C. Schultz[1]; Liang Li[1]; *[1]University of Alberta, Edmonton, AB, Canada*

MP 615 **Acute Dietary Effects of Cow Milk Consumption on the Urine Metabolome: Investigation by Chemical Isotope Labeling Liquid Chromatography Mass Spectrometry**; Dorothea Mung[1]; Liang Li[1]; *[1]University of Alberta, Edmonton, AB, Canada*

MP 616 **CIL LC-MS Metabolic Profiling of Sweat from Diseased and Healthy Areas of Lymphedema Patients Using A Non-occlusive Sweat Collection Kit**; Kevin Hooton[1]; Zeenat Ladak[1]; Ian Soles[2]; Liang Li[1]; *[1]University of Alberta, Edmonton, AB, Canada; [2]Salutaris Massage Therapy Centre, Edmonton, AB, Canada*

MP 617 **Performance Comparison of High-Throughput and Conventional Metabolomics Methods Based on Mass Spectrometry**; Peter Avar[1]; Andrew R. Korte[1]; Hang Li[1]; Lida Parvin[1]; Akos Vertes[1]; *[1]Department of Chemistry, The George Washington University, Washington, DC*

MP 618 **Non-Targeted Screening Using GC×GC-TOFMS for In-Depth Chemical Characterization and Comparison of Aerosols from a Heat-Not-Burn Tobacco Product and Cigarette Smoke**; Martin Almstetter[1]; Arno Knorr[1]; Mounir Rhouma[1]; Elyette Martin[1]; Antonio Castellon[1]; Pavel Pospisil[1]; Mark Bentley[1]; *[1]Philip Morris International R&D, Neuchatel, Switzerland*

MP 619 **Untargeted LC-MS Metabolomics of >2000 Fecal Samples Reveals Association between Pseudomonas spp Metabolites and Gastrointestinal Health**; Alan K. Jarmusch[1]; Daniel McDonald[2]; Ricardo da Silva[1]; Emmanuel O. Elijah[1]; Julia M. Gauglitz[1]; Robert A. Quinn[1]; Alexey V. Melnik[1]; Alexander Aksenov[1]; Paul Wischmeyer[3]; Rob Knight[2]; Pieter C. Dorrestein[1]; *[1]Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California, San Diego, La Jolla, CA; [2]Department of Pediatrics, University of California San Diego, La Jolla, CA; [3]Duke University School of Medicine, Durham, NC*

MP 620 **The Effect of the Gut Microbiome on the Plasma Metabolome:An LC-MS Metabolomic Investigation of Antibiotic Treatment in Rats**; Yutai Li[1]; Kara Michelle Pearson[1]; Peining Tao[2]; Jia Kang[2]; Raymond J. Gonzalez[1]; Warren E. Glaab[1]; Frank D Sistare[1]; Jose Lebron[1]; *[1]Merck Research Labs, West Point, PA; [2]Merck, Boston, MA*

MP 621 **Comparative Metabolomics by SWATH-MS of Adults-Onset Still's Disease and Systemic lupus Erythematosus**; Hsuan-Jen Chen[1]; Han-Ju Chien[1]; Chao-Yi Li[1]; Chien-Chen Lai*[1]; *[1]Institute of Molecular Biology,National Chung Hsing University,Taichung,Taiwan, Taichung, Taiwan*

MP 622 **The Secondary Effects of Hormone and Stimulants on Intestinal Bacteria,Bacteroides Fragilis 3_1_12**; Myedith Damba[1]; Javier S Quintanilla[1]; Erica M Forsberg[1]; Brijinder Soni[1]; Ellen Kuang[1]; *[1]San Diego State University, Department of Chemistry and Biochemistry, San Diego, CA*

MP 623 **Untargeted Metabolomics and Neuromodulatory Metabolites Produced by Lactobacillus rhamnosus GG**; Brijinder S Soni[1]; Nina Ly[1]; Ellen Kuang[1]; Javier Quintanilla[1]; Elizabeth A. Costa[1]; Erica M. Forsberg[1]; *[1]San Diego State University, Department of Chemistry and Biochemistry, San Diego, CA*

MP 624 **Data Independent Acquisition Improves Metabolite Coverage over Traditional Data Dependent Techniques for Untargeted Metabolomics**; Zuzana Demianova[1]; Cyrus Papan[2]; Joerg Dojahn[2]; Baljit K. Ubhi[3]; *[1]Sciex, Darmstadt, Germany; [2]SCIEX, Darmstadt, Germany; [3]SCIEX, Redwood City, CA*

MP 625 **LC-QToF Metabolomic Profiling on Determination of Non-Hodgkin Lymphoma's Tumor Biomarkers**; Gustavo Henrique Bueno Duarte[1]; Flavia Presta Fillietaz[2]; Jayr Schmidt Filho[3]; Vladmir Claudio Cordeiro de Lima[3]; Felipe D'Almeida Costa[4]; Victor Piana de Andrade[4]; Marcos Nogueira Eberlin[1]; Ana Valéria Colnaghi Simionato[2, 5]; *[1]ThoMSon Mass Spectrometry Laboratory, University of Campinas, Campinas, Brazil; [2]Laboratory of Analysis of Biomolecules Tiselius, University of Campinas, Campinas, Brazil; [3]Department of Clinical Oncology, AC Camargo Cancer Center, São Paulo, Brazil; [4]Department of Pathology, AC Camargo Cancer Center, São Paulo, Brazil; [5]National Institute of Science and Technology in Bioanalytics (INCTBio), Campinas, Brazil*

MP 626 **Metabolic Phenotyping of Human Atherosclerotic Plaques: Metabolic Alterations and Their Biological Relevance in Plaque-Containing Aorta**; Sunhee Jung; Do Hyun Ryu; Geum-Sook Hwang; *Korea Basic Science Institute, Seoul, South Korea; Sungkyunkwan University, Suwon, South Korea*

MP 627 **LC/MS- and NMR-Based Multiplatform Approach Revealsmyocardial Metabolic Alterations in Mice with Diet-Induced Atherosclerosis**; Jueun Lee[1]; Sunhee Jung[1, 2]; Geum-Sook Hwang[1]; *[1]Korea Basic Science Institute, Seoul, South Korea; [2]Sungkyunkwan University, Suwon-si, South Korea*

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MP 628 **A Rapid and Sensitive Multiplex Targeted LC-MS/MS Assay for ESKAPE Pathogens Identification**; Tao Liang[1]; Sung Hwan Yoon[2]; Benjamin Oyler[3]; Courtney Chandler[2]; Robert Ernst[2]; David Goodlett[1]; *[1]Department of Pharmaceutical Science, School of Pharmacy, University of Maryland, Baltimore, MD; [2]Department of Microbial Pathogenesis, School of Dentistry, University of Maryland, Baltimore, MD; [3]Department of Toxicology, School of Medicine, University of Maryland, Baltimore, MD, United States, Baltimore, MD*

MP 629 **Top-Down Proteomic Identification of a Novel Antibiotic-Induced Plasmid-Encoded Factor from Shiga Toxin-Producing Escherichia Coli (STEC) Using MALDI-TOF-TOF-MS/MS and Post-Source Decay**; Clifton K. Fagerquist[1]; Bertram G. Lee[1]; William J. Zaragoza[1]; Jaszemyn Yambao[1]; Beatriz Quinones[1]; *[1]USDA/ ARS, Albany, CA*

MP 630 **Deep Proteogenomics of Bacillus Subtilis Reveals the Presence of Uncharacterised Novel Open Reading Frames**; Nicolas C Nalpas[1]; Vaishnavi Ravikumar[2]; Karsten Krug[1]; Viktoria Anselm[1]; Ivan Andreas Stancik[2]; Ivan Mijakovic[2, 3]; Boris Macek[1]; *[1]Quantitative Proteomics, University of Tuebingen, Tuebingen, Germany; [2]Novo Nordisk Foundation Center for Biosustainability, Technical University of Denmark, Denmark; [3]Department of Biology and Biological Engineering, Chalmers University of Technology, Sweden*

MP 631 **Optimizing the Analysis of Metaproteomic Gut Samples for the Q Exactive HF**; Julia Rechenberger[1]; Juergen Behr[2]; Bernhard Kuster[1, 2, 3]; *[1]Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; [2]Bavarian Biomolecular Mass Spectrometry Center, Technical University of Munich, Freising, Germany; [3]German Cancer Consortium (DKTK), Heidelberg, Germany*

MP 632 **A Species Agnostic, Multi-Step Database Search Strategy for Metaproteomic Profiling of the Human Gut Microbiome**; Brian D Dill[1]; Smaranda Bodea[1]; Huijun Wang[2]; Anne Mai Wassermann[1]; Xudong Qiao[2]; An Chi[1]; Ivan Cornella-Taracido[1]; *[1]Merck, Boston, MA; [2]Merck Research Laboratories, Kenilworth, NJ*

MP 633 **Microwave Supported Hydrolysis Prepares Bacillus Spores for Proteomics Analysis**; Dapeng Chen[1]; Wayne A Bryden[2]; Catherine Fenselau[1]; *[1]Department of Chemistry and Biochemistry, University of Maryland, College Park, MD; [2]Zeteo Tech Inc, Sykesville, MD*

MP 634 **Unraveling the Functions of Microbiomes: a Comprehensive Evaluation of Software Tools for Functional Metaproteomics**; Caleb W Easterly[1]; Carolin Kolmeder[2]; Thilo Muth[3]; Bart Mesuere[4]; Subina Mehta[1]; Praveen Kumar[1]; James Johnson[1]; Shane L Hubler[5]; Jaime Huerta-Cepas[6]; Bjoern Gruening[7]; MIchael Riffle[8]; Damon May[8]; W. Judson Hervey[9]; Alessando Tanca[10]; Brook L Nunn[8]; Joel Rudney[1]; Timothy J. Griffin[1]; Pratik D Jagtap[1]; *[1]University of Minnesota, Minneapolis, MN; [2]University of Helsinki, Helsinki, Finland; [3]Robert Koch Institute, Berlin, Germany; [4]Ghent University, Ghent, Belgium; [5]Rhapsody Data LLC, Madison, WI; [6]EMBL, Heidelberg, Heidelberg, Germany; [7]University of Freiburg, Freiburg, Germany; [8]University of Washington, Seattle, WA; [9]Naval Research Laboratory, Washington, D.C., Washington, D.C.; [10]Porto Conte Ricerche Science and Technology Park of Sardinia, Alghero, Italy*

MP 635 **Characterization of Unique Gram-Positive Bacterial and Fungal Lipids Used as Chemical Bar Codes for Identification**; Sung Hwan Yoon[1]; Tao Liang[1]; Benjamin L. Oyler[1]; Courtney Chandler[1]; Belita O'Pene[1]; Lisa M. Leung[1, 2]; Robert K. Ernst[1]; David R. Goodlett[1]; *[1]University of Maryland, Baltimore, MD; [2]Maryland Department of Health, Baltimore, MD*

MP 636 **MS-Based Proteomic Characterization of Bacillus Subtilis Mutants Reveals Alterations in Membrane Proteins Related to Biofilm Formation**; Samantha Peters[1, 2]; Suresh Poudel[1, 2]; Paul E. Abraham[2]; Robert L. Hettich[1, 2]; *[1]University of Tennessee, Knoxville, TN; [2]Oak Ridge National Laboratory, Oak Ridge, TN*

MP 637 **A Novel Membrane-Based Protocol for Highly-Resolved MALDI- and MALDI-2- MS Imaging of Inactivated Bacterial Colonies**; Eike U. Brockmann[1, 2]; Daniel Steil[1, 2]; Andreas Bauwens[1]; Fabian Eiersbrock[1]; Klaus Dreisewerd[1, 2]; Jens Soltwisch[1, 2]; *[1]Institute for Hygiene, University of Muenster, Muenster, Germany; [2]Interdisciplinary Center for Clinical Research (IZKF), University of Muenster, Muenster, Germany*

MP 638 **Mass Spectrometry Analysis of Bacteriophage-infected Salmonella Determined the Temporal Expression of Viral Proteins and Identified a Major Virion Morphogenesis Protein**; Susan T. Weintraub[1]; Sammy Pardo[1]; Dana Molleur[1]; Melissa K. Barton[2]; Nur Amira Md Amin[2]; Michael V. Osier[2]; Lindsay W. Black[3]; Julie A. Thomas[2]; *[1]Univ. of Texas HSC, San Antonio, TX; [2]Rochester Institute of Technology, Rochester, NY; [3]Univ. of Maryland School of Medicine, Baltimore, MD*

MP 639 **Proteases and Protease Inhibitors Appear to Modulate a Microbe-Driven Model of Multiple Sclerosis**; Carlos G Gonzalez[1]; Stephanie K Tankou[2]; Laura M Cox[2]; Howard L Weiner[2]; Joshua Elias[1]; *[1]Stanford University, Chemical and Systems Biology Dept., Stanford, CA; [2]Ann Romney Center for Neurologic Diseases, Evergrande Center for Immunologic Diseases, Partners Multiple Sclerosis Center, Brigham and Women's Hospital, Department of Neurology, Harvard Medical School, Boston, MA*

MP 640 **Detecting Bacteria using MS and Multivariate Analysis Statistics: Comparing ESI and MAI Methods for Ionization**; Darrell Marshall[1]; Sarah Trimpin[1]; Charles N McEwen[2]; *[1]Wayne State University, Detroit , MI; [2]MSTM, LLC, Newark, DE*

MP 641 **Metaproteomics Reveals Potential Mechanisms by which Dietary Resistant Starch Supplementation Attenuates Chronic Kidney Disease Progression**; Boris Zybailov[1]; Galina Glazko[2]; Yasir Rahmatallah[2]; Dmitry Andreyev[1]; Taylor McElroy[1]; Oleg Karaduta[1]; Stephanie Byrum[1]; Lisa Orr[1]; Alan J. Tackett[1, 3]; Samuel Mackintosh[1, 3]; Rick Edmondson[3]; Dorothy Kieffer[4]; Roy J. Martin[4]; Sean Adams[5]; Nostratola Vaziri[6]; John Arthur[7]; *[1]Department of Biochemistry and Molecular Biology, UAMS, Little Rock, AR; [2]Department of Biomedical Informatics, UAMS, Little Rock, AR; [3]Proteomics Core Facility, UAMS, Little Rock, AR; [4]Department of Nutrition, University of California, Davis, CA; [5]Arkansas Children's Nutrition Center and Department of Pediatrics, UAMS, Little Rock, AR; [6]Division of Nephrology, University of California, Irvine, CA; [7]Division of Nephrology, UAMS, Little Rock, AR*

MP 642 **Identification of Candida Auris and Other Pathogenic Yeasts by MALDI-TOF Mass Spectrometry of Membrane Lipids**; Lisa M Leung[1]; Courtney E Chandler[2]; David R Goodlett[2]; Robert K Ernst[2]; Robert A Myers[1]; *[1]Maryland Department of Health, Baltimore, MD; [2]University of Maryland, Baltimore, MD*

MP 643 **Integrating Phylogenetic and Functional Information for Proteomic Analysis of Microbiomes: MPA Portable Presents a Full-Featured Solution for Characterizing Microbial Communities**; Thilo Muth[1]; Fabian Kohrs[2]; Robert Heyer[2]; Dirk Benndorf[2]; Erdmann Rapp[3]; Udo Reichl[3]; Lennart Martens[4]; Bernhard Y Renard[5]; *[1]Robert Koch Institute, Berlin, Germany; [2]Otto von Guericke University, Magdeburg, Germany; [3]Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany; [4]Ghent University, Ghent, Belgium; [5]Robert Koch Institute, Berlin, Germany*

MP 644 **Identification of Novel Bacteriophage Peptides Using a Combination of Gene Sequence, LC-MS-MS Analysis, and BLASTP**; Leslie A. Harden[1]; Yen-Te Liao[2]; Vivian C. H. Wu[3]; *[1]USDA/WRRC, Albany, CA; [2]USDA-ARS, Albany, CA; [3]USDA/ ARS, Albany, CA*

MP 645 **Oral Microbiological Changes in Critically Ill Septic Patients**; Monira Samaan Kallas[1]; Meriellen Dias[2]; Isaac Castro[1]; Maria Anita Mendes[3]; Luciano Cesar Pontes de Azevedo[1]; *[1]Sirio Libanes Hospital, São Paulo, Brazil; [2]Dempster MS Lab- Poli-USP, São Paulo, Brazil; [3]Dempster MS Lab- Poli-USP, Sao Paulo, Brazil*

MP 646 **Disease Severity in IBD: A Personalized and Community Based Microbial Proteomic Perspective**; Robert Mills[1]; James Morton[1]; Parambir Dulai[1]; Larry Smarr[1]; William Sandborn[1]; David J Gonzalez[1]; Rob Knight[1]; *[1]University of California, San Diego, La Jolla, CA*

MP 647 **Identification and Characterization of Pseudomonas Aeruginosa Metabolites Produced During Intraspecific Interactions**; Kisurb Choe[1]; Sage J. B. Dunham[2]; Stephanie Lozano[2]; Joseph F Ellis[2]; Nameera F Baig[3]; Tianyuan Cao[3]; Nydia Morales-Soto[4]; Joshua D Shrout[4]; Paul W Bohn[3]; Jonathan V Sweedler[2]; *[1]Department of Microbiology and Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign, Urbana, IL, United States, Urbana, IL; [2]Department of Chemistry and Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign, Urbana, IL; [3]Department of Chemistry and Biochemistry and Department of Chemical and Biomolecular Engineering, University of Notre Dame, Notre Dame, IN; [4]Department of Civil and Environmental Engineering and Earth Sciences and Department of Biological Sciences, University of Notre Dame, Notre Dame, IN*

MP 648 **Rapid Pathogen Identification Direct from Poly-Microbial Specimens**; David R. Goodlett[1]; William E. Fondrie[1]; Tao Liang[1]; Benjamin L. Oyler[1]; Lisa M. Leung[2]; Dudley K. Strickland[1]; Robert K. Ernst[1]; *[1]University of Maryland, Baltimore, MD; [2]Maryland Department of Health, Baltimore, MD*

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MP 649 **Molecular-Beam Mass Spectrometric Investigation of the Decomposition of Tetramethylsilane and Species Cluster Growth in Premixed Laminar Low-Pressure Flames**; Yasin Karakaya[1]; Tina Kasper[1]; *[1]University of Duisburg-Essen, Duisburg, Germany*

MP 650 **Analytical Tools Applicable for the Detection of ENMS in Aquatic Environments: Use of Single Particle Inductively Coupled Plasma Mass Spectrometry**; Hlengilizwe Nyoni[1]; Bhekie B Mamba[1]; Titius AM Msagati[1]; *[1]University Of South Africa(UNISA), Johannesburg, South Africa*

MP 651 **Proteomic Analysis of Gold Nanoparticle Surface Functionalization Influence on Protein Corona Complex Formation**; Marina Mulenos George[1]; Andreanna Burman[1]; Christie M Sayes[1]; *[1]Department of Environmental Science, Baylor University, Waco, TX*

MP 652 **Nanodiamond-Assisted Antibiotic Delivery for the Treatment of Multi-Drug Resistant Escherichia Coli.**; Yu Chi Lo; *Department of Applied Chemistry, National Chi Nan University, Nantou, Taiwan*

MP 653 **Nanostructured Tungsten Oxide Substrate with Oxygen Vacancies for Efficient Surface-Assisted Laser Desorption/Ionization Mass Spectrometry Analysis**; Yueguang Lv[1, 2]; Qiang Ma[1]; *[1]Chinese Academy of Inspection and Quarantine, Beijing, China; [2]University of Chinese Academy of Sciences, Beijing, China*

MP 654 **Nano Electrospray Differential Mobility Analysis Based Size-Selection of Liposomes for Offline Hyphenation to MALDI MS**; Victor U. Weiss[1]; Ernst Pittenauer[1]; Gernot Friedbacher[1]; Martina Marchetti-Deschmann[1]; Guenter Allmaier[1]; *[1]TU Wien, Vienna, Austria*

MP 655 **Mass Spectrometry Imaging Reveals Distribution of Nanozymes in Animal Tissues**; Laura Castellanos-García[1]; Gulen Y Tonga[1]; Yuanchang Liu[1]; Xianzhi Zhang[1]; Joseph Hardie[1]; Cao-Milán Roberto[1]; Vincent M. Rotello[1]; Richard W. Vachet[1]; *[1]University of Massachusetts-Amherst, Amherst, MA*

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MP 656 **Spatially-Resolved Proteomic Profiling of <100 Cells from Tomato Fruit Pericarp Integrating Nanodroplet Sample Preparation and Laser Capture Microdissection**; Yiran Liang[1]; Ying Zhu[1]; Maowei Dou[1]; Rosalie K. Chu[1]; William B. Chrisler[1]; Rui Zhao[1]; Ryan Kelly[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

MP 657 **Capillary Electrophoresis (CE) Separation Coupled to Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry Imaging (MALDI MSI) for the Enhanced Detection of Neuropeptides**; Kellen DeLaney[1]; Lingjun Li[1]; *[1]University of Wisconsin-Madison, Madison, WI*

MP 658 **Evaluating the Impact of Stationary Phases and Extra-Column Dispersion on Separation Efficiency in Trap-And-Elute Proteomic NanoLC-MS**; Moon Chul Jung[1]; Markus Wanninger[1]; *[1]Waters Corporation, Milford, MA*

MP 659 **Benchtop Sample Processing Workflow for In-Depth Proteome Profiling of <100 Cells**; Kerui Xu[1]; Ying Zhu[1]; Maowei Dou[1]; Yiran Liang[1]; Rui Zhao[1]; Ryan T. Kelly[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

MP 660 **Development of the Microflow LC Solvent Delivery Unit for Stable Pumping at µL/min Level**; Shinya Imamura[1]; Masahide Gunji[1]; Masataka Nikko[1]; Keisuke Ogawa[1]; Kyoko Watanabe[1]; Jun Yanagibayashi[1]; Yoshiaki Maeda[2]; Masateru Oguri[1]; Scott Kuzdzal[3]; Masami Tomita[1]; *[1]Shimadzu corp., Kyoto, Japan; [2]Shimadzu (China) Co., Ltd., Shanghai, China; [3]Shimadzu Scientific Instruments, Inc, Columbia, MD*

MP 661 **p53 Mutant Cell Line as a Model for a Proteogenomic Discovery Pipeline**; Jakub Faktor[1]; Goran Mitulovic[2]; David R. Goodlett[3]; Theodore Hupp[4, 5]; Borek Vojtesek[1]; *[1]RECAMO, Brno, Czech Republic; [2]Medical University of Vienna, Vienna, Austria; [3]University of Maryland, Baltimore, MD; [4]University of Edinburgh, Edinburgh, UK; [5]University of Gdansk, Gdansk, Poland*

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MP 662 **The Use of Computational De Novo Sequencing and Predictive Databases for Identification of Secondary Metabolites from Antarctic Pseudovibrio sp. Tun. PHSC045.I4**; Nicole E. Avalon[1]; Lucas Bishop[2]; Dale Chaput[1]; Alison E. Murray[2]; Bill J. Baker[1]; *[1]Department of Chemistry, University of South Florida, Tampa, FL; [2]Division of Earth and Ecosystem Sciences, Desert Research Institute, Reno, NV*

MP 663 **Dereplication of Icelandic Sponge Natural Products by UPLC-QTOF-MS**; Ana Margarida P Costa[1]; Finnur Freyr Eiríksson[1]; Margrét Thorsteinsdóttir[1]; *[1]Faculty of Pharmaceutical Sciences - University of Iceland, Reykjavík, Iceland*

MP 664 **Of Mangosteens and Mass Spectrometers: Non-Damaging Quantitative Chemical Analysis on a Herbarium Specimen**; Diana Kao[1]; Joshua M. Henkin[2, 3]; Djaja D. Soejarto[2, 4]; A. Douglas Kinghorn[3]; Nicholas H. Oberlies[1]; *[1]University of North Carolina at Greensboro, Greensboro, NC; [2]University of Illinois at Chicago, Chicago, IL; [3]Ohio State University, Columbus, OH; [4]The Field Museum, Chicago, IL*

MP 665 **Determination of the Enantiomers of Nicotine and Nornicotine in Cured Tobacco Leaf**; Huihua Ji[1]; Neil Fannin[1]; Lowell Bush[1]; *[1]University of Kentucky, Lexington, KY*

MP 666 **Chemometrics in the Quality Assessment of Botanical Products: a Case Study in Sandalwood Oils**; Ibtisam Ibtisam[1]; Corey Levenson[2]; Angela I. Calderon[1]; *[1]Department of Drug Discovery and Development, Harrison School of Pharmacy, 2316 Walker Building, Auburn University, Auburn, AL 36849; [2]Santalis Pharmaceuticals,18618 Tuscany Stone, Suite 100, San Antonio, TX 78258*

MP 667 **Affinity Selection MS Coupled with Metabolomics Software Enables Natural Product Screening**; Thomas O'Connell[1]; Melissa Wagenaar[1]; Thomas McLellan[1]; Edmund Graziani[1]; Greg Ciszewski[1]; Justin Stroh[2]; *[1]Pfizer, Groton, CT; [2]Eurofins Labs, Lancaster, PA*

MP 668 **Augmented Chemical Diversity of Fungal Cultures Facilitated by *in situ* Analysis via the Droplet -LMJ-SSP**; Chiraz Soumia M Amrine[1]; Michael Doyle[1]; Huzefa A Raja[1]; Cedric J Pearce[2]; Nicholas H Oberlies[1]; *[1]University of North Carolina at Greensboro, Greensboro, NC; [2]Mycosynthetix, Hillsborough, NC*

MP 669 **Spatial Mass Spectrometric Interrogation of Ant Gardens Reveals the Presence of Antimicrobials**; Andres M Caraballo-Rodriguez[1]; Ricardo R. da Silva[1]; Evan Fox[2]; Sara P. Puckett[3]; Marcy J. Balunas[3]; Jonathan L. Klassen[2]; Pieter C. Dorrestein[1]; *[1]Collaborative Mass Spectrometry Innovation Center, Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California, San Diego, CA; [2]Department of Molecular and Cell Biology, University of Connecticut, Storrs, CT; [3]Division of Medicinal Chemistry, Department of Pharmaceutical Sciences, University of Connecticut, Storrs, CT*

MP 670 **Quantification of Aristolochic Acids in Chinese Proprietary Medicines by LC-ESI-MS/MS and its Application in Product Safety Evaluation**; Yun Zeng[1]; Chee-Leong Kee[1]; Min-Yong Low[1]; Xiaowei Ge[1]; *[1]HSA, Singapore, Singapore*

MP 671 **Correlation of Pyrrolizidine Alkaloids in Crotalaria Host Plants with Chemistry of Their Herbivore, the Bella Moth (Utetheisa ornatrix)**; Jodie V Johnson[1]; Kari B Green[1]; Andrei Sourakov[2]; *[1]Chemistry Dept., University of Florida, Gainesville, FL; [2]McGuire Center for Lepidoptera and Biodiversity, Florida Museum of Natural History, University of Florida,, Gainesville, FL*

MP 672 **Identification and Structural Elucidation of Native Surfactins and Variants Produced by Bacillus Amyloliquefaciens Under Different Culture Conditions.**; Victoria Osorio[1]; Anthony Arguelles[2]; Nicolas Smargiasso[1]; Marc Ongena[2]; Edwin De Pauw[1]; *[1]Mass Spectrometry Laboratory (LSM-GIGA-R), Chemistry Department, University of Liege, Liege, Belgium; [2]Gembloux Agro-Bio Tech, University of Liege, Gembloux, Belgium*

MP 673 **Vibrio Natriegens Metabolic Profiling and Use for Natural Products Production**; Gregory A. Ellis[1]; Tanya Tschirhart[2]; Winifred Johnson[3]; Dagmar H. Leary[1]; Gary J. Vora[1]; *[1]Naval Research Laboratory, Washington, DC; [2]American Society of Engineering Education (ASEE) Postdoctoral Fellow, Washington, DC; [3]National Research Council (NRC) Postdoctoral Fellow, Washington, DC*

MP 674 **Biomolecular Fingerprints of Reishi and Cordyceps Mushrooms**; Chad C Nelson[1]; Douglas Stevenson[1]; *[1]Nu Skin Enterprises, Provo, UT*

MP 675 **Comprehensive Proteomic Analysis of Spider Fibers and Silk-Producing Glands Using Optimized Sample Preparation Methodology**; Mikayla Shanafelt[1]; Ryan Hekman[1]; Camille Larracas[2]; Simmone Dyrness[1]; Jared Deyarmin[1]; Michael Ysit[1]; Anish Patel[1]; Taylor Rabara[1]; Craig Vierra[1]; *[1]University of the Pacific, Stockton, CA; [2]University of the Pacific, Arthur Dugoni School of Dentistry, San Francisco, CA*

MP 676 **PepSAVI-MS Reveals Antifungal Cyclotides in Viola odorata**; Nicole C Parsley[1]; Christine L Kirkpatrick[2]; Leslie M Hicks[2]; *[1]UNC Chapel Hill, Durham, NC; [2]UNC Chapel Hill, Chapel Hill, NC*

MP 677 **Activation of Fungal Isolate, Pestalotiopsis microspora Silent Secondary Metabolite Gene Clusters for Discovery of Anti-infectives Against Drug-Resistant Pathogenic Bacteria**; Cassandra Naphen[1]; Lindsay K Caesar[1]; Huzefa A. Raja[1]; Nicholas H Oberlies[1]; Nadja B Cech[1]; *[1]University of North Carolina Greensboro, Greensboro, NC*

MP 678 **Monitoring the Secondary Metabolite Profile of Aspergillus Fischerithe Closest Relative to a Major Human Fungal Pathogen, *in situ*.**; Sonja L. Knowles[1]; Huzefa A. Raja[1]; Matthew E. Mead[2]; Jacob L. Steenwyk[2]; Antonis Rokas[2]; Nicholas H Oberlies[1]; *[1]University of North Carolina at Greensboro, Greensboro, NC; [2]Vanderbilt University, Nashville, TN*

MP 679 **Development of New LC-ERMS Approach for Analyzing Natural Positional Isomeric Oligomers**; Pai-Chi Syue[1]; Tsai-Fei Yu[1]; Nai-Yu Huang[1]; Ya-Zhu Zhang[1]; Mai-Su Lin[1]; Kuo-Lung Ku[1]; *[1]National Chiayi University, Chiayi City, Taiwan*

MP 680 **Towards the Development of a MALDI-MS Library of Fingerprint Spectra for Cannabis Products**; Baylie Gigolyk; *University of Manitoba, Winnipeg, MB, Canada*

MP 681 **Study on Natural Produced Drugs by LC-MS/MS**; Zenzaburo Tozuka[1]; Toshifumi Shiraga[2]; Yasuyuki Mitani[2]; *[1]Osaka University, Suita, Japan; [2]Astellas Pharmaceutical Inc., Suita, Japan*

PEPTIDES: FRAGMENTATION MECHANISMS 682-687

MP 682 **Effect of Molecular Structure and Ion Activation Conditions on Phosphate Rearrangement Chemistry**; Laura Bailey[1]; Nicolas C. Polfer[1]; *[1]University of Florida, Gainesville, FL*

MP 683 **Fragmentation of Modified Peptides Inspected with MALDI- and ESI-MSn**; Michael Ruehl[1]; Benjamin Kuehn[1]; Ilka Wittig[2]; Dieter Steinhilber[1]; Michael Karas[1]; *[1]Institute of Pharmaceutical Chemistry, Goethe University Frankfurt, Frankfurt am Main, Germany; [2]Functional Proteomics, SFB 815 Core Unit, Cluster of Excellence Frankfurt "Macromolecular Complexes", Goethe University, Frankfurt am Main, Germany*

MP 684 **CID of Deprotonated Peptides: Relative Abundance of Side-Chain Neutral Losses, Residue-Specific Product Ions, and Comparison with Protonated Peptides**; Yuxue Liang[1]; Pedatsur Neta[1]; Xiaoyu Yang[1]; Stephen E. Stein[1]; *[1]National Institute of Standards and Technology, Gaithersburg, MD*

MP 685 **The Fragments Analysis of Peptides by UVC Irradiation Using High-Resolution Mass Spectrometry**; Yuya Miyahara; *Osaka University, Suita-shi, Japan*

MP 686 **Optimizing Information Content in Collision-Induced Fragmentation Spectra of Peptides for Sequencing**; Nandhini Sokkalingam[1]; Luke Schneider[1]; William Wright[1]; Siamak Ashrafi[1]; Adam Tenderholt[1]; Jeffrey Peterson[1]; Mark Duncan[1]; *[1]Veritomyx Inc, Palo Alto, CA*

MP 687 **Middle-down Workflow and UVPD-MS for High Throughput Proteomics**; Edwin Escobar[1]; Sylvester M Greer[1]; Jennifer S Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX*

PHOSPHOPEPTIDES: QUANTITATIVE ANALYSIS 688-713

MP 688 **Measuring Kinase-Specific Protein Phosphorylation Stoichiometry by Motif-Targeting Quantitative Proteomic Method**; Pin-Lian Jiang[1, 2]; Yen-Chen Liao[1]; Chia-Feng Tsai[1, 3]; Yasushi Ishihama[3]; Yu-Ju Chen[1, 2]; *[1]Institute of Chemistry, Academia Sinica, Taipei, Taiwan; [2]Department of Chemistry, National Taiwan University, Taipei, Taiwan; [3]Graduate School of Pharmaceutical Sciences, Kyoto University, kyoto, Japan*

MP 689 **Custom Platform for Low-Abundance Phosphoproteomics by 2d LC-MS**; Nathan Hendricks[1]; Leo D Wang[1]; *[1]City of Hope, Duarte, CA*

MP 690 **Chemical and Phosphoproteomics for Mechanism of Action Analysis of AKT Inhibitors in Breast Cancer**; Svenja Petzoldt[1, 2, 3]; Benjamin Ruprecht[1]; Chen Meng[1]; Runsheng Zheng[1]; Elena Kunold[4]; Stefan Sieber[4]; Bernhard Kuster[1, 2, 5, 6, 7]; *[1]Technical University Munich, Chair of Proteomics and Bioanalytics, Freising, Germany; [2]German Cancer Consortium (DKTK), Munich, Germany; [3]German Cancer Center (DKFZ), Heidelberg, Germany; [4]Technical University Munich - Chair of Organic Chemistry II, Munich, Germany; [5]German Cancer Research Center (DKFZ), Heidelberg, Germany; [6]Center for Integrated Protein Science (CIPSM), Munich, Germany; [7]Bavarian Biomolecular Mass Spectrometry Center, Technical University of Munich, Freising, Germany*

MP 691 **Probing PLK4-Regulated Signalling Pathways by SILAC-Based Quantitative Phosphoproteomics**; Samantha Ferries; *University of Liverpool, Liverpool, UK*

MP 692 **Using MALDI-LTQ to Identify Specific HIV Protein Phosphorylation Sites**; Nhi Phan[1]; Pratikkumar Rathod[2, 3]; Hsin-Pin Ho[2, 4]; Kevin J Mark[1, 2]; Emmanuel J Chang[2, 3]; *[1]Department of Natural Science, LaGuardia Community College, City University of New York, Long Island, NY; [2]Department of Chemistry, York College, City University of New York, Jamaica, NY; [3]The Graduate Center, City University of New York, New York, NY; [4]Public Health Division, Rutgers University, Piscataway, NJ*

MP 693 **Phosphoproteomic Profiling of the Signaling Output of FLT3-ITD and an AC220- Resistant Mutant in Human Acute Myeloid Leukaemia**; Yanlong Ji[1, 2]; Johannes Kovar[1]; Julian Lohmeyer[1]; Silvia Münch[1]; Frank Schnütgen[1]; Anne Köhler[1]; Björn Häupl[1, 3, 4]; Henning Urlaub[2, 5]; Hubert Serve[1, 3, 4]; Thomas Oellerich[1, 3, 4]; Carmen Doebele[1, 3, 4]; *[1]Johann Wolfgang Goethe University, Frankfurt am Main, Germany; [2]Max-Planck-Institute for Biophysical Chemistry, Goettingen, Germany; [3]German Cancer Consortium (DKTK), Heidelberg, Germany; [4]German Cancer Research Center (DKFZ), Heidelberg, Germany; [5]Georg August University, Goettingen, Germany*

MP 694 **Characterising the PNUTS-Associated Protein Phosphatase 1 Signalling Network in Drosophila**; Amy Campbell[1]; Daimark Bennett[2]; Claire E. Eyers[2]; *[1]University of Liverpool, Liverpool, UK; [2]University of Liverpool, Liverpool, UK*

MP 695 **Sensing the Force: Mechanical Stimulation Induces Rapid Phosphorylation-Dependent Signaling in Xenopus Laevis Embryos**; Yutaka Hashimoto[1]; Noriyuki Kinoshita[2]; Todd M. Greco[1]; Pierre M. Jean Beltran[1]; Joel D. Federspiel[1]; Naoto Ueno[2]; Ileana M. Cristea[1]; *[1]Princeton University, Princeton, NJ; [2]NIBB, Okazaki, Japan*

MP 696 **PTMsigDB - A Curated Resource for Phosphosite-Specific Signature Analysis**; Karsten Krug[1]; Philipp Mertins[1, 2, 3]; Bin Zhang[4]; Peter Hornbeck[4]; Rajesh Raju[5]; Rushdy Ahmad[1]; Matt Szucs[1]; Filip Mundt[1]; Michael A Gilette[1]; Jennifer G Abelin[1]; Pablo Tamayo[6]; Jacob D Jaffe[1]; Steven A Carr[1]; D. R. Mani[1]; *[1]Broad Institute of MIT and Harvard, Cambridge, MA; [2]Proteomics Platform, Max Delbrück Center for Molecular Medicine in the Helmholtz Society, Berlin, Germany; [3]Berlin Institute of Health, Berlin, Germany; [4]Cell Signaling Technology, Danvers, MA; [5]Rajiv Gandhi Centre for Biotechnology, Thiruvananthapuram, India; [6]School of Medicine, University of California San Diego, La Jolla, CA*

MP 697 **Cytokine-Induced Phosphorylation Dynamics Reveals Molecular Mechanisms Underlying Human Beta Cell Stress**; Lian Yi[1]; Brittney N. Newby[2]; Marina Gritsenko[1]; Adam C. Swensen[1]; Ronald Monroe[1]; Richard D. Smith[1]; Clayton E Mathews[2]; Wei-Jun Qian[1]; *[1]PNNL, Richland, WA; [2]Department of Pathology, Immunology, and Laboratory Medicine, University of Florida, Gainesville, FL*

MP 698 **MS3-IDQ: Utilizing MS3 Spectra Beyond Quantification Yields Increased Coverage of the Phosphoproteome in Isobaric Tag Experiments**; Matthew J. Berberich[1]; Joao A. Paulo[2]; Robert A. Everley[1, 2]; *[1]Harvard Program In Therapeutic Science/Harvard Medical School, Boston, MA; [2]Department of Cell Biology, Harvard Medical School, Boston, MA*

MP 699 **Towards a High-Throughput Workflow for Quantitative Middle-Down Phosphoproteomics Using Isobaric Labeling**; Victoria C. Cotham[1]; Beatrix M. Ueberheide[1]; *[1]NYU Langone Health, Proteomics Laboratory, New York, NY*

MP 700 **Cross-Talk of Lysine Acetylome and Tyrosine Phosphoproteome Unveils Abnormal Cell Signaling of Acquired Resistance to EGFR Inhibitors in Lung Adenocarcinoma**; Yue Qi[1]; Tapan Maity[1]; Xu Zhang[1]; Udayan Guha[1]; *[1]NIH/NCI, Bethesda, MD*

MP 701 **SigPath300: A High Throughput Ms-Based Assay to Quantify over 300 Phosphosites of Known Biological Relevance in Cells and Tissues**; Hasmik Keshishian[1]; Luke Wallace[1]; Harrison Specht[2]; Judith Jané -Valbuena[1]; Rob McDonald[3]; Dale Petterson[1]; Eric Kuhn[1]; Michael Burgess[1]; D. R. Mani[1]; Tomas Rejtar[3]; Javad Golji[3]; Karen Wang[3]; William Sellers[1]; Steven A. Carr[1]; *[1]Broad Institute of MIT and Harvard, Cambridge, MA; [2]Northeastern University, Boston, MA; [3]Novartis, Cambridge, MA*

MP 702 **Targeted Single Precursor Selection Analysis of Phospho-Proteomic Changes in Strained Human Uterine Smooth Muscle**; Craig Ulrich[1]; Christian Copley Salem[1]; Dave Quilici[2, 3]; Rebekah Woolsey[2, 3]; Karen Schlauch[4]; Heather Burkin[1]; *[1]University of Nevada, Reno School of Medicine, Reno, NV; [2]University of Nevada, Reno, Reno, NV; [3]Mick Hitchcock, Ph.D. Nevada Proteomics Center, Reno, NV; [4]Desert Research Institute, Reno, NV*

MP 703 **Targeted TMT Assays Enabled via a Real-Time Instrument API (IAPI): Application to Phoshotyrosine Anlaysis**; Alison R Erickson[1]; Brian K Erickson[1]; Craig Braun[1]; David Nusinow[1]; Mirra Chung[1]; Peter K Sorger[1]; Steven P Gygi[1]; *[1]Harvard Medical School, Boston, MA*

MP 704 **Autophagy Inhibitor LYS05 Enhances Impact of Ionizing Radiation on Human Lung Cancer Cells H1299: Phosphoproteomic Analysis**; Martin Ondrej[1]; Lucie Cechakova[1]; Ravi Amaravadi[2]; Ales Tichy[1]; *[1]University of Defence, Hradec Kralove, Czech Republic; [2]Perelmann School of Medicine, Philadelphia, PA*

MP 705 **Functional Analysis of TAZ Phosphorylation by High Resolution Mass Spectrometry**; Panayiotis Vacratsis[1]; Justin Roberto[2]; Catherine Sykes[2]; *[1]University of Windsor, Windsor, ON, Canada; [2]University of WIndsor, Windsor, On*

MP 706 **CORAL: An Interactive and Highly Customizable Kinase Enrichment and Visualization Platform**; Ivan Jimenez Ruiz[1]; Douglas H Phanstiel[1]; *[1]UNC Chapel Hill, Chapel Hill, NC*

MP 707 **Quantitative Targeted Proteomic Analysis of Potential Markers of Tyrosine Kinase Inhibitor (TKI) Sensitivity in EGFR Mutated Lung Adenocarcinoma**; Shivangi Awasthi[1, 2]; Tapan Maity[2]; Benjamin L Oyler[3]; Xu Zhang[2]; David R Goodlett[1]; Udayan Guha[2]; *[1]University of Maryland, School of Pharmacy, Baltimore, MD; [2]Thoracic & Gastrointestinal Oncology Branch, Center for Cancer Research, NCI, Bethesda, MD; [3]University of Maryland School of Medicine, Baltimore, MD*

MP 708 **Global Ion Suppression Limits the Potential of Mass Spectrometry Based Phosphoproteomics**; Roland Felix Dreier[1]; Erik Ahrné[1]; Petr Broz[2]; Alexander Schmidt[1]; *[1]Biozentrum University of Basel, Basel, Switzerland; [2]University of Lausanne, Lausanne, Switzerland*

MP 709 **Evaluation of 1DLC and 2DLC for Phosphoproteomics Analysis Combined with Different Mass Spectrometry Fragmentation Methods**; Ramon Diaz[1]; Renuka Sabris[1]; Km Shams Ud Doha[1]; Alicia Richards[1]; Alexandre Rosa Campos[1]; *[1]Sanford Burham Prebys Medical Discovery Institute, San Diego, CA*

MP 710 **Withdrawn**

MP 711 **Quantitative Phosphoproteomic Analysis in Yeast Metabolic Pathways**; Peng Xue[1, 2]; Brendan Ryback[1]; Zrinka Nakic Raguz[1]; Ludovic Gillet[1]; Wenguang Shao[1]; Uwe Sauer[1]; Ruedi Aebersold[1]; *[1]Institute of Molecular Systems Biology (IMSB), ETH, Zurich, Switzerland; [2]Institute of Biophysics ,Chinese Academy of Sciences, Beijing, China*

MP 712 **Quantitative Phosphoproteomics Reveals a Novel Extended Basophilic RxRxxp[S/T]xxp[S/T] Motif as PI3K/Akt Signaling Switch**; Lena Reimann[1]; Anja N. Schwaeble[1]; Yvonne Leber[2]; Anna Lena Fricke[1]; Sascha Schaeuble[3]; Heike Wiese[1, 4]; Christian D. Peikert[1]; Peter F.M. van der Ven[2]; Gerald Radziwill[1]; Dieter O. Fürst[2]; Bettina Warscheid[1]; *[1]Faculty of Biology and BIOSS Centre for Biological Signalling Studies, University of Freiburg, Freiburg, Germany; [2]Department of Molecular Cell Biology, Institute for Cell Biology, Bonn, Germany; [3]Jena University Language & Information Engineering (JULIE) Lab, Friedrich-Schiller-University Jena, Jena, Germany; [4]Institute of Pharmacology and Toxicology, University of Ulm, Ulm, Germany*

MP 713 **Comparison of MS Methods for Analysis of TMT Labeled Phosphopeptides in an Orbitrap Fusion Lumos MS**; Roger E Moore[1]; Helen Y. Ge[1]; Gabriel B Gugiu[1]; *[1]City of Hope, Duarte, CA*

PROTEINS: COMPLEXES/NON-COVALENT INTERACTIONS
714-736

MP 714 **Engineering Nanodisc Scaffold Proteins for Native Mass Spectrometry of Integral and Peripheral Membrane Proteins**; Deseree J. Reid[1]; James Keener[1]; Andrew P. Wheeler[1]; Dane Zambrano[1]; Jessica M. Diesing[1]; Michael T. Marty[1]; *[1]The University of Arizona, Tucson, AZ*

MP 715 **Modelling Simplified Natural Lipid Membranes in Nanodiscs for Native MS**; Marius Kostelic[1]; Michael Thomas Marty[1]; *[1]University of Arizona, Tucson, AZ*

MP 716 **Ion Mode Affects Membrane Protein-Lipid Binding in Native MS**; Idlir Liko[1, 2]; Matteo T. Degiacomi[3]; Eamonn Reading[4]; Jonathan T.S. Hopper[1]; Joseph Gault[2]; Justin L.P. Benesch[2]; Timothy M. Allison[5]; Carol V. Robinson[2]; *[1]OMass Technologies Ltd., Oxford, UK; [2]University of Oxford,*

Oxford, UK; [3]Durham University, Durham, UK; [4]King's College London, London, UK; [5]University of Canterbury, Christchurch, New Zealand

MP 717 **Impact of Ligand Binding on Photodissociation of Multimeric Protein Complexes**; Sarah Sipe[1]; Jennifer S Brodbelt[1]; *[1]University of Texas Austin, Austin, TX*

MP 718 **ITEM-TWO: Nano-Electrospray Mass Spectrometry Enables Simultaneous Characterization of Specificities and Affinities of Epitope – Antibody Complexes in the Gas Phase**; Bright D. Danquah[1]; Yelena Yefremova[1]; Cornelia Koy[1]; Kwabena F.M. Opuni[2]; Michael O. Glocker[1]; *[1]Proteome Center Rostock, Rostock, Germany; [2]University of Ghana, School of Pharmacy, Legon, Ghana*

MP 719 **Interaction of Transcription Factor TEAD1 and Its DNA Response Elements Studied by Structural Mass Spectrometry**; Ruzena Liskova[1, 2]; Lukas Slavata[1, 2]; Karel Valis[1, 2]; Petr Novak[1, 2]; *[1]Institute of Microbiology of the CAS, Prague 4, Czech Republic; [2]Faculty of Science, Charles University, Prague 2, Czech Republic*

MP 720 **Using FTICR and Multimode Tandem Mass Spectrometry to Analyse Inhibitors of Amyloid Protofibrils**; Pui Yiu Lam[1]; Cookson K. C. Chiu[1]; Christopher A. Wootton[1]; Ji Inn Song[1]; Meng Li[1]; Ian Hands-Portman[1]; Mark P. Barrow[1]; Peter B. O'Connor[1]; *[1]University of Warwick, Coventry, UK*

MP 721 **Norovirus-Like VP1 Particles Exhibit Isolate-Dependent Stability Profiles**; Ronja Pogan[1]; Carola Schneider[1]; Rudolph Reimer[1]; Grant Hansman[2, 3]; Charlotte Uetrecht[1, 4]; *[1]Heinrich Pette Institute, Hamburg, Germany; [2]Department of Infectious Diseases, Heidelberg University, Heidelberg, Germany; [3]Schaller Research Group at the University and the DKFZ, Heidelberg, Germany; [4]European XFEL, Schenefeld, Germany*

MP 722 **Determining the Binding Interface of a Leader Peptide with Class IV Lanthipeptide Synthetase by HDX and FPOP Mass Spectrometry**; Rachel Liuqing Shi[1]; Julian D. Hegemann[2]; Bojie Zhang[3]; Wilfred A. van der Donk[2]; Michael L. Gross[3]; *[1]Washington University, Clayton, MO; [2]University of Illinois at Urbana-Champaign, Urbana, Illinois; [3]Washington University, St. Louis, St. Louis, MO*

MP 723 **Structural Characterization of a Bacterial Replicative Helicase and Helicase Loader Complex by Native and Crosslinking Mass Spectrometry**; Paul Dominic B. Olinares[1]; Jillian Chase[2, 3]; Kelly R. Molloy[1]; David Jeruzalmi[2, 4]; Brian T. Chait[1]; *[1]The Rockefeller University, New York, NY; [2]Department of Chemistry and Biochemistry, City College of New York, New York, NY; [3]Ph.D. Program in Biochemistry, The Graduate Center of the City University of New York, New York, NY; [4]Ph.D. Programs in Biochemistry, Biology and Chemistry, The Graduate Center of the City University of New York, New York, NY*

MP 724 **Determining Charge and Mass Information from Extremely Congested Mass Spectra of Large Biomolecular Complexes Using Fourier-Domain Harmonics**; Sean P Cleary[1]; Daniel Ko[1]; JAMES S PRELL[1, 2]; *[1]University of Oregon, Eugene; [2]Materials Science Institute, University of Oregon, Eugene, OR*

MP 725 **Significant Improvements in Spectral Quality of Non-Covalent Protein Complexes using SEC-Native MS**; Jonathan P. Williams[1]; Christopher Hughes[1]; Dale A Cooper-Shepherd[1]; Jeffery M. Brown[1]; *[1]Waters Corporation, Wilmslow, UK*

MP 726 **Monitoring Changes of Complexome in Yeast Hybrids Using SILAC-SEC-Based Proteomics**; Yi-Yun Chen[1]; Krishna. B. S. Swamy[2]; Hsin-Yi Lee[2]; Jung-Chi Chao[2]; Shu-Yu Lin[3]; Jun-Yi Leu[2]; *[1]Institute of Biological Chemistry, Academia Sinica, Taipei, Taiwan; [2]Institute of Molecular Biology, Academia Sinica, Taipei, Taiwan; [3]Institute of Biological Chemistry, Academia Sinica, Taipei, Taiwan*

MP 727 **Mass Spectrometry Reveals a Multi-Faceted Role of Glycosaminoglycan Chains in Factor Xa Inactivation by Antithrombin**; Burcu Minsky[1]; Rinat R. Abzalimov[2]; Yunlong Zhao[3, 4]; Chendi Niu[5]; Paul Dubin[5]; Sergey Savinov[5]; Igor A. Kaltashov[5]; *[1]Smith College, Northampton; [2]CUNY Advanced Science Research Center, New York, NY; [3]University of Massachusetts Amherst, Amherst, MA; [4]Regeneron Pharmaceuticals, Tarrytown, NY; [5]University of Massachusetts-Amherst, Amherst, MA*

MP 728 **Advances in Orbitrap™ Instrumentation for Native Top-Down Analysis of Non-Covalent Protein Complexes**; Eugen Damoc[1]; ROSA VINER[2]; Albert Konijnenberg[3]; Kyle Fort[1]; Maria Reinhardt-Szyba[1]; Mikhail Belov[1]; Alexander Makarov[1]; *[1]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [2]Thermo Scientific, San Jose, CA; [3]Thermo Fisher Scientific, Eindhoven, Netherlands*

MP 729 **"Gold Finger" Protein Complexes Characterized Through Native Ion Mobility Mass Spectrometry**; Wenjing Li[1]; Kiwon Ok[1]; Sarah L. J. Michel[1]; Maureen A. Kane[1]; *[1]University of Maryland, Baltimore, Baltimore, MD*

MP 730 **Toward Understanding Gag Assembly *in vivo***; Yisong Deng[1]; John A Hammond, Ph.D. [1]; Ilean Chai[2]; Bruce E. Torbett, Ph.D. [1, 2]; James R. Williamson, Ph.D. [1]; *[1]The Scripps Research Institute, La Jolla, CA; [2]University of California San Diego, San Diego, CA*

MP 731 **Oligosaccharide Affinities for Anti-Ganglioside Antibodies Quantified by ESI-MS**; Jianing Li[1, 2]; Ling Han[1, 2]; Jun Li[1, 2]; Elena N. Kitova[1, 2]; John S. Klassen[1, 2]; *[1]University of Alberta, Edmonton, AB, Canada; [2]Alberta Glycomics Centre, Edmonton, Alberta*

MP 732 **Heparinase Digestion Combined with Online SEC/MS Assay Reveals That Heparin/Protein Binding Is Kinetically Controlled Resulting in Apparent Promiscuity**; Chendi Niu[1]; Yunlong Zhao[2]; Cedric Bobst[1]; Igor A. Kaltashov[1]; *[1]University of Massachusetts Amherst, Amherst, MA; [2]Regeneron Pharmaceuticals, Tarrytown, NY*

MP 733 **Deciphering the Contribution of H-bonds and Salt Bridges to the Gas-Phase Stability of Coiled-Coil-Complex Using Native Top-Down MS and MDs**; Huilin Li[1]; Reza Malmirchegini[2]; Shirin Jamshidi[3]; Shao-Qing Zhang[2]; *[1]Sun Yat-Sen University, Guangzhou, China; [2]Department of Pharmaceutical Chemistry, School of Pharmacy, University of California, San Francisco, San Francisco, CA; [3]University of Warwick, Coventry, UK*

MP 734 **Charge Detection Mass Spectrometry of Virus Like Particles Assembled Around Short Genomic Fragments**; Kevin M. Bond[1]; Irina B. Tsvetkova[1]; Bogdan Dragnea[1]; Martin F. Jarrold[1]; *[1]Indiana University Bloomington, Bloomington, IN*

MP 735 **To What Extent Can the Fitting of Biological Structure to Biological Function Be Formalized?**; Yeva Mirzakhanyan[1]; Paul Gershon[1]; *[1]UC-Irvine, Irvine, CA*

MP 736 **Characterization of Hydroxymethylbilane Synthase and its Acute Intermittent Porphyria Associated Mutants by Fourier Transform Ion Cyclotron Resonance Mass Spectrometry**; Janne Jänis; *University of Eastern Finland, Joensuu, Finland*

PROTEINS: CONFORMATION ANALYSIS AND STRUCTURAL BIOLOGY
737-754

MP 737 **Chemo-Selection Strategy for Increasing the Information Content in Proteome-Wide Studies of Ligand Binding Utilizing the Pulse Proteolysis Technique**; Renze Ma[1]; Michael C. Fitzgerald[1]; *[1]Duke University, Durham, NC*

MP 738 **Probing Activation Mechanism of Adhesion GPCR by In-Cell Crosslinking and Quantitative Mass Spectrometry**; Bill Huang[1]; Xin Hu[2]; Heung Sun Kwon[1]; Cheng Fu[1]; Ji-won Lee[1]; Margugan Juan[2]; Hee-Yong Kim[1]; *[1]NIAAA/NIH, Rockville, MD; [2]NCATS/NIH, Rockville, MD*

MP 739 **Cross-Linking Mass Spectrometry and Molecular Dynamics to Analyze the Flexible Neuronal Calcium-Sensor Synaptotagmin-1**; Julian Bender[1]; Caroline Haupt[1]; Matteo T. Degiacomi[2]; Carla Schmidt[1]; *[1]IWE ZIK HALOmem, Martin Luther University Halle-Wittenberg, Halle (Saale), Germany; [2]Department of Chemistry, Durham University, Durham, UK*

MP 740 **Discovery of Subglutinol A Protein Targets using Energetics-Based Proteomics Approaches**; Michael C. Fitzgerald[1]; Renza Ma[1]; He Meng[1]; Hyeri Park[1]; Do-Yeon Kwon[1]; Laura Chrisitan[2]; Qi-Jing Li[2]; Jiyong Hong[1]; *[1]Duke University, Durham, NC; [2]Duke University School of Medicine, Durham, NC*

MP 741 **pH Time Window Expansion of HDX on GCase Points to MoA for Chaperones**; Graham West[1]; Laura J Byrnes[1]; Felix Vajdos[1]; Xiayang Qiu[1]; *[1]Pfizer, Groton, CT*

MP 742 **Structural characterization of the knot protein YibK using TIMS-MS and molecular dynamics**; Juan Camilo Molano-Arevalo[1]; Kevin Jeanne Dit Fouque[1]; Daniel Gimeno[1]; Fenfei Leng[1]; Francisco Fernandez Lima[1]; *[1]Florida International University, Miami, FL*

MP 743 **Trapped Ion Mobility Spectrometry and PASEF for Enhanced Observation of Chemically Crosslinked Peptides**; Chris Adams[1]; Stijn van Dorp[2]; Richard Lewis[2]; Kratika Singhal[1]; Allis S Chien[1]; Ryan D Leib[1]; *[1]Stanford University Mass Spectrometry, Stanford, CA; [2]Stanford University, Stanford, CA*

MP 744 **Effects of Oxidative Stress on the Conformational Stability of Hemoglobin Measured by IMS-MS**; Daniel W. Woodall[1]; Tarick J. El-Baba[1]; Shannon A. Raab[1]; Daniel R. Fuller[1]; David E. Clemmer[1]; *[1]Indiana University, Bloomington, IN*

MP 745 **Collision-Induced Unfolding and Dissociation Reveal the Location of Ni(II) Binding in the Dimer of the Alpha-Crystallin Domain of HSPB5**; Seoyeon Hong[1]; Matthew F Bush[1]; *[1]University of Washington, Seattle, WA*

MP 746 **Epoxides Are New Footprinting Reagents for Interrogating Protein Higher-Order Structure**; Weidong Cui[1]; Ming Cheng[1]; Michael L Gross[1]; *[1]Washington University, St. Louis, MO*

MP 747 **Molecular Mechanism of Structural Rearrangements During Photoregulation of OCP and Binding of FRP**; Sayan Gupta[1]; Corie Y Ralston[1]; Cheryl A Kerfeld[1, 2]; Christopher J. Petzold[1]; Maria Agustina Dominguez-Martin[2]; Han Bao[2]; Markus Sutter[1, 2]; Ashlee Feng[1]; Emily G Pawlowski[2]; Jun Feng[1]; Leanne-Jade G Chan[1]; *[1]Lawrence Berkeley National Laboratory, Berkeley; [2]Michigan State University, East Lansing, MI*

MP 748 **Evaluating the Utility of Submicron (0.07 to 0.2 µM) Static Nanoelectrospray Capillaries for Native Mass Spectrometry**; Joshua Gilbert[1]; Erin M Panczyk[2]; Gargi Jagdale[3]; Lane A Baker[3]; Vicki H. Wysocki[2]; *[1]Ohio State University, Columbus, OH; [2]The Ohio State University, Columbus, OH; [3]Indiana University, Bloomington, IN*

MP 749 **Extensive Trajectory Method Calculations Reveal the Charge-State Effects on Protein CCSs**; Joana Costeira-Paulo[1]; Erik G. Marklund[1]; *[1]Uppsala University, Uppsala, Sweden*

MP 750 **A Tandem Mass Spectrometry Study of pH-Dependent Modification of Peptides by Epoxides**; Ming Cheng[1]; Zhengxuan Cui[1]; Bojie Zhang[1]; Michael L Gross[1]; *[1]Washington University, St.louis, MO*

MP 751 **Crosslinking Mass Spectrometry to Probe Solution Conformations of Tau as Monomer and in Triage Complex**; Lolita Piersimoni[1]; Eric Tse[2]; Angela Wiggins[2]; Daniel Southworth[2]; Hollis Showalter[2]; Philip C. Andrews[3]; *[1]University of Michigan Medical School, Ann Arbor, MI; [2]University of Michigan, Ann Arbor, MI; [3]University of Michigan Medical School, Ann Arbor, MI*

MP 752 **Protein Footprinting Probes the Conformational Changes During Aβ42 Aggregation Upon Binding to Small Molecule Inhibitors**; Ke Sherry Li[1]; Saketh Chemuru[1]; Don L. Rempel[1]; Justin Paulose[2]; George Mathai[2]; Michael L Gross[1]; *[1]Washington University in St. Louis, St. Louis, MO; [2]Sacred Heart College, Cochin, India*

MP 753 **Using SIM-XL and Quantitative Cross-Linking Mass Spectrometry to Characterize Homodimer Interfaces of Isotopically-Labeled Proteins**; Juliana de S. da G. Fischer[1]; John Melchior[2]; Diogo B Lima[3]; Jamie Morris[2]; Valmir C Barbosa[4]; Tatiana A C B Souza[1]; Julia Chamot-Rooke[3]; Mariana Fioramonte[5]; Fabio C Gozzo[5]; Sean Davidson[2]; Paulo C Carvalho[1]; *[1]Fiocruz, Curitiba, Brazil; [2]University of Cincinnati, Cincinnati, OH; [3]Institute Pasteur, Paris, France; [4]Federal University of Rio de Janeiro, Rio de Janeiro, Brazil; [5]University of Campinas, Campinas, Brazil*

MP 754 **Heteromeric Self-Assembly of Amyloid β 1-42 and 1-40 in the Early Stage of Fibrillation**; Chae Eun Heo[1]; Tau Su Choi[2]; Hugh I. Kim[2]; *[1]Korea university, Seoul, South Korea; [2]Korea University, Seoul, South Korea*

PROTEINS: GENERAL AND MEMBRANE
755-775

MP 755 **Investigating a Membrane-Bound Globin Coupled Sensor and Its Oxygen-Mediated Channel Formation: a Native Mass Spectrometry Approach**; Dietmar Hammerschmid[1]; Catherine Venien-Bryan[2]; Sylvia Dewilde[1]; Frank Sobott[3, 4]; *[1]Department of Biomedical Sciences, University of Antwerp, Antwerp, Belgium; [2]Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie, Paris, France; [3]Astbury Centre for Structural Molecular Biology, Leeds, UK; [4]School of Molecular and Cellular Biology, Leeds, UK*

MP 756 **Important Considerations for LC-MS Based Drug Transporter Quantitation**; Buyun Chen[1]; Liling Liu[2]; Hoadung Ho[2]; Yuan Chen[2]; xiaorong Liang[2]; jian payandeh[2]; Brian Dean[2]; Yuzhong Deng[2]; *[1]Genentech, South San Francisco, CA; [2]Genentech Inc., South San Francisco, CA*

MP 757 **Native Mass Spectrometry of Membrane Proteins in Physiological Salts Preserve Binding of Endogenous Lipids**; Mark T Agasid[1]; Idlir Liko[2]; Joseph Gault[3]; Carol V. Robinson[3]; *[1]University of Oxford, Oxford, UK; [2]OMass Technologies Ltd., Oxford, UK; [3]University of Oxford, UK, Oxford, UK*

MP 758 **Investigation on the Effect of Temperature and Acetonitrile on Microwave-Assisted Weak Acid Protein Hydrolysis**; Jeongkwon Kim[1]; Dabin Lee[1]; Yeoseon Kim[1]; *[1]Chungnam National University, Daejeon, South Korea*

MP 759 **Probing the Structural Changes of Biological Complexes with Internal Cavities After Transfer to the Gas-Phase Using Native IM-MS and MD**; Jesse W Wilson[1]; Amber D Rolland[1]; Grant M Klausen[1]; Daniel Ko[1]; Nathan J Hardenbrook[2]; Bryan A Krantz[2]; James S Prell[1, 3]; *[1]University of Oregon Department of Chemistry and Biochemistry, Eugene, OR; [2]Department of Microbial Pathogenesis, School of Dentistry, University of Maryland, Baltimore, MD; [3]Materials Science Institute, University of Oregon, Eugene, OR*

MP 760 **Characterization of Compositional Heterogeneity in Intact Nanodisc Ions Containing Two Different Types of Lipids using Fourier-Transformed Native Mass Spectra**; James S Prell[1, 2]; Sean P Cleary[1]; *[1]University of Oregon Department of Chemistry and Biochemistry, Eugene, OR; [2]Materials Science Institute, University of Oregon, Eugene, OR*

MP 761 **Automated Sample Preparation Enables Miniaturization of Cell Surface Capture for Identification of Cell Surface N-Glycoproteins from Small Sample Sizes**; Rachel A. Jones Lipinski[1]; Matthew Waas[1]; Theodore R. Keppel[1, 2]; Ranjuna Weerasekera[1]; Polly A. Hansen[1]; John A. Corbett[1]; Rebekah L. Gundry[1, 2]; *[1]Medical College of Wisconsin,*

Milwaukee, WI; [2]Center for Biomedical Mass Spectrometry Research, Medical College of Wisconsin, Milwaukee, WI

MP 762 **Mass Spectrometry of Collagen Preserved in Neolithic Animal Bones for the Identification of Species**; Takashi Nakazawa[1]; Mao Karino[1]; Saiji Arai[2]; Keiko Ohnishi[3]; Kazuki Kawahara[4]; Yoko Taniguchi[5]; Akira Tsuneki[5]; Seiji Kadowaki[3]; Yoshihiro Nishiaki[6]; *[1]Nara Women's University, Nara, Japan; [2]The Graduate University of Advanced Studies, Miura-Gun Hayama-Cho, Japan; [3]Nagoya University, Nagoya, Japan; [4]Osaka University, Suita, Japan; [5]Tsukuba University, Tsukuba, Japan; [6]The University of Tokyo, Bunkyo, Japan*

MP 763 **Best Practices and Benchmarks for Mass Spectrometry of Intact Proteins**; Daniel p Donnelly[1]; Catherine M Rawlins[1]; Caroline J. DeHart[2]; Luca Fornelli[2]; Luis F Schachner[2]; Ziqing Lin[3]; Jeremy J Wolff[4]; Jennifer Lippens[5]; Iain D. G. Campuzano[5]; Jared R Auclair[1]; Ljiljana Pasa Tolic[6]; Julia Chamot-Rooke[7]; Paul O Danis[8]; Lloyd M. Smith[9]; Yury Tsybin[10]; Joseph A Loo[11]; Ying Ge[12]; Neil L. Kelleher[2]; Jeffrey N Agar[1]; *[1]Northeastern University, Boston, MA; [2]Northwestern University, Evanston, IL; [3]University of Wisconsin-Madison, Madison, Wisconsin; [4]Bruker Daltonics Inc., Billerica, MA; [5]Amgen, Thousand Oaks, CA; [6]Pacific Northwest National Laboratory, Richland, WA; [7]Institute Pasteur, Paris, France; [8]Eastwood Consulting, Boylston, MA; [9]University of Wisconsin–Madison, Madison, WI; [10]Spectroswiss, Lausanne, Switzerland; [11]UCLA, Los Angeles, CA; [12]Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI*

MP 764 **Application of Isotope Dilution Mass Spectrometry Method in Low-level CHO Cell Impurity Protein Quantification**; Feng Yan[1]; Zi Wang[1]; *[1]GSK Vaccines, Rockville, MD*

MP 765 **High-Throughput Accurate Mass UPLC-MS of GPCR's, Water Channels and a Start Domain Superfamily Binding Protein: a Structural Biology Support Effort**; Jennifer L Lippens[1]; Pascal F Egea[2]; Christopher Spahr[1]; Joseph A Loo[2]; Iain D. G. Campuzano[1]; *[1]Amgen, Thousand Oaks, CA; [2]UCLA, Los Angeles, CA*

MP 766 **Detecting Low Abundance Proteins in the Complex Background of the Cochlea by Mass Spectrometry**; Miguel Ramirez[1]; Nopporn Jongkamonwiwat[1]; Jeffrey N. Savas[1]; *[1]Northwestern University, Chicago, IL*

MP 767 **A Comparative Proteomics Study of Five Serum Exosome Isolation Procedures**; Hongbin Zhu[1]; Betsy Benton[1]; Chris Wojewodzki[1]; Barbara Kaboord[1]; John C. Rogers[1]; *[1]Thermo Fisher Scientific, Rockford, IL*

MP 768 **Investigating Peptide Assembly in a Membrane Environment**; Megan Murray Gessel[1]; Megan Kober[1]; Zoe Maxwell[1]; Samantha Swain[1]; *[1]University of Puget Sound, Tacoma, WA*

MP 769 **Characterization of Native Proteins Using Enhanced-Fluidity Hydrophobic Interaction Chromatography-Mass Spectrometry**; Yanhui Wang[1]; Susan Olesik[1]; *[1]Ohio State University, Columbus, OH*

MP 770 **Proteomic Analysis of Detergent Insoluble Pathogenic Proteins in the Amygdala of Cognitively Impaired Elderly Persons for Novel Misfolded Proteins**; Jing Chen[1]; Jozsef Gal[1]; Yuriko Katsumata[1]; David W Fardo[1]; Wang-Xia Wang[1]; Sergey Artiushin[1]; Douglas Price[1]; Sonya Anderson[1]; Ela Patel[1]; Haining Zhu[1]; Peter T. Nelson[1]; *[1]University of Kentucky, Lexington, KY*

MP 771 **Native MS Provides Insight into Eye Lens Aquaporins**; Sophie R Harvey[1]; Erin M Panczyk[1]; Yue Ju[1]; Wendy L White[2]; Kevin L. Schey[2]; Vicki H Wysocki[1]; *[1]The Ohio State University, Columbus; [2]Vanderbilt University Medical Center, Nashville, TN*

MP 772 **Effect of Exercise on Metabolism of Fluoride in Kidney of Mice: Proteomic Analysis**; Mileni S Fernandes[1]; Aline Lima Leite[1]; Mayara Florencio Fabrício[2]; Sandra Lia Amaral[3]; Marília Afonso Rabelo Buzalaf[1]; *[1]USP-FOB, Bauru, Brazil; [2]UFSCAR, São Carlos, Brazil; [3]UNESP, BAURU, Brazil*

MP 773 **Using Native Ion Mobility Mass Spectrometry to Investigate Membrane Protein – Lipid Interactions**; John Patrick; *Texas A&M, College Station, TX*

MP 774 **Apparatus for High-throughput Filtration of Cell Lysates**; Asha A Oroskar[1]; Babu S Antharavally[1]; Anil R Oroskar[1]; *[1]Orochem Technologies Inc., Naperville, IL*

MP 775 **Effects of Temperature and Acetonitrile Amount on Microwave- Assisted Tryptic Digestion of Horse Skeletal Muscle Myoglobin and Bovine Serum Albumin**; Yeoseon Kim[1]; Dabin Lee[1]; Jeongkwon Kim[1]; *[1]Chungnam National University, Daejeon, South Korea*

PROTEOMICS: QUANTITATIVE I
776-807

MP 776 **Mass Spectrometry based Proteomics to Investigate the Molecular Changes in Rat Atria During Obstructive Sleep Apnea**; Madhuri Jayathirtha[1]; Devika Channaveerappa[1]; Cristiana Dumbraveanu[1]; Jacob Lux[2]; Meredith McLerie[2]; Brian K. Panama[2]; Costel C. Darie[1]; *[1]Clarkson University, Potsdam, NY; [2]Masonic Medical Research Laboratory, Utica, NY*

MP 777 **Genetic Wiring Maps of Single Protein States Reveal an Off-Switch for GPCR Signaling**; Onno Bleijerveld[1]; Markus Brockmann[2]; Vincent A Blomen[2]; Joppe Nieuwenhuis[2]; Elmer Stickel[2]; Matthijs Raaben[2]; Maarten Altelaar[1, 3]; Lucas Jae[2]; Thijn R Brummelkamp[2, 4]; *[1]The Netherlands Cancer Institute, Proteomics Facility, Amsterdam, Netherlands; [2]The Netherlands Cancer Institute, Amsterdam, Netherlands; [3]Biomolecular Mass Spectrometry and Proteomics, Utrecht University, Utrecht, Netherlands; [4]cancergenomics.nl, Amsterdam, Netherlands*

MP 778 **Quantitative Proteomics of Murine Bronchoalveolar Lavage Fluid Following Respiratory Exposures to 4,4'-Methylene Diphenyl Diisocyanate**; Justin M. Hettick[1]; Brandon F. Law[1]; Chen-Chung Lin[1]; Paul D. Siegel[1]; *[1]NIOSH, Morgantown, WV*

MP 779 **Proteome-Wide Modulation of Degradation Dynamics in Response to Growth Arrest**; Sina Ghaemmaghami[1]; Tian Zhang[2]; Kevin Welle[1]; Jennifer Hryhorenko[1]; *[1]University of Rochester, Rochester, NY; [2]Harvard Medical School, Boston, MA*

MP 780 **Resistome Profiling in Gram-Negative Bacteria to Identify Selection-Averse Antimicrobial Drug Targets**; Anaamika Campeau[1]; Connor Olson[1]; Adam Feist[1]; Bernhard Palsson[1]; David Gonzalez[1]; *[1]UC San Diego, San Diego, CA*

MP 781 **Evaluation of a Dual Isolation Mode Method for Improved Isobaric Labelling Protein Quantification**; Theodoros I Roumeliotis[1]; Jyoti S Choudhary[1]; *[1]The Institute of Cancer Research, London, UK*

MP 782 **Quantitative Temporal Proteomics Captures Differential Antiviral Immune Responses Between GM-CSF- and M-CSF-Stimulated Macrophages Following Exposure to Oncolytic Reovirus**; Michael Giacomantonio[1]; Andra M Sterea[1]; Patrick Murphy[1]; Youra Kim[1]; Derek R Clements[1]; Joao A. Paulo[2]; Steven P Gygi[2]; Shashi Gujar[1]; *[1]Dalhousie University, Halifax, NS, Canada; [2]Harvard Medical School, Boston, MA*

MP 783 **A Targeted Quantitative Proteomic Method Uncovers DNAJB4 as a Novel Suppressor for Melanoma Metastasis**; Weili Miao[1]; Yinsheng Wang[2]; *[1]University of California, Riverside, CA; [2]UC Riverside, Riverside, CA*

MP 784 **Integrated Proteomic Approaches to Dissect Complex Signaling Pathways in the Epithelial to Mesenchymal Transition**; Paola Cavaliere[1]; Michal Nagiec[1]; Adnan Ahmed[1]; Vijay J Raja[1]; John Blenis[1]; Noah Dephoure[1]; *[1]Weill Cornell Medicine, New York City, NY*

MP 785 **Drosophila Melanogaster Head Proteomics with Amyloid Beta 42 Expression**; Chris Brown[1]; Melissa A Phelps[1]; Robert C Eisman[1]; Jonathan C Trinidad[1]; Thomas C Kaufman[1]; David E Clemmer[1]; *[1]Indiana University, Bloomington, IN*

MP 786 **Multi-Proteomic Approach for Studying Drug Resistance in Ovarian Cancer**; Vijay J Raja[1]; Adnan Achmed[1]; Paola Cavaliere[1]; Noah Dephoure[1]; *[1]Weill Cornell Medicine, New York City, NY*

MP 787 **Identification of Guanine-Quadruplex-Binding Proteins Zi Gao, Preston Williams, Lin Li and Yinsheng Wang**; Zi Gao; *University of California, Riverside, Riverside, CA*

MP 788 **Evaluation of a Two-Proteome Quality Control Standard for TMT-Based Proteomics: the HYPER Standard**; Steven P Gygi[1]; Jose Navarrete-Perea[1]; Edward L Huttlin[1]; Devin K Schweppe[1]; Joao A Paulo[1]; *[1]Harvard Medical School, Boston, MA*

MP 789 **Accurate, Sensitive, and Precise Multiplexed Proteomics using the Complement Reporter Ion Cluster**; Matthew Sonnett[1]; Eyan Yeung[1]; Martin Wühr[1]; *[1]Princeton University, Princeton, NJ*

MP 790 **Highly Streamlined Sample Processing for TMT-SPS-MS3: Proteomics and Phosphoproteomics in a Simple Workflow**; Joao A Paulo[1]; Jose Navarrete-Perea[1]; Steven P Gygi[1]; *[1]Harvard Medical School, Boston, MA*

MP 791 **Workflow Dependent Bias in Whole Proteome Analysis: Gene Ontologies and Modification Artifacts**; Lynn A. Spruce[1]; Hua Ding[1]; Asif Amin Dar[1]; Hossein Fazelinia[1]; Steven H. Seeholzer[2]; *[1]Children's Hospital of Philadelphia, Philadelphia, PA; [2]Children's Hospital of Philadelphia, Philadelphia, PA*

MP 792 **Quantitative Chemical Proteomic Strategy for Site-Specific Stoichiometric Analysis of Ubiquitination**; Jonathan Evers[1]; Zachary Postler[1]; Mohamed Jama[1]; Yue Chen[1]; *[1]University of Minnesota at Twin Cities, Minneapolis, MN*

MP 793 **Proteomics of Honey Bee (Apis melliferaL)–Quantification of Proteome Changes Following Oral Sterol Intake**; Liping Yang[1]; Priyadarshini Chakrabarti[2]; Ramesh R. Sagili[2]; Claudia S Maier[3]; *[1]Oregon State University, Corvallis, OR; [2]Department of Horticulture, Oregon State University, Corvallis, OR; [3]Department of Chemistry, Oregon State University, Corvallis, OR*

MP 794 **Targeted MS-based Assay to Assess Real Time Performance of Immunoaffinity Depletion Columns for Plasma**; Michael W. Burgess[1]; Harrison M. Specht[2]; Luke J. Wallace[1]; Michael A. Gillette[1]; Hasmik Keshishian[1]; Steven A. Carr[1]; *[1]Broad Institute, Cambridge, MA; [2]Northeastern University, Boston, MA*

MP 795 **High-Throughput Quantitative Profiling of Small GTPases in Tamoxifen-Resistant and Radio-Resistant Breast Cancer Cells**; MING HUANG[1]; Yinsheng Wang[1]; *[1]University of California, Riverside, Riverside, CA*

MP 796 **A Comparison of Different Protein Extraction Methods from Mammalian Cells to Optimize Proteome Coverage and Reproducibility**; Km Shams Ud Doha[1]; Renuka Sabnis[1]; Alicia Richards[1]; Ramon Diaz Pena[1]; Alexandre Rosa Campos[1]; *[1]Sanford Burnham Prebys Medical Discovery Institute, San Diego, CA*

MP 797 **Methanosarcina Mazei Proteomic Response to Different Methylotrophic Substrates**; Deborah Jarrett[1]; Farzaneh Sedighian[1]; Hong Hanh Nguyen[1]; Robert P Gunsalus[1]; Joseph A Loo[1]; Rachel O. Loo[1]; *[1]UCLA, Los Angeles, CA*

MP 798 **Application of Data Independent Acquisition to Identify Proteins Involved in the Intestinal Mucosa of Early-Weaning Piglets**; Bing Xia[1]; Qingshi Meng[1]; Xiaohui Feng[1]; Hongfu Zhang[1]; *[1]State Key Laboratory of Animal Nutrition, Institute of Animal Sciences; Chinese Academy of Agricultural Sciences, Beijing, China*

MP 799 **Effects of New Combination Therapy in Gemcitabine-Sensitive and Resistant Pancreatic Cancer Cell Lines Using Highly Reproducible, Ion-Current Based Quantitative Proteomics**; Sailee Rasam[1, 2]; Shichen Shen[2]; Qingxiang Lin[3, 4]; Xue Wang[2, 4]; Robert Straubinger[2, 3, 4]; Jun Qu[1, 2, 3, 4]; *[1]Department of Biochemistry, State University of New York, Buffalo, NY; [2]New York State Center of Excellence in Bioinformatics and Life Sciences, 701 Ellicott Street, Buffalo, NY; [3]Department of Pharmaceutical Sciences, State University of New York, Buffalo, NY; [4]Department of Cell Stress Biology, Roswell Park Cancer Institute, Elm and Carlton Streets, Buffalo, NY*

MP 800 **Integrated Proteome and HLA Peptidome Quantitation with Tandem Mass Tags**; Patrick Murphy[1]; Prathyusha Konda[2]; Joao A. Paulo[3]; Heiko Schuster[4]; Daniel J Kowalewski[4]; Youra Kim[1]; Derek R Clements[2]; Michael Giacomantonio[2]; Stefan Stevanovic[4]; Steven P Gygi[5]; Shashi Gujar[2]; *[1]Dalhousie University, Halifax; [2]Dalhousie University, Halifax, NS, Canada; [3]Harvard Medical School, Boston, MA; [4]Tubingen Univeristy, Tubingen, Germany; [5]Harvard Medical School, Boston, MA*

MP 801 **Determining Late-Stage Ribosome Assembly with SWATH-MS**; Jessica N Rabuck-Gibbons[1]; Joseph H Davis[2]; James R. Williamson[1]; *[1]The Scripps Research Institute, La Jolla, CA; [2]Massachusetts Institute of Technology, Cambridge, MA*

MP 802 **Label Free Comparative Protein Expression Profiling of MCf7 and K562 Cancer Cells Treated with Mitomycin C and Decarbamoylmitomycin C**; Cristina C Clement[1]; Shu-Yuan Cheng[2]; Monika Dzieciatkowska[3]; William Aguilar[4]; Elise Champeil[4]; *[1]Albert Einstein College Medicine, Bronx, NY; [2]Department of Science, John Jay College of Criminal Justice, CUNY, New York, NY, United States, New York City, NY; [3]Biological Mass Spectrometry Core Facility, University of Colorado Denver, Aurora, CO; [4]John Jay College of Criminal Justice, New York, NY*

MP 803 **Multiplexed Analysis of Purifications from Biold and AP-MS Workflows Using Isobaric Tags**; Stefan K Maier[1]; Cassandra Wong[1]; Brett Larsen[1]; Anne-Claude Gingras[1]; *[1]Lunenfeld-Tanenbaum Research Institute, Toronto*

MP 804 **Kinetics of β-Adrenergic Phosphorylation in Proximity of Cardiac Cav1 Channels: proximity-Phosphoproteomics in Hearts of APEX Mice**; Marian Kalocsay[1]; Guoxia Liu[2]; Steven O. Marx[2]; Steven P Gygi[1]; *[1]Harvard Medical School, Boston, MA; [2]Columbia University, New York, NY*

MP 805 **Proteome-Wise Comparison of PAXgene Fixed to Fresh Frozen Human Tissue Samples**; Ruiqi Jian[1]; Lihua Jiang[1]; Joanne Chan[1]; Hua Tang[1]; Michael Snyder[1]; *[1]Stanford University, Palo Alto, CA*

MP 806 **A Novel Bioinformatic Pipeline for Data Analysis Reduction in Reporter Ion Quantification Experiments**; Conor Jenkins[1, 2]; Alexis L Norris[3]; Benjamin Orsburn[1]; *[1]National Cancer Institute @ Frederick, Frederick, MD; [2]Hood College, Frederick, MD; [3]The Johns Hopkins University, Baltimore, MD*

MP 807 **Ion-Current-Based Temporal Proteomic Analysis Identifies RGS12 as a Novel Regulator of Osteoclast Redox State Through NRF2**; Andrew Ng[1, 2, 3]; Chengjian Tu[1, 2]; Jun Qu[1, 2]; Shuying Yang[4]; *[1]University at Buffalo, Buffalo, NY; [2]New York State Center of Excellence in Bioinformatics and Life Sciences, Buffalo, NY; [3]University of Pennsylvania, Philadelphia, PA; [4]University of Pennsylvania, PA*

SYSTEMS BIOLOGY
808-824

MP 808 **Integrated Omics Analyses Reveal the Proteins and Lipids and Their Associated Pathways Crucial for the Swarming Motility in Panenibacillus Polymyxa**; Suresh Poudel[1]; Richard J. Giannone[2]; Abigail T. Farmer[1]; Shawn R. Campagna[1]; Amber N. Bible[2]; Jennifer L. Morrell-Falvey[2]; James G. Elkins[2]; Robert L. Hettich[2]; *[1]University of*

Tennessee, Knoxville, TN; [2]Oak Ridge National Laboratory, Oak Ridge, TN

MP 809 **Proteomic Characterization of the Embryonic Neural Ectoderm Cells in the Xenopus laevisEmbryo**; Aparna Baxi[1, 2]; Camille Lombard-Banek[1]; Sally A Moody[2]; Peter Nemes[1, 2]; *[1]Department of Chemistry & Biochemistry, University of Maryland, College Park, MD; [2]Department of Anatomy & Regenerative Biology, The George Washington University, Washington, District of Columbia*

MP 810 **Global Mapping of Protein Subcellular Localisation in an Apicomplexan Parasite Toxoplasma Gondii by a Quantitative Mass Spectrometry-Based Proteomics Approach**; Konstantin Barylyuk[1]; Ludek Koreny[1]; Huiling Ke[1]; Simon Butterworth[1]; Imen Lassadi[1]; Tobias Mourier[2]; Laurent Gatto[1]; Arnab Pain[2]; Kathryn S. Lilley[1]; Ross F. Waller[1]; *[1]Department of Biochemistry, University of Cambridge, Cambridge, UK; [2]Biological and Environmental Science and Engineering Division, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia*

MP 811 **DIA Analysis of Cellular Reprogramming Using SWATH-MS**; Uxue Ulanga Amondarain[1]; Dave Lee[2]; Julie Brazzatti[2]; Stefano Patassini[3]; Stella Pearson[3]; Ciaren Graham[4]; Anthony Whetton[2, 3]; Robert Graham[1, 2]; *[1]Clinical Proteomics Research Group, Division of Molecular and Clinical Cancer Sciences, Faculty of Biology, Medicine and Health, University of Manchester, Oxford Road, Manchester, UK; [2]Stoller Biomarker Discovery Centre, Division of Molecular and Clinical Cancer Sciences, Faculty of Biology, Medicine and Health, University of Manchester, Oxford Road, Manchester, UK; [3]Stem Cell & Leukaemia Proteomics Laboratory, Manchester Cancer Research Centre, Division of Molecular and Clinical Cancer Sciences, Faculty of Biology, Medicine & Health, University of Manchester, Manchester, UK; [4]Centre for Biosciences, School of Healthcare Science, Manchester Metropolitan University, Manchester, UK*

MP 812 **Profiling the Kinome and Phosphoproteome of Mutant KRAS-driven Pancreatic Ductal Adenocarcinoma**; Laura E Herring[1, 2]; Thomas SK Gilbert[2]; Nely Dicheva[1, 2]; Emily G Werth[3]; Emily M Wilkerson[1, 2]; Angelina V Vaseva[4]; Kirsten L Bryant[5]; Devon R Blake[2]; J Nathaniel Diehl[6]; Naim Rashid[5, 7]; Channing J Der[2, 5]; Lee M Graves[1, 2, 5]; *[1]UNC Proteomics Core Facility, UNC-Chapel Hill, Chapel Hill, NC; [2]Department of Pharmacology, UNC-Chapel Hill, Chapel Hill, NC; [3]Department of Chemistry, UNC-Chapel Hill, Chapel Hill, NC; [4]University of Texas Health Science Center, San Antonio, TX; [5]Lineberger Cancer Center, UNC-Chapel Hill, Chapel Hill, NC; [6]Genetics and Molecular Biology, UNC-Chapel Hill, Chapel Hill, NC; [7]Department of Biostatistics, UNC-Chapel Hill, Chapel Hill, NC*

MP 813 **Serial-Omics Characterization of Equine Urine and Mane Hair by LC-MS/MS**; Min Yuan[1]; Susanne B Breitkopf[1]; John M Asara[1]; *[1]Beth Israel Deaconess Medical Center/ Harvard Medical School, Boston, MA*

MP 814 **Unraveling FGF-2 Signaling to Chromatin in Cancer Cell Lines Using an Optimized Phospho-Epi-Proteomics Strategy**; Mariana Lopes[1]; Francisca Vitorino[1]; Simone Sidoli[2]; Benjamin A Garcia[2]; Julia Cunha[1]; *[1]Laboratório Especial de Ciclo Celular (LECC/CeTICs), Center of Toxins, Immune-Response and Cell Signaling - CeTICS, Instituto Butantan, São Paulo, Brazil; [2]Epigenetics Institute, Department of Biochemistry and Biophysics, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA*

MP 815 **Evaluation of Advanced Peak Determination (APD) for Tandem Mass Tag (TMT)-Based Quantitative Proteomics Across Instrument Platforms**; Samuel Myers[1]; Susan Klaeger[2]; ROSA VINER[3]; jae Choi[4]; John C. Rogers[4]; Tabiwang N Arrey[5]; Namrata Udeshi[2]; Karl Clauser[2]; Steven A Carr[2]; *[1]Broad Institute, Cambridge, CA; [2]Broad Institute, Cambridge; [3]Thermo Fisher Scientific, San Jose, CA; [4]Thermo Fisher Scientific, Rockford, IL; [5]Thermo Fisher Scientific, Bremen, Germany*

MP 816 **Leveraging Microbial Community Proteomics to Elucidate the Development of the Gut Microbiome's Metabolic Network in Preterm Infants**; J. Alfredo Blakeley-Ruiz[1, 2]; Suresh Poudel[1, 2]; Weili Xiong[2]; Christopher T. Brown[3]; Michael J. Morowitz[4]; Jillian F. Banfield[3]; Robert L. Hettich[1, 2]; *[1]Genome Science and Technology Program, University of Tennessee, Knoxville, Tennessee; [2]Oak Ridge National Laboratory, Oak Ridge, TN; [3]University of California Berkeley, Berkeley, CA; [4]University of Pittsburgh, Pittsburgh, PA*

MP 817 **Quantification of Transcriptional Regulatory Proteome Dynamics Using Data Independent Acquisition**; Alexander J Federation[1]; Tanya Kutyavin[1]; John A Stamatoyannopoulos[1]; Michael J MacCoss[2]; *[1]Altius Institute, Seattle, WA; [2]University of Washington Genome Sciences, Seattle, WA*

MP 818 **Experimental Design and Data Normalization in a Large-Scale Multiplexed Proteomics Project**; David Nusinow[1]; John Szpyt[1]; Christopher Rose[1]; Marian Kalocsay[1]; Mahmoud Ghandi[2]; Steven P Gygi[1]; *[1]Harvard Medical School, Boston, MA; [2]Broad Institute of MIT and Harvard, Cambridge, MA*

MP 819 **An Integrative Experimental and Mathematical Approach Discovers a Critical Role for Peroxisomes in Viral Infection**; Pierre M. Jean Beltran[1]; Yutaka Hashimoto[1]; Katelyn Cook[1]; Cyril Galitzine[2]; Morgan Jones[1]; Olga Vitek[2]; Ileana M. Cristea[1]; *[1]Princeton University, Princeton, NJ; [2]Northeastern University, Boston, MA*

MP 820 **Multiplexed Protein Turnover Profiling for Large-Scale Identification of Drug Targets and Characterization of Drug Mode-Of-Action**; Miguel Martin Perez[1]; Judit Villén[1]; *[1]University of Washington Genome Sciences, Seattle, WA*

MP 821 **Systems Biology of MHC Class I Antigen Presentation Studied in Human Cancer Cell Lines**; Jennifer Hahlbrock[1]; Pedro Navarro[2]; Sebastian Boegel[3]; Maike Wagner[3]; Ugur Sahin[3]; Hansjörg Schild[1]; Stefan Tenzer[1]; *[1]University Medical Center Mainz, Mainz, Germany; [2]Thermo Fisher Scientific, Bremen, Germany; [3]TRON, Mainz, Germany*

MP 822 **Label-Free Quantification of T-Cell Proteome in Nephrotic Syndrome**; Cerina Chhuon[1]; Pauline Vachin[2, 3]; Kelhia Sendeyo[2, 3]; André Pawlak[2, 3]; Dil Sahali[2, 3, 4, 5]; Mario Ollero[2, 3]; Chiara Guerrera[1]; *[1]Proteomics Platform Necker, Paris, France; [2]Institut National de la Santé et de la Recherche Médicale (INSE RM), UMRS 955, Equipe 21, Créteil, France; [3]Université Paris Est, Faculté de Médecine, UMRS 955, Equipe 21, Créteil, F-94010, France, Créteil, France; [4]AP-HP, Groupe Henri-Mondor Albert-Chene vier, Service de Néphrologie, Créteil, F-14 94010 France, Créteil, France; [5]Institut francilien de recherche en néphrologie et transplantation, Créteil, France*

MP 823 **Real-Time, Millisecond Assignment of Sub-Proteome Peptides Unravels Cellular Systems Within Cancer Cell Lines**; Brian Erickson[1]; Julian Mintseris[1]; Alison Erickson[1]; Joao A. Paulo[1]; Devin K. Schweppe[1]; Jose Navarrete-Perea[1]; Jiaming Li[1]; David Nusinow[1]; Edward Huttlin[1]; Derek J Bailey[2]; Steven Gygi[1]; *[1]Harvard Medical School, Boston, MA; [2]Thermo Fisher Scientific, San Jose, CA*

MP 824 **A Proteome- and Lipidome-Wide Systems Genetic Analysis of Hepatic Lipid Metabolism**; Benjamin Leo Parker[1]; Anna C Calkin[2]; Marcus M Seldin[3]; Elizabeth J Tarling[3]; Yingying Liu[2]; Eser J Zerenturk[2]; Pengyi Yang[1]; Kaushala Jayawardana[2]; Calvin Pan[3]; Natalie A Mellet[2]; Jacquelyn M Weir[2]; Ross Lazarus[2]; Aldons J Lusis[3]; Peter J. Meikle6 J Meikle[2]; David E James[1]; Thomas Q. de Aguiar Vallim[3]; Brian G Drew[2]; *[1]The University of Sydney, Sydney, Australia; [2]Baker Heart & Diabetes Institute, Melbourne, Australia; [3]UCLA, Los Angeles, CA*

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

AMBIENT IONIZATION: FUNDAMENTALS AND INSTRUMENTATION
001-026

TP 001 **Effect of Solvent Composition on the Analysis of Aerosol Generated by Pyrolized Cellulose Using Coaxial EESI-MS**; Anne L. Worth[1]; Kenneth D. Swanson[1]; Gary L. Glish[1]; *[1]University of North Carolina at Chapel Hill, Chapel Hill, NC*

TP 002 **Probing the Mechanism of Coaxial Extractive Electrospray Ionization**; Kenneth Swanson[1]; Paul S. Soma[1]; Gary L. Glish[1]; *[1]University of North Carolina, Chapel Hill, NC*

TP 003 **Characterization of Novel Plasma-Ionization Source for Real-Time Breath Analysis**; Christopher Gongar[1]; Michael Wei[1]; Richard A. Yost[1]; *[1]University of Florida Department of Chemistry, Gainesville, FL*

TP 004 **A Versatile Integrated Ambient Ionization Source Platform**; Ai Wanpeng[1]; Nie Honggang[1]; Song Shiyao[1]; Liu Xiaoyun[1]; Bai Yu[1]; Liu Huwei[1]; *[1]Peking Univ, Beijing, China*

TP 005 **Development of Polystyrene-Impregnated Paper Substrate for Direct Mass Spectrometric Analysis of Proteins and Peptides in Complex Matrices**; Jin Li[1]; Yajun Zheng[1]; Wei Mi[1]; Weiwei Han[1]; Yue Ji[1]; Zhiping Zhang[1]; *[1]Xi'an Shiyou University, Xi'an, China*

TP 006 **Rapid Quantitationof Free Fatty Acids in Blood for Type 2 Diabetes Diagnosis Using Functionized Capillaries**; Wenpeng Zhang[1, 2]; Spencer Chiang[1, 2]; Qinhua Chen[3]; Zheng Ouyang[1, 2]; *[1]State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instruments, Tsinghua University, Beijing, China; [2]Weldon School of Biomedical Engineering, Purdue University, West Lafayette, IN; [3]Affiliated Dongfeng Hospital, Hubei University of Medicine, Shiyan, China*

TP 007 **Single Cell Analysis of Infected Cellular Subpopulations by Fiber-Based Laser Ablation Electrospray Ionization Mass Spectrometry with Multimodal Microscopy Targeting**; Rikkita Khattar[1]; Sylwia A Stopka[1]; Laith Z Samarah[1]; Beverly J Agtuca[2]; Christopher R Anderton[3]; David W Koppenaal[3]; Ljiljana Pasa Tolic[3]; Gary Stacey[2]; Akos Vertes[1]; *[1]The George Washington University, Washington, DC; [2]University of Missouri, Columbia, MO; [3]Pacific Northwest National Laboratory, Richland, WA*

TP 008 **Utilisation of Mid - Infrared Lasers for Rapid Evaporative Ionization Mass Spectrometry Imaging and High Throughput Sampling**; Daniel Simon[1]; Tamas Karancsi[1]; Julia Balog[1]; Richard Schaffer[1]; Steven D Pringle[2]; Julia Abda[3]; Zoltan Takats[3]; *[1]Waters Research Center, Budapest, Hungary; [2]Waters Corporation, Wilmslow, UK; [3]Imperial College London, London, UK*

TP 009 **Development of a New Ambient Ionization Mass Spectrometry Using Dark Current Discharge with Argon Gas**; Kanako Sekimoto[1]; Motoshi Sakakura[2]; Hiroshi Hike[2]; Takatomo Kawamukai[2]; Teruhisa Shiota[2]; Mitsuo Takayama[1]; *[1]Yokohama City Univ., Yokohama, Japan; [2]AMR Inc., Meguro-ku, Japan*

TP 010 **Two-Laser Ablation Electrospray Ionization Mass Spectrometry**; Remi O Lawal[1]; Fabrizio Donnarumma[1]; Kermit K Murray[1]; *[1]Louisiana State University, Baton Rouge, LA*

TP 011 **Molecular Characterization of Exhaust Particulate Matters Using Extractive Atmospheric Pressure Chemical Ionization Mass Spectrometry**; Yi Li[1]; Yong Tian[2]; Hua Zhang[3]; Kun Liu[4]; FeiFang Jie[4]; Huanwen Chen[4]; *[1]Jiangxi Key Laboratory for Mass Spectrometry and Instrumentation, East China University of Technology, Nan Chang, China; [2]CAS Key Laboratory of Biobased Materials, Qingdao Institute of Bioenergy and Bioprocess Technology, Chinese Academy of Sciences, Qingdao, China; [3]State Key Laboratory of Inorganic Synthesis and Preparative Chemistry, College of Chemistry, Jilin University, Changchun, China; [4]East China University of Technology, Jiangxi Key Laboratory for Mass Spectrometry and Instrumentation, NanChang, China*

TP 012 **Solid-State RF Energy Powered Coaxial Wave-Guided Microwave Ion Sources for Small Molecule & Elemental Mass Spectrometry**; Gregory Sven Katzmann[1]; Alberto Torreño Núñez[1]; Arno Wortmann[1]; Ralf Dieter Dumler[1]; *[1]NovionX GmbH, Lindau, Germany*

TP 013 **Studying and Modifying Paper Properties and to Improve Detection Limits of Synthetic Cannabinoids and Fentanyl Using Paper Spray Mass Spectrometry**; Brandon Bills[1]; Jeffrey Kinkade[1]; Greta Ren[1]; Nicholas E. Manicke[1]; *[1]IUPUI Department of Chemistry & Chemical Biology, Indianapolis, IN*

TP 014 **Evaluation of Analytical Capabilities of Direct Spray-From-Tissue Ionization Method for a Brain Tumor Analysis**; Stanislav Pekov[1, 2]; Savva Semenov[1]; Alexander Vorobyev[1]; Konstantin Bocharov[1, 2]; Vsevolod Shurkhay[1, 3]; Anatoly Sorokin[1, 4]; Igor Popov[1, 2]; Eugene (Evgeny) Nikolaev[2, 5]; *[1]Moscow Institute of Physics and Technology, Moscow, Russia; [2]Institute for Energy Problems of Chemical Physics of RAS, Moscow, Russia; [3]N. N. Burdenko Scientific Research Neurosurgery Institute, Moscow, Russia; [4]Institute of Cell Biophysics RAS, Pushchino, Russia; [5]Skolkovo Institute of Science and Technology, Moscow Region, Russian Federation*

TP 015 **Investigating and Comparing Internal Standard Addition Methods for Direct Analyte Probed Nanoextraction (Dapne)**; Janella Marie de Jesus[1, 2]; Josephine Bunch[2]; Catia Costa[1]; Roger Webb[1]; Guido Verbeck[3]; Melanie Bailey[1]; *[1]University of Surrey, Guildford, UK; [2]National Physical Laboratory, Teddington, UK; [3]University of North Texas, Denton, Texas*

TP 016 **Comparison of Continuous Flow Infrared Desorption Electrospray Ionization and ESI in Measurement of Peptide Solution Containing Detergent or Buffer**; Koichi Kimura[1]; Hisanao Hazama[1]; Kunio Awazu[1, 2, 3]; *[1]Graduate School of Engineering, Osaka University, Osaka, Japan; [2]Graduate School of Frontier Biosciences, Osaka University, Suita, Japan; [3]Global Center for Medical Engineering and Informatics, Osaka University, Suita, Japan*

TP 017 **"On-Droplet" Chemical Reactivity of Cycloadditions and Epoxide Openings *via* theta Tip Capillaries and Electrosonic Spray Ionization Mass Spectrometry**; Ryan M Bain[1]; Shyam Sathyamoorthi[1]; Yin-Hung Lai[1]; Richard N Zare[1]; *[1]Stanford University, Palo Alto, CA*

TP 018 **Measuring the Sizes of Electrosprayed Droplets Smaller Than the Diffraction Limit of Light Using Super Resolution Fluorescence Microscopy**; Adam Hollerbach[1]; David Logsdon[1]; Kiran Iyer[1]; Anyin Li[1]; J. Andy Schaber[2]; R. Graham Cooks[1]; *[1]Purdue University, West Lafayette, IN; [2]Bioscience Imaging Facility, Bindley Bioscience Center, Purdue University, West Lafayette, IN*

TP 019 **Determining The Universality of a Model to Predict the Ionization Efficiency of Negative Electrospray Ionization**; Melanie Odenkirk[1]; Erika Hutchinson[1]; Chrisi Hughey[1]; Jeff Jones[2]; *[1]James Madison University, Harrisonburg, VA; [2]SoCal Bioinformatics Inc., Montrose, CA*

TP 020 **Direct Chemical Analysis of Sap from Living Plants by Electrospray Ionization Mass Spectrometry**; Laith Z. Samarah[1]; Tina H. Tran[1]; Beverly J. Agtuca[2]; Ljiljana Pasa-Tolic[3]; Dong Xu[2]; David G. Mendoza Cozatl[2]; Gary Stacey[2]; Akos Vertes[1]; *[1]The George Washington University, Washington, DC; [2]University of Missouri, Columbia, MO; [3]Pacific Northwest National Laboratory, Richland, WA*

TP 021 **Need for Speed? Coated Blade Spray-Mass Spectrometry: Towards Targeted and Untargeted Analysis under 10 Seconds Per Sample**; Alexander Kasperkiewicz[1]; German Augusto Gomez-Rios[1]; Daniel Rickert[1]; Marcos Tascon[1]; Vinicius Acquaro[2]; Varoon Singh[1]; Sofia Lendor[1]; Nathaly Reyes-Garces[1]; Janusz Pawliszyn[1]; *[1]University of Waterloo, Department of Chemistry, Waterloo, ON, Canada; [2]University of Sao Paulo, Sao Paulo, Brazil*

TP 022 **Effects of Interfacial Surface Tension on the Cone-Jet Mode Electrospray Ionization in Microspray**; Sau Lan Staats[1]; Anna Stoltzfus[1]; Andris Suna[1]; *[1]Phoenix S & T, Inc, Chadds Ford, PA*

TP 023 **Efficient Preparation of Organoimido Derivatives of Lindqvist Hexamolybdate in Leidenfrost Droplets**; Jie Cao; *Beijing Institute of Technology, LiangXiang Campus, Beijing, China*

TP 024 **Microdroplets Accelerate Epoxides Ring Opening**; Yin-Hung Lai[1]; Shyam Sathyamoorthi[1]; Ryan M Bain[1]; Richard N Zare[1]; *[1]Stanford University, Palo Alto, CA*

TP 025 **Inclusion of ASAP on a Multi-Ionization Platform for Analysis of Low Polarity Compounds Using Mass Spectrometry**; Charles N McEwen[1, 2]; Veronica Smith[1]; Milan Pophristic[2]; Anil Kumar Meher[2]; Santosh Karki[2]; Ellen D. Inutan[2]; *[1]Univ. of the Sciences, Philadelphia, PA; [2]MSTM, LLC, Newark, DE*

TP 026 **Metrological Study of Reims, Towards a More Robust Sampling and Ionisation Technique**; Efstathios Elia[1]; Alex Dexter[1]; Josephine Bunch[1]; *[1]National Physical Laboratory, Teddington, UK*

BIOMARKERS: QUANTITATIVE ANALYSIS
027-055

TP 027 **Enhanced Screening of Antibodies for Immuno-Mass Spectrometric Assays Using Post Immuno-Enrichment On-Bead Digestion Immuno-MALDI**; Huiyan Li[1, 2]; Claudia Fredolini[3]; Vincent R. Richard[1]; Jochen M. Schwenk[3]; Christoph H. Borchers[1, 2, 4, 5]; *[1]Jewish General Hospital Proteomics Centre, McGill University, Montreal, QC; [2]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [3]Science for Life Laboratory, School of Biotechnology, Solna, Sweden; [4]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada; [5]Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC, Canada*

TP 028 **An LC-MS/MS Method for the Quantitative Determination of Leukotriene B4 (LTB4) in Human K2EDTA Plasma**; Shuming Yang[1]; Jinshui Chen[1]; Elise Snider[1]; Yon-Xi Li[1]; *[1]Medpace Inc, Cincinnati, OH*

TP 029 **Simultaneous Measurement of Six Phytosterols in Human Plasma by UPLC-APCI-MS/MS Method**; Aiping Zhu[1]; Emily Epure[2]; Tian-Sheng Lu[1]; Yong-Xi Li[1]; *[1]Medpace, Cincinnati, OH; [2]Medpace Inc., Cincinnati, OH*

TP 030 **Validation of Candidate Biomarkers for Prediction of Future Stricturing Disease in a Prospective Pediatric Crohn's Disease Cohort by Prm Assays**; Jing Wu[1]; Mingrui An[2]; Jianhui Zhu[2]; David M. Lubman[2]; Ryan W. Stidham[2]; *[1]University of Michigan, Ann Arbor, MI; [2]University of Michigan, Ann Arbor, MI*

TP 031 **Analysis of Short Chain Fatty Acids in Biological Samples Using GC-MS**; Takero Sakai[1]; Tasuku Murata[1]; Riki Kitano[1]; Toyohito Wada[1]; *[1]Shimadzu corp., Kyoto, Japan*

TP 032 **Targeted Proteomics Assay Development for Precise Quantification of Hepcidin in Human Plasma**; Ahmed Moghieb[1]; Marina Gritsenko[1]; Lia Tesfay[2]; Song Nie[1]; Thomas Fillmore[1]; Jon Jacobs[1]; Richard Smith[1]; Suzy Torti[2]; Tujin Shi[1]; Charles K. Ansong[1]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]University of Connecticut, Storrs, CT*

TP 033 **Lipidomics Identifies Brain Cardiolipins in Plasma as a Prognostic Marker after Cardiac Arrest**; Tamil S. Anthonymuthu[1]; Elizabeth M. Kenny[2]; Andrew M. Lamade[2]; Hitesh Gidwani[2]; Nicholas M. Krehel[2]; Andrew A. Amoscato[2]; Adam C. Straub[2]; Valerian E. Kagan[2]; Cameron Dezfulian[2]; Hülya Bayır[2]; *[1]University of Pittsburgh, Pittsburgh, PA; [2]University of Pittsburgh, Pittsburgh, PA*

TP 034 **Quantification Reporting Using Targeted Mass Spec Assays with Panorama and Skyline**; Josh Eckels[1]; Marty Pradere[1]; Ron Dashwood[1]; Kristin Geddes[2]; Nicholas J Shulman[3]; Daniel S. Spellman[2]; Michael J MacCoss[3]; Brendan X MacLean[3]; *[1]LabKey, San Diego, CA; [2]Merck, West Point, PA; [3]University of Washington, Seattle, WA*

TP 035 **Quantification of Urinary Protein Biomarkers of Autosomal Dominant Polycystic Kidney Disease by Parallel Reaction Monitoring**; Navin Rauniyar[1]; Xiaoqing Yu[2]; TuKiet Lam[1]; Lloyd Cantley[1]; *[1]Yale University, New Haven, CT; [2]Moffitt Cancer Center, Tampa, FL*

TP 036 **Advancing Mass Spectrometry-Based Large-Cohort Proteomics for Precision Medicine – An International Cancer Moonshot Multiple Site Study**; Yue Xuan[1, 2]; Thomas P. Conrads[3, 4]; Yu-ju Chen[5]; Albert Sickmann[6]; Bernd Wollscheid[7]; Connie R. Jimenez[8]; John Koomen[9]; Martin R. Larsen[10]; Hu Zhou[11]; Siqi Liu[12]; Zhinan Chen[13]; Thomas Kislinger[14]; Ben Crossett[15]; Sebastien Gallien[1, 16]; Pedro Navarro[2]; Yue Zhou[17]; Nicholas W. Bateman[3, 4]; Reta Birhanu Kitata[5]; Christin Lorenz[6]; Sandra Goetze[7]; Sander Piersma[8]; Davide Chiasserini[8]; Bin Fang[9]; Victoria Izumi[9]; Muhammad Tahir[10]; Hongwen Zhu[11]; Guixue Hou[12]; Xiuxuan Sun[13]; Andrew Macklin[14]; Ankit Sinha[14]; Benjamin L. Parker[18]; Stuart J. Cordwell[18]; *[1]Thermo Fisher Scientific, Precision Medicine Science Center, Cambridge, MA; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [3]Gynecologic Cancer Center of Excellence, Murtha Cancer Center, Uniformed Services University of the Health Sciences, Bethesda, MD; [4]Inova Schar Cancer Institute, Annandale, VA; [5]Institute of Chemistry, Academia Sinica, Taipei, Taiwan; [6]Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Dortmund, Germany; [7]Institute of Molecular Systems Biology (IMSB), ETH, Zurich, Switzerland; [8]Dept. Medical Oncology, Cancer Center Amsterdam, VU University Medical Center, Amsterdam, Netherlands; [9]Moffitt Cancer Center, Tampa, FL; [10]Department of Biochemistry and Molecular Biology University of Southern Denmark, Odense, Denmark; [11]Shanghai Institute of Materia Medica, Chinese Academy of Sciences, Shanghai, China; [12]BGI-Shenzhen, Shenzhen, China; [13]The Fourth Military Medical University, Xi'an, China; [14]Princess Margaret Cancer Centre, Toronto, ON, Canada; [15]Sydney Mass Spectrometry, The University of Sydney, Sydney, Australia; [16]Thermo Fisher Scientific, Paris, France; [17]Thermo Fisher Scientific, Shanghai, China; [18]School of Life and Environmental Science, The University of Sydney, Sydney, Australia*

TP 037 **Trouble Shooting LC/MS/MS Biomarker Assay Transfer for Sphingolipids with Multiple Isomers in Human Dried Blood Spots**; Allena J. Ji[1]; Nan Zhao[2]; Yi Zhu[1]; Mona Hdeib[1]; Troy Voelker[2]; Scott Reuschel[2]; *[1]Sponsor, Biomarkers and Clinical Bioanalyses-Boston, Sanofi, Framingham, MA; [2]Covance, Salt Lake City, UT*

TP 038 **Development of Multi-Chronic Diseases Screening Method with Human Plasma through Multiple Reaction Monitoring Mass spectrometry (MRM-MS)**; Jihyeon Lee[1]; Jaenyeon Kim[2]; Areum Sohn[1]; Injoon Yeo[2]; Hyunsoo Kim[1]; Youngsoo Kim[1, 2]; *[1]Department of Biomedical Sciences, Seoul National University, Seoul, South Korea; [2]Department of Biomedical Engineering, Seoul National University, Seoul, South Korea*

TP 039 **Longitudinal Stability of Urinary Mercapturic Acids of Acrolein, Crotonaldehyde, and Acrylonitrile in Smokers Determined by APCI-LC-MS/MS-SRM**; Menglan Chen[1]; Steven G. Carmella[1]; Xianghua Luo[1]; Dorothy K. Hatsukami[1, 2]; Stephen S. Hecht[1]; *[1]Masonic Cancer Center, University of Minnesota, Minneapolis, Minnesota; [2]Department of Psychiatry, University of Minnesota, Minneapolis, Minnesota*

TP 040 **Quantitative Assessment of Methylmalonic Acid in Human Blood and Serum Using Direct Isotope Dilution Mass Spectrometry**; Jeremiah Jamrom[1]; Logan Miller[1]; Scott Faber[2]; Matt Pamuku[3]; Fredrick D Foster[4]; H. M. Skip Kingston[1]; *[1]Duquesne University, Pittsburgh, PA; [2]The Children's Institute of Pittsburgh, Pittsburgh, PA; [3]Applied Isotope Technologies, PITTSBURGH, PA; [4]Gerstel, Inc., Linthicum, MD*

TP 041 **Quantification of Urinary Bile Acids as Potential Biomarkers for Human Kidney Diseases Using UPLC-HRMS**; Yao Shi[1]; Dennis Milanowski[1]; Brian Dean[2]; xiaorong Liang[2]; *[1]Covance, Madison, WI; [2]Genentech, Inc., South San Francisco, CA*

TP 042 **Protein-Specific Glycomic Analysis Yielded Extensive Iga Glycosylation and Biologically Important Tissue Specific Variations**; Elisha Goonatilleke[1]; Mariana Barboza Gardner[1]; Jennifer T Smilowitz[2]; Carlito B. Lebrilla[1]; *[1]Chemistry Department, University of California, Davis, California; [2]Department of Food Science and Technology, University of California, Davis, California*

TP 043 **Selective Depletion of Abundant Acidic Serum Proteins Using Amphiphilic Polymeric Reverse Micelles Improves Mass Spectrometric Detection of Low-Level Proteins**; Mahalia Serrano[1]; Jingjing Gao[1]; S. Thayumanavan[1]; Richard W. Vachet[1]; *[1]University of Massachusetts Amherst, Amherst, MA*

TP 044 **A Multiplexed Absolute Quantification Strategy for Candidate Biomarker Verification in Preclinical Alzheimer's Disease**; Xiaofang Zhong[1]; Qinying Yu[1]; Fengfei Ma[1]; Dustin Frost[1]; Lei Lu[1]; Zhengwei Chen[1]; Henrik Zetterberg[2]; Cynthia Carlsson[1]; Ozioma Okonkwo[1]; Lingjun Li[1]; *[1]University of Wisconsin-Madison, Madison, WI; [2]University of Gothenburg, Gothenburg, Sweden*

TP 045 **Quantification of N-ε (1-carboxymethyl)-L-Lysine and Pentosidine *via* LC-MS/MS: Assessment of Biomarkers for Chronic Disease**; Katherine L. O'Grady[1]; Jolaine M. Hines[1]; Olga P. Bondar[1]; Ravinder J. Singh[1]; *[1]Mayo Clinic, Rochester, MN*

TP 046 **Quantitative Analysis of Total Soluble CD73 in Human Serumas a Pharmacodynamic (PD)Biomarkerby Immuno-Capture-LC-MS/MS**; Yue Zhao[1]; Huidong Gu[1]; Jennifer Postelneck[1]; Yan J. Zhang[1]; Jianing Zeng[1]; *[1]Bristol-Myers Squibb Co., Princeton, NJ*

TP 047 **Hemoglobin Analysis by Capillary Electrophoresis – Mass Spectrometry (CE-MS) and Ion Exchange Liquid Chromatography (IEX-HPLC)**; Joseph T Snodgrass[1]; Eric Chan[1]; Shunyan Mo[1]; Sudipta Mahajan[1]; Alexander Langston[1]; Ricardo J Borjas[1]; *[1]Vertex Pharmaceuticals Incorporated, Boston, MA*

TP 048 **Immuno-MRM-Based Protein Quantification in Archived Cancer Tissues Recapitulates Biomarker Classification Based on IHC**; Jacob Kennedy[1]; Jeffrey R. Whiteaker[1]; Chenwei Lin[1]; Regine M Schoenherr[1]; Lei Zhao[1]; Dongqing Huang[1]; Melissa Lerch[2]; Geoffrey Baird[2]; Melissa Shipley[1]; Kimberly Allison[3]; Andy Hoofnagle[2]; Amanda G Paulovich[1]; *[1]Fred Hutchinson CRC, Seattle, WA; [2]University of Washington, Seattle, WA; [3]Stanford University, Palo Alto, CA*

TP 049 **Improved High-Throughput Quantitative Analysis of a Biomarker of X-Linked Adrenoleukodystrophy (X-ALD) Using a Self-Cleaning ESI Source**; Sara E Smith[1]; James DiPerna[1]; Heather Cicco[1]; Joe Trometer[2]; *[1]PerkinElmer Genetics, Pittsburgh, PA; [2]PerkinElmer, Waltham, MA*

TP 050 **Top-Down and Bottom-Up Mass Spectrometry Approaches for Alpha-Synuclein Analysis in Biological Matrixes**; Arthur Viodé[1]; Foudil Lamari[2]; Pierre-Olivier Fernagut[3]; Benjamin Dehay[3]; Christophe Junot[1]; Alain Pruvost[4]; François Fenaille[1]; François Becher[1]; *[1]CEA Saclay, DRF, Institut Joliot, Service de Pharmacologie et d'Immunoanalyse- CEA-INRA UMR 0496, Laboratoire d'Etude du Métabolisme des Médicament, Gif-sur-Yvette, France; [2]UF Biochimie des Maladies Neurométaboliques, Service de Biochimie Métabolique Hôpital Pitié-Salpêtrière, Paris, France; [3]Institut des Maladies Neurodégénératives, CNRS UMR 5293, Université de Bordeaux, Bordeaux, France; [4]CEA Saclay, DRF, Institut Joliot, Service de Pharmacologie et d'Immunoanalyse- CEA-INRA UMR 0496, Laboratoire d'Etude du Métabolisme des Médicament, Gif-sur-Yvette, France*

TP 051 **An LC-MS/MS Method for Simultaneous Determination of Seven Unconjugated Bile Acids in Human Feces**; Wuyi (charlie) Zha[1]; Kinnari Patel[1]; Xuejun Sun[1]; *[1]WuXi AppTec. Inc, Plainsboro Township, NJ*

TP 052 **A Double Surrogate Approach for the Quantitation of 2-HG – a Biomarker - in Human Brain Tumors via LC-MS/MS**; Feng Yin[1]; Jennifer Keller[2]; Dennis Kraus[2]; Heidi Mangus[1]; Fumin Li[2]; Guowen Liu[1]; *[1]Agios Pharmaceuticals, Cambridge, MA; [2]PPD Laboratories, Middleton, WI*

TP 053 **LC-MS/MS Method for Determining Endogenous Guanidino Compounds in Human Plasma and Application in Clinical Studies**; Changyu Quang[1]; Joelle M. Lucarell[1]; Hua Wang[1]; Seth R. Bell[1]; Jennifer L. Simko[1]; Susan E. Alters[2]; Liam B. Moran[1]; Elizabeth A. Groeber[1]; *[1]Charles River, Ashland, OH; [2]Aeglea Biotherapeutics, Austin, TX*

TP 054 **Human Plasma Oxyntomodulin Quantitation Using High Resolution Q-TOF**; Megan Wang[1]; Anita Lee[1]; Michael Lassman[1]; Omar Laterza[1]; *[1]Merck & Co., Inc., Kenilworth, NJ*

TP 055 **Rapid Profiling and Quantification of 17 Bile Acids in Human Plasma by LC-MS/MS**; Connor Flannery[1]; Dan Li[1]; Frances Carroll[1]; Shun-Hsin Liang[1]; Ravali Alagandula[1]; Justin Steimling[1]; Landon Wiest[1]; Ty Kahler[1]; Susan Steinike[1]; Paul Connolly[1]; *[1]Restek Corporation, Bellefonte, PA*

BIOMOLECULAR STRUCTURE ANALYSIS: CHEMICAL CROSSLINKING AND COVALENT LABELING 056-088

TP 056 **Characterization of IL-7/ IL-7Rα Binding Interface and Structural Dynamics through Chemical Cross-Linking**; Mengru Zhang; *Washington University, St. Louis, St. Louis, MO*

TP 057 **Cross-Linking Structural Validation: Why We Must Stop Using Euclidean Distances in Favor of Topological Ones**; Allan Jhonathan Ramos Ferrari[1]; Leandro Martínez[1]; Fabio C Gozzo[1]; *[1]University of Campinas, Campinas, Brazil*

TP 058 **Analysis of Chemically Crosslinked Proteins by Ultraviolet Photodissociation**; Luis A Macias[1]; Michael B Cammarata[1]; Jennifer S Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX*

TP 059 **Chemical Crosslinking Studies Provide Insight into the Molecular Basis for Oligomerization Of Helicobacter Pylori Vaca Toxin**; Marcus B. M. Nagel[1]; Mark S. McClain[2]; Hayes W. McDonald[1]; Kristie L. Rose[1]; Timothy L. Cover[2]; Kevin L. Schey[1]; *[1]Vanderbilt Mass Spectrometry Research Center and Department of Biochemistry, Vanderbilt University School of Medicine, Nashville, TN; [2]Department of Medicine and Dept. of Pathology, Microbiology and Immunology, Vanderbilt University School of Medicine, Nashvile, TN*

TP 060 **Studying Crosslinking of Dopa-Containing Peptides by High-Resolution Tandem Mass Spectrometry**; Maxime Sansoucy[1]; Lekha Sleno[1]; *[1]Université du Québec à Montréal, Montreal, QC, Canada*

TP 061 **An Optimized Enrichment Strategy for Improved Mass Spec Analysis of Chemically Cross-Linked Peptides**; Rosa Viner[1]; Erum Raja[2]; Leigh Foster[2]; Chris Etienne[2]; Ryan Bomgarden[2]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Rockford, IL*

TP 062 **Cross-Linking Mass Spectrometry for Optimized Large Scale Interaction Proteomics**; Zheng Ser[1]; Alex Kentsis[1]; *[1]Memorial Sloan Kettering Cancer Center, New York, NY*

TP 063 **An Integrated Approach with an ETD Cleavable Cross-linker for More Confident Identifications of Cross-linked Peptides**; Bingqing Zhao[1]; Santosh A. Misal[1]; Colin P. Reilly[1]; James P. Reilly[1]; *[1]Indiana University, Bloomington, IN*

TP 064 **Protein Complexes in Synaptic Vesicle Membranes Mediate Signal Transduction In Neurons**; Sabine Wittig[1]; Caroline Haupt[1]; Marcelo Ganzella[2]; Susann Kostmann[1]; Reinhard Jahn[2]; Carla Schmidt[1]; *[1]HALOmem, University of Halle, Halle / Saale, Germany; [2]MPI for Biophysical Chemistry, Goettingen, Germany*

TP 065 **Withdrawn**

TP 066 **Identification of Cleavable and Non-Cleavable Chemically Crosslinked Peptides with MetaMorpheus**; Lei Lu[1]; Michael R. Shortreed[1]; Stefan Solntsev[1]; Robert J. Millikin[1]; Zach Rolfs[1]; Lloyd M. Smith[1]; *[1]University of Wisconsin–Madison, Madison, WI*

TP 067 **Evaluation of Different Stationary Phases in the Separation of Inter-Crosslinked Peptides**; Zixiang Fang[1]; Yehia Z. Baghdady[1]; Kevin A. Schug[1]; Saiful M. Chowdhury[1]; *[1]University of Texas Arlington, Arlington TX*

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TP 070 **Identification of a Novel Lysinoalanine Covalent Crosslink of Spirochaete Flagella Hook Proteins by CID-ETD MS/MS Double-Play Analysis**; Michael J. Lynch[1]; Elizabeth T. Anderson[2]; Nyles W. Charon[3]; Brian R. Crane[1]; Sheng Zhang[2]; *[1]Department of Chemistry and Chemical Biology, Cornell University, Ithaca, NY; [2]Institute of Biotechnology, Cornell University, Ithaca, NY; [3]Robert C. Byrd Health Sciences Center, West Virginia University, Morgantown, WV*

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TP 073 **Identification and Quantification of a Prion Protein Tertiary Structural Interaction Using APDC4, a Novel Mass Spectrometry Cleavable Cross-Linker**; Deborah R Leon[1]; Alex J McDonald[1]; Christian F Heckendorf[1]; Hollis D Showalter[2]; Mark E McComb[1]; Philip C. Andrews[2]; David A Harris[1]; Catherine E. Costello[1]; *[1]Boston University School of Medicine, Boston, MA; [2]University of Michigan Medical School, Ann Arbor, Michigan*

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TP 075 **Protein Interactions at the Presynaptic Terminal Studied by Cross-Linking and Mass Spectrometry**; Caroline Haupt[1]; Melissa Frick[1]; Susann Kostmann[1]; Sabine Wittig[1]; Carla Schmidt[1]; *[1]HALOmem, University of Halle, Halle / Saale, Germany*

TP 076 **OpenPepXL: a Versatile and Sensitive XL-MS Identification Tool**; Eugen Netz[1]; Tjeerd M. H. Dijkstra[1]; Oliver Kohlbacher[1, 2, 3]; *[1]Max Planck Institute for*

Developmental Biology, Tuebingen, Germany; [2]Applied Bioinformatics, Center for Bioinformatics Tuebingen, University of Tuebingen, Tuebingen, Germany; [3]Quantitative Biology Center (QBiC), University of Tuebingen, Tuebingen, Germany

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Auger[1]; Pier-Luc Plante[2]; Jean Lacoursière[1]; Pierre Picard[1]; *[1]Phytronix Technologies, Quebec, QC, Canada; [2]Universite Laval, Quebec, QC, Canada*

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TP 198 **Enabling Photodissociation on a Commercial Q-TOF Instrument for Structural Analysis of Biomolecules**; Hai-Fang Li[1]; Yu Xia[2]; Zheng Ouyang[3]; *[1]State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instrument, Tsinghua University, Beijing, China; [2]Department of Chemistry, Tsinghua University, Beijing, China; [3]State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instruments, Tsinghua University, Beijing, China*

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TP 211 **Confirmation of Dioxins and Dioxin-like Substances at Sub-Femtogram Levels Using Atmospheric Pressure Gas Chromatography (APGC) MS/MS**; Keith Hall[1]; Rhys Jones[2]; David Douce[2]; Jody Dunstan[2]; Kenneth Rosnack[3]; Adam Ladak[3]; *[1]GC2 Chromatography Ltd, Cheshire, UK; [2]Waters Corporation, Wilmslow, UK; [3]Waters Corporation, Milford, MA*

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TP 213 **Targeted and Untargeted Analysis of Pesticides and Other Contaminants in Fruits and Vegetables Using Multi-Platform GC-MS/MS and GC/Q-TOF**; Jing Qiu[1]; Qi Jia[1]; Yihong Yang[1]; Wenwen Wang[2]; *[1]Institute of Quality Standards and Testing Technology for Agro-products, Chinese Academy of Agricultural Sciences, Beijing, China; [2]Agilent Technologies (China) Co.,Ltd, Beijing, China*

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TP 218 **Improved Analysis of Environmental Samples Using Soft Ionization and Novel GCxGC-HR-TOFMS**; George Tikhonov[1]; Viatcheslav Artaev[1]; David E Alonso[1]; Scott Pugh[1]; *[1]LECO Corporation, Saint Joseph, MI*

TP 219 **Determination of 18 Polycyclic Aromatic Hydrocarbons in Air by Online Super Critical Fluid CO2 Extraction - Gas Chromatography Mass Spectrometry**; Yuyang wu[1]; Xiaodong Li[2]; Satoshi Yamaki[2]; Mona Hamada[2]; Yuki Hashi Hashi[3]; *[1]Shimadzu (China) Co., Ltd, Shanghai, China; [2]Shimadzu, Beijing, China; [3]Shimadzu (China) Co., Ltd,, Shanghai, China*

TP 220 **Screening of Phthalate Esters in the Rubber Sample, as per RoHS(II) Directives Using Single Quadrupole GCMS with Multi-Shot Pyrolyzer**; Subodh Budakoti[1]; Sanket Anand Chiplunkar[2]; Dheeraj Handique[2]; Prashant Hase[2]; durvesh sawant[2]; Nitish Suryavanshi[2]; Ajit Datar[2]; Jitendra Kelkar[2]; Pratap Rasam[2]; *[1]Shimadzu Analytical (India) Pvt. Ltd., Delhi, India; [2]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India*

TP 221 **Trace Level Determination of Epichlorohydrin (ECH) in Active Pharmaceutical Ingredient (API) by HSGCMS**; Nitish Ramchandra Suryawanshi[1]; Prashant Hase[1]; Durvesh Sawant[1]; Sanket Anand Chiplunkar[1]; Dheeraj Handique[1]; Subodh Budakoti[2]; Ajit Datar[1]; Jitendra Kelkar[1]; Pratap Rasam[1]; *[1]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India; [2]Shimadzu Analytical (India) Pvt. Ltd., Delhi, India*

TP 222 **Analysis of Volatiles in Food Packaging Paper Board Using ITEX Dynamic Headspace**; Daniel a Abate Pella[1]; Douglas Doster[1]; Ken Rice[1]; Edward Koleski[1]; Roger Pearson[1]; Tom Flug[2]; *[1]Aspen Research, Maple Grove, MN; [2]CTC Analytics, Zwingen, Switzerland*

TP 223 **A Novel Approach by APGC-MS/MS to Increase the Sensitivity of POPs Measurement (PCBs, PBDEs, Dioxins and Furans) in Human Serum**; Eric Gaudreau[1]; Pierre Dumas[1]; René Bérubé[1]; Alain LeBlanc[1]; David Bisson[1]; Normand Fleury[1]; *[1]Centre de Toxicologie du Québec (CTQ/INSPQ), Québec, QC, Canada*

TP 224 **Using Multi-Dimensional GC with a GC-Orbitrap to Separate Isomers for Identification of Unknowns**; Jason Cole[1]; Xin Zheng[2]; Suresh Seethaphathy[3]; *[1]Thermo Fisher Scientific, Runcorn, NA; [2]Thermo Fisher Scientific, Austin, TX; [3]Thermo Fisher Scientific, Somerset, NJ*

TP 225 **A New Extraction Technique for Determination of SVOCs in Water Samples by GCMS Using Vacuum Assisted Sorbent Extraction (VASE)**; Victoria L Noad[1]; Daniel B Cardin[1]; *[1]Entech Instruments, Simi Valley, CA*

TP 226 **Simultaneous Determination of Toxic Volatiles in Sanitary Products Using Headspace-GC/MS**; Minyeong Kim[1]; Hye-Jin Park[1]; Ok-Nam Bae[2]; Seung-Hoon Baek[1]; *[1]College of Pharmacy and Research Institute of Pharmaceutical Sciences and Technology, Ajou University, Suwon, South Korea; [2]College of Pharmacy and Research Institute of Pharmaceutical Sciences and Technology, Hanyang University, Ansan, South Korea*

H/D EXCHANGE: HARDWARE, SOFTWARE AND METHODOLOGY
227-240

TP 227 **Internal Exchange Standards Enable Cross-Platform Reproducibility in Measuring Gas-Phase Hydrogen/Deuterium Exchange Kinetics by Mass Spectrometry**; Sanjit S. Uppal (Sunny)[1]; Sarah E. Beasley[1]; Rick Harkewicz[1]; Abhigya Mookherjee[1]; Miklos Guttman[1]; *[1]Department of Medicinal Chemistry, University of Washington, Seattle, WA*

TP 228 **Automated Removal of Phospholipids from Membrane Proteins for Hydrogen Deuterium Exchange Mass Spectrometry Workflows**; Kyle W Anderson[1, 2]; Elyssia S Gallagher[1, 2]; Jeffrey W Hudgens[1, 2]; *[1]National Institute of Standards and Technology, Gaithersburg, MD; [2]Institute for Bioscience and Biotechnology Researc, Rockville, MD*

TP 229 **Sparse Representation for Hydrogen Exchange Mass Spectrometry (HX-MS) Data by Using LASSO Optimization**; Yuqi Shi[1]; Jarod Hart[1]; David D Weis[1]; *[1]University of Kansas, Lawrence, KS*

TP 230 **Protein Conformation Study by Hydrogen/Deuterium Exchange Mass Spectrometry with Electron Transfer Dissociation**; Terry Zhang[1]; Stephane Houel[1]; Jonathan Josephs[1]; *[1]ThermoFisher, San Jose, CA*

TP 231 **Volcano Plot Analysis of HX-MS Measurements for Reliable Identification of Significant Differences in Comparability Studies**; Tyler Hageman[1]; Jukyung Kang[2]; Anna Schwendeman[2, 3]; David D Weis[1, 4]; *[1]Department of Chemistry, University of Kansas, Lawrence, KS; [2]Department of Pharmaceutical Sciences, University of Michigan, Ann Arbor, MI; [3]Biointerfaces Institute, University of Michigan, Ann Arbor, MI; [4]Department of Pharmaceutical Chemistry, University of Kansas, Lawrence, KS*

TP 232 **Expanded Functionality in Mass Spec Studio 2.0 for Full HDX-MS Workflow Support**; Shaunak Raval[1]; Vladimir Sarpe[1]; David Schriemer[1]; *[1]University of Calgary, Calgary, AB, Canada*

TP 233 **Applying Internal Standards to In-Electrospray – Hydrogen/Deuterium Exchange – Mass Spectrometry to Differentiate Carbohydrate Isomers**; Tara Liyanage[1]; Chinthaka A Seneviratne[2]; Elyssia S Gallagher[1]; *[1]Department of Chemistry and Biochemistry, Baylor University, Waco, TX; [2]Mass Spectrometry Center, Baylor University, Waco, TX*

TP 234 **A New Method for HX-MS Without Dilution Applied to a Reversibly Associating Monoclonal Antibody**; Mihiri Weerasinghe[1]; Reza Esfandiary[2]; Bishop Steven[2]; Sangeeta B Joshi[3]; Russell Middaugh[4]; David B Volkin[3]; David D Weis[4, 5]; *[1]University of Kansas, Lawrence, KS; [2]Department of Formulation Sciences, MedImmune LLC, , MD, Gaithersburg, MD; [3]Department of Pharmaceutical Chemistry, University of Kansas, Lawrence, KS; [4]Department of Pharmaceutical Chemistry,University of Kansas, Lawrence, KS; [5]Department of Chemistry, University of Kansas, Lawrence, KS*

TP 235 **Thiol-Ene Microchips for Efficient and Diversified Online Enzymatic Treatment of Proteins during an HDX-MS Workflow**; Gerard Comamala[1]; Rasmus R. Svejdal[1]; Vibe S. Nielsen[1]; Jörg P. Kutter[1]; Kasper D. Rand[1]; *[1]University of Copenhagen, Copenhagen, Denmark*

TP 236 **Rapid Hydrogen/Deuterium Exchange of Carbohydrates Using Theta-Capillary Electrospray Emitters**; H. Jamie Kim[1]; Elyssia S Gallagher[1]; *[1]Baylor University, Waco, TX*

TP 237 **Electrochemical Reduction of Disulfide Bonds in Proteins for Enhanced Characterization by LC-MS and HDX-MS**; Jean-Pierre Chervet[1]; Hendrik-Jan Brouwer[1]; Martin Eysberg[2]; *[1]Antec Scientific, Zoeterwoude, Netherlands; [2]Antec Scientific, Boston, MA*

TP 238 **Integrated Software Platform for Analyzing Hydrogen-Deuterium Exchange and Oxidative Footprinting Data**; Wilfred Tang[1]; Marshall Bern[1]; Chris Becker[1]; K. Ilker Sen[1]; Yong J. Kil[1]; Eric Carlson[1]; Henry Rohrs[2]; Elizabeth Bergman[2]; Yining Huang[2]; Manolo Plasencia[2]; Jagat Adhikari[2]; Melissa Barrow[2]; Daved Fremont[2]; Greg Bowman[2]; Michael L Gross[2]; *[1]Protein Metrics Inc., San Carlos, CA; [2]Washington University in St. Louis, St. Louis, Missouri*

TP 239 **Ultrafast Isolation of Proteins to Extend HDX-MS into Complex Sample Matrices**; Shaunak Raval[1]; David Schriemer[1]; *[1]University of Calgary, Calgary, AB, Canada*

TP 240 **Simplified Method Development for Targeted Hydrogen-Deuterium Exchange Studies of ABL using MALDI**; Laxmi Sinduri Vuppala[1]; Theresa Evans-Nguyen[1]; John Koomen[2]; Ioannis Gelis[1]; *[1]University of South Florida, Tampa; [2]Moffitt Cancer Center, Tampa, FL*

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TP 241 **Metabolite Conservation in Mass Spectrometry Imaging: Comparing Flash Frozen and Formalin Fixed Paraffin Embedded (FFPE) Pancreatic Cancer Spheroids**; Jillian Johnson[1]; W. John Kao[2]; Melissa C Skala[1]; Kevin W Eliceiri[1]; Lingjun Li[1]; *[1]University of Wisconsin-Madison, Madison, WI; [2]The University of Hong Kong, Pokfulam, Hong Kong*

TP 242 **Mass Spectrometry: from Imaging to Metabolic Networks**; Paolo Inglese[1]; Nicole Strittmatter[2]; M Luisa Doria[2]; Anna Mroz[2]; Abigail V M Speller[2]; Liam R Poynter[2]; Andreas Dannhorn[2]; Hiromi Kudo[2]; Reza Mirnezami[2]; Robert D Goldin[2]; Jeremy K Nicholson[2]; Robert C Glen[2, 3]; Zoltan Takats[2]; *[1]Imperial College, London, UK; [2]Imperial College London, London, UK; [3]University of Cambridge, Cambridge, UK*

TP 243 **Evaluation of Target Proteins in Ovary and Breast TMAs and Single Tissue Sections Datasets**; Yovany Cordero Hernandez[1]; Tobias Boskamp[1, 2]; Rita Casadonte[3]; Lena Hauberg-Lotte[1]; Delf Lachmund[1]; Janina Oetjen[1]; Dennis Trede[2]; Jörg Kriegsmann[3, 4]; Peter Maass[1, 2]; *[1]University of Bremen, Bremen, Germany; [2]SCiLS, Bremen, Germany; [3]Proteopath GmbH, Trier, Germany; [4]Center for Histology, Cytology and Molecular Diagnostic, Trier, Germany*

TP 244 **Novel Computational Methods for Large Cohort Mass Spectrometry Imaging Studies**; Alex Dexter[1]; Spencer Thomas[1]; Rory T. Steven[1]; Andrew D. Campbell[2]; Yulia Panina[3, 4]; Paolo Inglese[5]; James McKenzie[5]; Jean-Luc Vorng[4]; Adam J Taylor[4]; Teresa Murta[4]; Arafath K Najumudeen[2]; Bin Yan[4]; Stephanie Ling[6]; Gregory Hamm[6]; Rasmus Havelund[4]; Ala Al-Afeef[4]; Robin Phillip[4]; Renata Filipe-Soares[5]; Chelsea Nikula[4]; Efstathios Elia[1]; David Gay[2]; Tingting Fu[4]; Ian S Gilmore[4]; Mariia O Yuneva[3]; Richard J.A. Goodwin[6]; Zoltan Takats[5]; Owen J Sansom[2]; Josephine Bunch[4, 5]; *[1]National Physical Laboratory, Teddington, UK; [2]Cancer Research UK Beatson Institute, Glasgow, UK; [3]The Francis Crick Institute, London, UK; [4]National Physical Laboratory, Teddington, UK; [5]Imperial College, London, UK; [6]AstraZeneca, UK, Cambridge, UK*

TP 245 **Evaluating Robustness and Feature Extraction in T-Sne-Based Dimensionality Reduction for Mass Spectrometry Imaging Data Using Noise Injection**; Tina Smets[1]; Nico Verbeeck[1]; Marc Claesen[1]; Bart De Moor[1]; Etienne Waelkens[2]; *[1]KU Leuven, Dept. of Electrical Engineering (ESAT), STADIUS Center for Dynamical Systems, Signal Processing, and Data Analytics, Kasteelpark Arenberg 10, B-3001, Leuven, Belgium; [2]Dept. Cellular and Molecular Medicine, KU Leuven, Leuven, Belgium*

TP 246 **Evaluation of Digital Image Recognition Methods for Mass Spectrometry Imaging Data Analysis**; Maans Ekeloef[1]; Kenneth P Garrard[1]; Elias P Rosen[2]; Angela DM Kashuba[2]; David C Muddiman[1]; *[1]North Carolina State University, Raleigh, NC; [2]University of North Carolina at Chapel Hill, Chapel Hill, NC*

TP 247 **Single Day, Full Organism Imaging with DESI-MS; Creating and Exploring a Three Dimensional Chemical Map of a Mouse**; Emrys A Jones[1, 2]; Lukasz Migas[3]; Richard Chapman[1]; Steven D Pringle[1]; Zoltan Takats[2]; *[1]Waters Corporation, Wilmslow, UK; [2]Imperial College, London, UK; [3]University of Manchester, Manchester, UK*

TP 248 **Target Exposure Scoring with Mass Spectrometry Imaging**; Fabien Pamelard[1]; Manon Beuque[1]; Gaël Picard de Muller[1]; Rima Ait-Belkacem[1]; Raphael Legouffe[1]; David bonnel[1]; Jonathan Stauber[1]; *[1]Imabiotech, Loos, France*

IMAGING MS: DISEASE MARKERS
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TP 249 **Imaging of Hyaluronan in Mouse Breast Tumor Tissue Using Desorption Electrospray Ionization Mass Spectrometry**; Matej Simek[1]; Petra Zadnikova[1]; Martina Hermannova[1]; Tereza Foglova[1]; Vladimir Velebny[1]; *[1]Contipro, Dolni Dobrouc, Czech Republic*

TP 250 **Imaging of Antibody Arrays by MALDI FT-ICR Mass Spectrometry for High-Throughput Glycoprotein Cancer Biomarker Discovery from Biological Samples**; Alyson P Black[1]; Peggi M Angel[2]; Richard R Drake[2]; Anand S Mehta[2]; *[1]Medical University of South Carolina, Charleston; [2]Medical University of South Carolina, Charleston, SC*

TP 251 **Glycan and Lipid MALDI IMS Integrated with a Genomic and Metabolomic Defined Clinical Breast Cancer Cohort**; Danielle A Scott[1]; Jeffrey R Marks[2]; Richard R Drake[1]; *[1]Medical University of South Carolina, Charleston, SC; [2]Duke University, Durham, NC*

TP 252 **Extracellular Matrix Glycoproteins as Potential Cancer Markers by MALDI Imaging Mass Spectrometry**; Peggi M Angel[1, 2]; Susana Comte-Walters[1, 2]; Lauren E Ball[1, 2]; Richard R Drake[1, 2]; *[1]Medical University of South Carolina, Charleston, SC; [2]MUSC Proteomics Center, Medical University of South Carolina, Charleston, SC*

TP 253 **Understanding Lipid Localization in the Developing Lung using Nano-DESI Mass Spectrometry Imaging**; Hilary M. Brown[1]; Son N Nguyen[2]; Jennifer E. Kyle[2]; Sydney E. Dautel[2]; Ryan Sontag[2]; Teresa Luders[2]; Charles K. Ansong[2]; James Carson[3]; Julia Laskin[1]; *[1]Purdue University, West Lafayette, IN; [2]Pacific Northwest National Laboratory, Richland, WA; [3]University of Texas at Austin, Austin, TX*

TP 254 **MALDI Imaging to Characterize Breast Cancer Receptor Status in a Large Scale Clinical Cohort**; Kristina Schwamborn[1]; Christine Bollwein[2]; Carsten Denkert[3]; Anne Jacob[2]; Aurelia Noske[2]; Sibylle Loibl[4]; Wilko Weichert[2]; *[1]Institute of Pathology, Technical University Munich, Munich, Germany; [2]Institute of Pathology, Technical University Munich, Munich, Germany; [3]Institute of Pathology, Charité Universitätsmedizin Berlin, Berlin, Germany; [4]GBG German Breast Group, Neu-Isenburg, Germany*

TP 255 **Multimodal Investigation for Novel Biomarkers in Niemann-Pick Disease, Type C1: A Spatial and Temporal Profiling Lipidomics Study**; Fernando Tobias[1]; Chandimal Pathmasiri[1]; Stephanie M. Cologna[1]; *[1]University of Illinois at Chicago, Chicago, IL*

TP 256 **Discovery of Oncometabolites in Human Glioma Using *in situ* Metabolomics Based on Air Flow-Assisted Desorption Electrospray Ionization Mass Spectrometry**; Xiangyi Hui[1]; Chenglong Sun[1]; Meiying Lin[2]; Jiuming He[1]; Huicong Shen[2]; Xin Li[1]; Zeper Abliz[1, 3]; *[1]Institute of Materia Medica, Beijing, China; [2]Beijing Tiantan Hospital, Beijing, China; [3]Minzu University of China, Beijing, China*

TP 257 **DESI Imaging of Intact Proteins in Human Liver Samples of Non-Alcoholic Steatohepatitis**; James W Hughes[1]; Rian L Griffiths[1]; Mark Towers[2]; Emmanuelle Claude[2]; Patricia F Lalor[1]; Helen J Cooper[1]; *[1]University of Birmingham, Birmingham, UK; [2]Waters Corporation, Wilmslow, UK*

TP 258 **An Integrated Proteomic and Glycomic MALDI-IMS Study Towards the Characterization of Breast Cancer Subtypes**; Rita Casadonte[1]; Danielle A. Scott[2]; Mark Kriegsmann[3]; Richard R. Drake[2, 4]; Jörg Kriegsmann[1, 5]; *[1]Proteopath GmbH, Trier, Germany; [2]Department of Cell and Molecular Pharmacology, Medical University of South Carolina, Charleston, SC; [3]Institute of Pathology, University of Heidelberg, Heidelberg, Germany; [4]MUSC Proteomics Center, Medical University of South Carolina, Charleston, SC; [5]Center for Histology, Cytology and Molecular Diagnostic, Trier, Germany*

TP 259 **Comparing Molecular Abundance at the Host-Pathogen Interface through Multi-modal MALDI Imaging Mass Spectrometry**; William J. Perry[1, 2]; N. Heath Patterson[1, 3]; Jessica R. Sheldon[4]; Jessica L. Moore[1, 3]; Caroline Grunenwald[4]; Boone M. Prentice[1, 3]; James E. Cassat[4, 5]; Raf Van de Plas[1, 3, 6]; Eric P. Skaar[4]; Jeffrey M. Spraggins[1, 2, 3]; Richard M. Caprioli[1, 2, 3, 7, 8]; *[1]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [2]Department of Chemistry, Vanderbilt University, Nashville, TN; [3]Department of Biochemistry, Vanderbilt University, Nashville, TN; [4]Department of Pathology, Microbiology, and Immunology, Vanderbilt University Medical Center, Nashville, TN; [5]Department of Pediatrics, Division of Pediatric Infectious Diseases, Vanderbilt University Medical Center, Nashville, TN; [6]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [7]Department of Pharmacology, Vanderbilt University, Nashville, TN; [8]Department of Medicine, Vanderbilt University, Nashville, TN*

TP 260 **DESI-MS Imaging of Metabolites and Lipids in Brain Samples from Rats Submitted to Blood flow Reduction**; Géssica A Vasconcelos[1]; Onésia C Oliveira[1]; Dryelle L Severiano[1]; Carlos H X Custódio[1]; Mauro C Pinto[1]; Boniek G Vaz[1]; *[1]Federal University of Goias, Goiania, Brazil*

TP 261 **Targeted Imaging Mass Spectrometry of Malaria-Causing Plasmodia in Mouse Liver**; Michael Tuck[1]; Michelle L. Reyzer[1]; Nathan H. Patterson[1]; David M.G. Anderson[1]; Adam Lewis[2]; Alexis Kaushansky[2]; Richard M. Caprioli[1]; *[1]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [2]Center for Infectious Disease Research, Seattle, WA*

TP 262 **Molecular Characterization and Diagnosis of Endometriosis to Aid in Surgical Resection Using Ambient Ionization Mass Spectrometry**; Clara Feider[1]; Spencer Woody[1]; Jialing Zhang[1]; Suzanne Ledet[2]; Katherine Sebastian[2]; Michael T. Breen[3]; Livia S Eberlin[1]; *[1]University of Texas at Austin, Austin, TX; [2]Seton Medical Center, Austin, TX; [3]Dell Medical School, Austin, TX*

TP 263 **Molecular Signatures of Uterine Receptivity through High-Resolution Nanospray Desorption Electrospray Ionization Mass Spectrometry Imaging**; Ruichuan Yin[1]; Kristin Burnum-Johnson[2]; Jia Yuan[3]; Sudhansu K. Dey[3]; Julia Laskin[1, 2]; *[1]Department of Chemistry, Purdue University, West Lafayette, IN; [2]Pacific Northwest National Laboratory, Richland, WA; [3]Division of Reproductive Sciences, Cincinnati Children's Hospital Medical Center, Cincinnati, OH*

TP 264 **Mass Spectrometry Imaging Exposes Novel Neurotransmitter Alterations in Parkinson's disease and L-DOPA-Induced Dyskinesia**; Elva Fridjonsdottir[1]; Mohammadreza Shariatgorji[1]; Anna Nilsson[1]; Theodosia Vallianatou[1]; Per Svenningsson[2]; Erwan Bezard[3]; Per E. Andren[1]; *[1]Uppsala University, Uppsala, Sweden; [2]Karolinska Institutet, Stockholm, Sweden; [3]University of Bordeaux, Bordeaux, France*

TP 265 **MALDI-TOF MS and MALDI-FTICR MS Imaging of Mouse Brain after Traumatic Brain Injury (TBI)**; Nivedita Bhattacharya[1]; Bo Yan[1]; Andrew M. Fisher[1]; Mark E. McComb[1]; Ann C. McKee[1]; Lee E. Goldstein[1]; Catherine E. Costello[1]; *[1]Boston University School of Medicine, Boston, MA*

TP 266 **MALDI-MSI Investigation into N-Linked Glycan Alterations Following Radiation-Induced Lung Injury: Correlations to Inflammation and Fibrosis**; Claire L. Carter[1]; Kim Hankey[2]; George W. Parker[3]; Ann M. Farese[2]; Thomas J. MacVittie[2]; Maureen A. Kane[1]; *[1]University of Maryland, School of Pharmacy, Baltimore, MD; [2]University of Maryland School of Medicine, Baltimore, MD; [3]Charles River Laboratories, Pathology Associates,, Raleigh-Durham, NC*

TP 267 **High Resolution Imaging Mass Spectrometry of Human Donor Eyes with and without Age-Related Macular Degeneration**; David M. G. Anderson[1]; Jeffrey D. Messinger[2]; Nathan Heath Patterson[1]; Jeffrey M. Spraggins[1]; Christine A. Curcio[2]; Kevin L. Schey[1]; *[1]Vanderbilt Mass Spectrometry Research Center and Department of Biochemistry, Vanderbilt University School of Medicine, Nashville, TN; [2]University of Alabama at Birmingham, Department of Ophthalmology, Birmingham, AL*

TP 268 **MALDI Imaging of Proteins in Frozen or Fixed/Paraffin-Embedded Sections from Human Skin**; Gerhard Saalbach[1]; Damon Bevan[2]; Marielle Vigouroux[3]; Marc Moncrieff[4]; Jelena Gavrilovic[2]; *[1]John Innes Centre, Norwich, UK; [2]University of East Anglia, Norwich, UK; [3]John Innes*

Centre, Norwich, UK; [4]Norfolk and Norwich University Hospital NHS Foundation Trust, Norwich, UK

TP 269 **3D Imaging of a 14-Patient Cohort of Formalin Fixed Paraffin Embedded Human Bladder Cancer**; D. R. Naomi Vos[1]; Ilaria Jansen[2, 3]; Marit Lucas[3]; Martin R. L. Paine[1]; Benjamin Balluff[1]; C. Dilara Savci-Heijink[4]; Sybren L. Meijer[4]; Onno J. de Boer[4]; Henk A. Marquering[3, 5]; D. Martijn de Bruin[2, 3]; Ron M.A. Heeren[1]; Shane R. Ellis[1]; *[1]Maastricht MultiModal Molecular Imaging (M4I) insitute, Division of Imaging Mass Spectrometry (IMS), Maastricht, Netherlands; [2]Department of Urology and Department of Biomedical Engineering & Physics, Academic Medical Center, University of Amsterdam, Amsterdam, Netherlands; [3]Department of Biomedical Engineering & Physics, Academic Medical Center, University of Amsterdam, Amsterdam, Netherlands; [4]Department of Pathology, Academic Medical Center, University of Amsterdam, Amsterdam, Netherlands; [5]Department of Radiology, Academic Medical Center, University of Amsterdam, Amsterdam, Netherlands*

TP 270 **Desorption Electrospray Ionization and Data Independent Analysis Profiling of the Lipid Complement of Lysosomal Storage Disorders**; Philippa Hart[1]; Lee A Gethings[1]; Emmanuelle Claude[1]; Mina Mirzaian[2]; Jose Castro-Perez[3]; Johannes M.F.G Aerts[2]; Johannes P.C Vissers[1]; *[1]Waters Corporation, Wilmslow, UK; [2]Department of Biochemistry, Leiden Institute of Chemistry, University of Leiden, Netherlands; [3]Waters Corporation, Milford, MA*

TP 271 **Distinct Deposition of Amyloid-β Species in Brains with Alzheimer's Disease Pathology Visualized with MALDI Imaging Mass Spectrometry**; Nobuto Kakuda[1]; Tomohiro Miyasaka[1]; Takashi Nirasawa[2]; Shigeo Murayama[3]; Yasuo Ihara[1]; Masaya Ikegawa[4]; *[1]Doshisha university, Kyotanabe City, Japan; [2]Bruker Japan K.K., Yokohama, Japan; [3]The Brain Bank for Aging Research, Tokyo Metropolitan Geriatric Hospital, Itabashi, Japan; [4]Doshisha University, Kyotanabe City, Japan*

TP 272 **Elucidation of Metabolite Markers for Medulloblastoma Metastasis with Three-Dimensional Mass Spectrometry Imaging**; Martin R. L. Paine[1, 2]; Jingbo Liu[3]; Shane R. Ellis[2]; Dennis Trede[4]; Jan H. Kobarg[4]; Ron M.A. Heeren[2]; Facundo M. Fernandez[1]; Tobey J. MacDonald[1]; *[1]Georgia Institute of Technology, Atlanta, GA; [2]Maastricht Multimodal Molecular Imaging (M4I) Institute, Division of Imaging Mass Spectrometr, Maastricht, Netherlands; [3]Emory University School of Medicine, Atlanta, GA; [4]SCiLS, Bremen, Germany*

TP 273 **Examination of a Wounded Living Skin Equivalent Model by Mass Spectrometry Imaging**; Emily Lewis[1]; Maggie Barrett[1]; Louise Freeman-Parry[2]; Richard Bojar[1]; Alex Chapman[1]; Malcolm R Clench[2]; *[1]Innovenn(UK) Ltd, York, UK; [2]Sheffield Hallam University, Centre for Mass Spectrometry Imaging, Sheffield, UK*

TP 274 **Identification and Mapping of Lipid Biomarkers in Crohn's Disease and Ulcerative Colitis**; Jone Garate[1]; Albert Maimó-Barceló[2]; Roberto Fernandez[3]; Joan Bestard-Escalas[2]; Lucía Martin[3]; Daniel H Lopez[2]; Rebeca Reigada[2]; Sam Khorrami[2]; Daniel Ginard[2]; Igor Galetich[3]; Gwendolyn Barcelo-Coblijn[2]; Jose A Fernandez[3]; *[1]Univeristy of the Basque Country, Leioa, Spain; [2]Hospital Universitari Son Espases (HUSE), Palma, Spain; [3]Universidad del Pais Vasco, Leioa, Spain*

TP 275 **MALDI Imaging Mass Spectrometry-Based Classification of 10 Cancer Types**; Rita Casadonte[1]; Mark Kriegsmann[2]; Dennis Trede[3]; Jan H. Kobarg[4]; Tobias Boskamp[4]; Soeren O. Deininger[5]; Rémi Longuespée[2]; Katharina Kriegsmann[6]; Aurel Perren[7]; Jörg Kriegsmann[1, 8]; *[1]Proteopath GmbH, Trier, Germany; [2]Institute of Pathology, University of Heidelberg, Heidelberg, Germany; [3]SCiLS, Bremen, Germany; [4]SCiLS, Bremen, Germany; [5]Bruker Daltonik GmbH, Bremen, Germany; [6]Department of Hematology, Oncology and Rheumatology, University of Heidelberg, Heidelberg, Germany; [7]Institute of Pathology, University of Bern, Bern, Switzerland; [8]Center for Histology, Cytology and Molecular Diagnostic, Trier, Germany*

TP 276 **MALDI Imaging Mass Spectrometry for the Study of Cardiovascular Pathology**; Takashi Nirasawa[1]; Megumi Terada[2]; Hiroko Namba[2]; Nobuto Kakuda[2]; Patrick Bruneval[3]; Hatsue Ishibashi-Ueda[4]; Masaya Ikegawa[2]; *[1]Bruker Japan K.K., Yokohama, Japan; [2]Department of Life and Medical Systems, Doshisha University, Kyotanabe, Japan; [3]Georges-Pombidou European Hospital, Anatomy-Pathology, Rue Leblanc, France; [4]National Cerebral and Cardiovascular Research Center, Suita-Shi, Japan*

TP 277 **In Situ Proteomics of Kidney from Type 2 Diabetes Mellitus (T2DM) Rat Using MLDI-Imaging Mass Spectrometry**; Yuki Kuzuhara[1]; Yume Mukasa[1]; Takashi Nirasawa[2]; Nobuto Kakuda[1]; Masaya Ikegawa[1]; *[1]Department of Life and Medical Systems, Doshisha University, Kyotanabe City, Japan; [2]Bruker Japan, Yokohama, Japan*

IMAGING MS: PHARMACEUTICAL APPLICATIONS
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TP 278 **Imaging of Drug, Biomarker and Metabolites by Repeat Analysis of Single Tissue Sections Using Multiple Modalities and Polarities**; Alex Dexter[1]; Rory Thomas Steven[1]; Aateka Patel[2]; Lea Ann Dailey[3]; Josephine Bunch[1]; *[1]National Physical Laboratory, Teddington, UK; [2]King's College London, London, UK; [3]Martin-Luther-Universität, Halle-Wittenberg, Germany*

TP 279 **Developing IR-MALDESI Mass Spectrometry Imaging of HIV Medications in Hair as a Clinical Tool for Measuring Patient Adherence**; William M Gilliland, Jr. [1]; Kristen Moody[1]; Amanda Poliseno[1]; Heather Prince[1]; Monica Gandhi[2]; David C Muddiman[3]; Angela DM Kashuba[1]; Elias P Rosen[1]; *[1]UNC-Chapel Hill, Chapel Hill, NC; [2]UCSF, San Francisco, CA; [3]North Carolina State University, Raleigh, NC*

TP 280 **Investigation of the Hepatic Metabolism of Amodiaquine Using MALDI Imaging Mass Spectrometry**; Kerri J. Grove[1]; Shaila Hoque[1]; Patrick J. Rudewicz[1]; *[1]Novartis Institutes for BioMedical Research, Emeryville, CA*

TP 281 **Collisional Cross Section Enabled DESI Ion Mobility Mass Spectrometry Imaging**; Anthony Midey[1]; Hernando Olivos[1]; Bindesh Shrestha[1]; *[1]Waters Corp., Beverly, MA*

TP 282 **Metabolic Profile of Bile Acids and Lipids in Fibrosis of NASH-Model Liver Using MALDI Imaging at 20 µm Spatial Resolution**; Yuzo Yamazaki[1]; Daisuke Miura[2]; Shinichi Yamaguchi[1]; Tomonori Oshikawa[1]; Makoto Yamazaki[3]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]Innovation Center for Medical Redox Navigation, Kyusyu University, Fukuoka, Japan; [3]Mitsubishi Tanabe Pharma Corporation, Toda, Japan*

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TP 286 **Direct Chemical Imaging of Small Molecules in Single Cells Using High-Resolution Gas Cluster Ion Beam Secondary Ion Mass Spectrometry (GCIB-SIMS)**; Hua Tian[1]; Jeniffer Campbell[2]; Nicholas Winograd[3]; *[1]Pennsylvania State University, State College, PA; [2]Global Discovery Chemistry – Analytics, Novartis Institutes for Biomedical Research, Boston, MA; [3]Chemistry Department, Pennsylvania State University, University Park, PA*

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TP 351 **Integrating Genomics and Proteomics Data in the UniProt Resource**; Emanuele Alpi[1]; Maria Martin[1]; Consortium UniProt[1, 2, 3]; *[1]EMBL-EBI, Cambridge, UK; [2]SIB, Geneva, Switzerland; [3]PIR, Washington DC*

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TP 353 **An Interactive Tool for Exploring Peptide Tandem Mass Spectra**; Dain Ryan Brademan[1, 2]; Nicholas W. Kwiecien[1, 2]; Michael S Westphall[2]; Joshua J Coon[1, 2, 3, 4]; *[1]Department of Chemistry, University of Wisconsin–Madison, Madison, WI; [2]Genome Center of Wisconsin, Madison, WI; [3]Morgridge Institute for Research, Madison, WI; [4]Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI*

TP 354 **PROSIT: Deep Learning Enables Proteome Wide Prediction of Peptide Tandem Mass Spectra with High Accuracy**; Siegfried Gessulat[1, 2]; Tobias K Schmidt[3]; Daniel P Zolg[3]; Patroklos Samaras[3]; Martin Frejno[3]; Karsten Schnatbaum[4]; Johannes Zerweck[4]; Tobias Knaute[4]; Ulf Reimer[4]; Pedro Navarro[5]; Bernard Delanghe[5]; Andreas Huhmer[6]; Hans-Christian Ehrlich[2]; Stephan Aiche[2]; Mathias Wilhelm[3]; Bernhard Kuster[3, 7, 8]; *[1]Technical University of Munich, Chair of Proteomics and Bioanalytics, Freising, Germany; [2]SAP SE, Potsdam, Germany; [3]Technical University Munich, Chair of Proteomics and Bioanalytics, Freising, Germany; [4]JPT Peptide Technologies GmbH, Berlin, Germany; [5]Thermo Fisher Scientific, Bremen, Germany; [6]Thermo Fisher Scientific, San Jose, CA; [7]Center for Integrated Protein Science (CIPSM), Munich, Germany; [8]Bavarian Center for Biomolecular Mass Spectrometry, Freising, Germany*

TP 355 **Spectral Library Search Improves Peptide Identification in TMT Based Proteomics Analysis**; Jianqiao Shen[1]; Vishwajeeth R Pagala[2]; Bin Ma[1]; Junmin Peng[3]; Xusheng Wang[3]; *[1]University of Waterloo, Waterloo, ON, Canada; [2]St. Jude Children's Research Hospital, Memphis, TN; [3]St. Jude Children's Hospital, Memphis, TN*

TP 356 **Aggregated Signal Quality Based Filtering of FT MS/MS to Improve Peptide and Protein Identification**; Eduardo Jacobo Miranda Ackerman; *Max Plank Institute for Molecular Cell Biology and Genetics, Dresden, Germany*

TP 357 **Including Target Crosslink-Peptide Spectrum Matches that Lack Crosslinker-Cleavage Fragment Ions with Decoy-Based Negative Examples for Classifier Training Improves Crosslink Identification**; Karl A.T. Makepeace[1, 2]; Evgeniy V. Petrotchenko[1]; Christoph H. Borchers[1, 2, 3, 4]; *[1]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [2]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada; [3]Jewish General Hospital Proteomics Centre, McGill University, Montreal, QC, Canada; [4]Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC, Canada*

TP 358 **Open-pFind Enables Precise, Comprehensive and Rapid Peptide Identification in Shotgun Proteomics**; Hao Chi[1]; Chao Liu[1]; Hao Yang[1]; Wen-Feng Zeng[1]; Wen-Jing Zhou[1]; Xiu-Nan Niu[1]; Zhen-Lin Chen[1]; Rui-Xiang Sun[1]; Si-Min He[1]; *[1]Institute of Computing Technology, CAS, Beijing, China*

TP 359 **Speeding up Percolator**; Hantian Zhang[1]; Kaan Kara[1]; Damon H May[2]; Matthew The[3]; Lukas Käll[3]; William S Noble[2]; Ce Zhang[1]; *[1]ETH Zurich, Zurich, Switzerland; [2]University of Washington, Seattle, WA; [3]Royal Institute of Technology, Stockholm, Sweden*

TP 360 **The Promise of Fragmentation Prediction to Improve Peptide Identification in Bottom-Up Tandem Mass-Spectrometry**; Ufuk Kirik[1]; Jan C Refsgaard[2]; Lars Juhl Jensen[1]; *[1]University of Copenhagen, Center for Protein Research, Copenhagen, Denmark; [2]Intomics A/S, Lyngby, Denmark*

TP 361 **Spectral Cluster Refinement by DBSCAN Clustering for Proteomics Data**; Justin Lee[1]; Ka Po To[1]; Long Wu[1]; Henry Lam[1]; *[1]Hong Kong University of Science and Technology, Hong Kong*

TP 362 **Computational Solutions for Large-Scale Phosphoproteomics Experiments**; Ryan Smith[1]; Jon Hays[1]; Pedro Cutillas[1]; Conrad Bessant[1]; *[1]Queen Mary University of London, London, UK*

TP 363 **ProteoClade: An Open-Source Tool to Characterize and Quantify Taxon-Specific Peptides in Mixed-Species Samples Such as Patient-Derived Xenografts and Microbiota**; Arshag D. Mooradian[1]; Sjoerd van der Post[1]; Kristen M. Naegle[2]; Jason M. Held[1]; *[1]Washington University School of Medicine, St. Louis, MO; [2]Washington University in St. Louis, St. Louis, MO*

TP 364 **Evaluation of Database Searching Engines for Accurate Identification of Histone Post-Translational Modifications**; Zuofei Yuan[1]; Simone Sidoli[1]; Benjamin A. Garcia[2]; *[1]University of Pennsylvania, Philadelphia, PA; [2]University of Pennsylvania, Philadelphia, PA*

TP 365 **Prediction of Relative Retention Time of Glycopeptides Separated By C18 Reverse Phase Liquid Chromatography with Polar Characteristic**; Joshua Klein[1]; Deborah Chang[1]; Joseph Zaia[1]; *[1]Boston University, Boston, MA*

TP 366 **Benchmarking Computational Methods for Mass-Spec Based Protein Identification**; Liang Xue[1]; Simon Xi[1]; *[1]Pfizer, Cambridge, MA*

TP 367 **Software for the Processing of PASEF Identification and Label-Free Quantitation Data**; Markus Lubeck[1]; Heiner Koch[1]; Scarlet Koch[1]; Paul Savage[2]; Oliver Raether[1]; Schmit Pierre-Olivier[3]; Paul Shan[4]; Gary Kruppa[2]; *[1]Bruker Daltonik GmbH, Bremen, Germany; [2]Bruker Daltonics Inc., Billerica, MA; [3]Bruker France S.A.S., Wissembourg, France; [4]Bioinformatics Solutions Inc., Waterloo, ON, Canada*

TP 368 **Global Amino Acid Variant and Modification Analysis Using Comet and the HUPO PSI Enhanced Fasta Format (PEFF)**; Jimmy Eng[1]; Luis Mendoza[2]; Eric W Deutsch[2]; *[1]University of Washington, Seattle, WA; [2]Institute for Systems Biology, Seattle, WA*

TP 369 **SLTAG: Efficient and Expansive Spectral Library Search Using SLGF and Tag Filters.**; Duong Nguyen[1]; Nuno Bandeira[1, 2]; *[1]University of California San Diego, Department of Computer Science and Engineering, La Jolla, CA; [2]University of California San Diego, Skaggs School of Pharmacy and Pharmaceutical Sciences, La Jolla, CA*

TP 370 **Tartare: Adding RawMeat Functionality to the Xcalibur Workbench**; Michael W. Senko[1]; Romain Huguet[1]; Derek J Bailey[1]; Michael P Goodwin[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

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TP 371 **Next Generation Superconducting Tunnel Junction Cryodetection for Heavy Ion Mass Spectrometry**; Logan D Plath[1]; Jackson T. Harris[2]; William K. Warburton[2]; Robin Cantor[3]; Jonathan S. Feldman[1]; Stephan Friedrich[4]; Mark E. Bier[1]; *[1]Carnegie Mellon University, Pittsburgh, PA; [2]XIA LLC, Hayward, CA; [3]STAR Cryoelectronics, Santa Fe, NM; [4]Lawrence Livermore National Laboratory, Livermore, CA*

TP 372 **Investigation of the Performance of Low Pressure Nano-Electrospray Ioniztion-Ion Funnel-Linear Ion Trap Mass Spectrometer**; Chuan-Fan Ding[1]; Fuxing Xu[1]; Hangyu Ding[1]; Keqi Tang[2]; *[1]Fudan University, Shanghai, China; [2]Pacific Northwest National Laboratory, Richland, WA*

TP 373 **Characterization of MCP/Scintillator Sandwich by Use of High Speed Multichannel Photon Sensors for Purposes of Ion Detection**; Oleg Silivra[1]; Tsung-Chi Chen[1]; Alan Schoen[1]; Eric Hemenway[1]; Raman Mathur[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

TP 374 **Development of a Dual Mode Ion Detector with a Long Lifetime Using Discreet Dynodes and an Avalanche Diode (AD)**; Hiroshi Kobayashi; *HAMAMATSU Photonics K.K., Iwata, Japan*

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TP 375 **Desorption Ionization Using Through Hole Alumina Membrane (DIUTHAME)**; Yasuhide Naito[1]; Masahiro Kotani[2]; Takayuki Ohmura[2]; Kayoko Itou[3]; Keiko Kuwata[3]; *[1]GPI, Hamamatsu, Japan; [2]Hamamatsu Photonics K.K., Iwata, Japan; [3]ITbM, Nagoya, Japan*

TP 376 **Pulsed Liquid Droplet Inductive Injection. A 1000x Sample Input Rate Increase Compared To ESI Sprays?**; Drew Sauter[1]; Andrew D Sauter III[1]; Gary G groenewold[2]; Ron S Shomo[3]; *[1]Nanoliter, LLC, Henderson, NV; [2]Idaho National Lab, Idaho Falls, ID; [3]Scientific Instrument Services, Ringoes, NJ*

TP 377 **Online Membrane Acid/Base Addition for 'No Dilution' Electrospray Ionization Enhancements**; Hannah N. Damer[1]; Scott A. Borden[1, 2]; Erik T. Krogh[1, 2]; Christopher G. Gill[1, 2, 3, 4]; *[1]Appl. Env. Res. Labs. (AERL), Nanaimo, BC, Canada; [2]Chemistry, University of Victoria, Victoria, BC, Canada; [3]Chemistry, Simon Fraser University, Burnaby, BC, Canada; [4]University of Washington, Seattle, WA*

TP 378 **Direct Single-Cell Analysis Using Electro-Migration and Electroporation in NanoESI Capillary**; Zishuai Li[1]; Chao Xie[2]; Xiaoxiao Ma[1]; Gugangshuo Ou[2]; Zheng Ouyang[1, 3]; *[1]State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instrument, Tsinghua University, Beijing, China; [2]Tsinghua-Peking Center for Life Sciences, School of Life Sciences and MOE Key Laboratory for Protein Science, Tsinghua University, Beijing, China; [3]Weldon School of Biomedical Engineering, Purdue University, West Lafayette, Indiana*

TP 379 **Chemically Modified Anti-Reflection Metal Surfaces for Laser Desorption Ionization**; Jing Yang[1]; Wenpeng Zhang[1, 2]; Zheng Ouyang[1, 2]; *[1]State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instruments, Tsinghua University, Beijing, China; [2]Weldon School of Biomedical Engineering, Purdue University, West Lafayette, IN*

TP 380 **Monolithically-Fabricated Micro-Nano Mass Exchanger for Dynamic ESI-MS Monitoring of Bioreactors for Therapeutic Cell Manufacturing**; Mason A. Chilmonczyk[1]; Hazel Y. Stevens[1]; Peter A. Kottke[1]; Robert E. Guldberg[1]; Andrei G. Fedorov[1]; *[1]Georgia Institute of Technology, Atlanta, GA*

TP 381 **Acoustic Mist Ionization of Organic Fluids: Expanding the Chemical Space of High-Throughput, Label-Free Mass Spectrometry**; Eric Hall[1]; Deepshikha Angrish[1]; Jeremy Kowalczyk[1]; Lucien Ghislain[1]; Sammy Datwani[1]; *[1]Labcyte, San Jose, CA*

TP 382 **Real-Time Electro-Organic Reaction Screening Platform for In-situ Oxide Generation and C=C Bond Oxidation**; Kavyasree Chintalapudi[1]; Abraham Kwame Badu-Tawiah[1]; *[1]The Ohio State University, Columbus, OH*

TP 383 **Charging and Charge Switching of Unsaturated Lipids and Apolar Compounds Using Paternò-Büchi Reactions**; Patrick Esch[1]; Bernhard Spengler[1]; Sven Heiles[1]; *[1]Justus Liebig University Giessen, Giessen, Germany*

TP 384 **Comparing Inlet Ionization Techniques (SAII/ESII) and Submicron Emitter NanoESI for Native MS of Proteins Using CIU & CID**; Raul Villacob[1]; Luke T Richardson[1]; Touradj Solouki[1]; *[1]Baylor University, Waco, TX*

TP 385 **A Novel Robust Direct Extraction EI Source for GC-TOFMS and GCxGC-TOFMS**; Matthew Soyk[1]; Viatcheslav Artaev[1]; Tim Judkins[1]; *[1]LECO Corporation, St. Joseph, MI*

TP 386 **Capillary Electrophoresis Nano-Electrospray Ionization Mass Spectrometry for Analysis of Single Plant Cell Sap**; Shôn G Jones[1]; Bela Paizs[1]; Deri Tomos[1]; *[1]Bangor University, Bangor, UK*

TP 387 **Multiple-Corona H2/N2 Ion Source for AP GC-MS Coupling Stages**; Steffen Bräkling[1]; Walter Wißdorf[1]; Hendrik Kersten[1]; Thorsten Benter[1]; Bradley B. Schneider[2]; Tom Covey[2]; Peter Kovarik[2]; *[1]Bergische Universität Wuppertal, Wuppertal, Germany; [2]SCIEX, Concord, ON, Canada*

TP 388 **Atmospheric Pressure Chemical Ionization at Low Sample Flow Rates**; Josef Cvacka[1, 2]; Vladimír Vrkoslav[1]; Timotej Strmeň[1, 2]; Barbora Rumlová[2]; Ondřej Pačes[1]; *[1]Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences, Prague, Czech Republic; [2]Charles University in Prague, Faculty of Sciences, Prague, Czech Republic*

TP 389 **Smart Blood Spots for Whole Blood Protein Analysis**; Øystein Skjærvø[1]; Trine Grønhaug Halvorsen[1]; Léon Reubsaet[1]; *[1]School of Pharmacy, University of Oslo, Oslo, Norway*

TP 390 **High-Pressure Photoionization Induced O2+ Cation Chemical Ionization Mass Spectrometry for Direct Detection of Small N-alkanes at Sub-ppbv Level**; Lei Hua[1]; Yan Wang[1]; Qingyun Li[2]; Jichun Jiang[1]; Keyong Hou[1]; Haiyang Li[1]; *[1]Dalian Institute of Chemical Physics, Dalian, China; [2]Jilin University, Changchun, China*

TP 391 **Use of Dielectric Barrier Discharge Ionization to Minimize Matrix Effects and Expand Coverage in Pesticide Residue Analysis by LC-MS**; Juan F Garcia-Reyes[1]; Felipe J Lara-Ortega[1]; Alexander Schütz[2]; Sebastian Brandt[3]; Bienvenida Gilbert-López[1]; Antonio Molina-Diaz[1]; Joachim Franzke[3]; *[1]University of Jaen, Jaen, Spain; [2]Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Dortmund, Germany; [3]Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Dortmund, Germany*

TP 392 **Toluene-Assisted APCI Using a Compact Mass Spectrometer (CMS)**; Daniel Eikel[1]; Simon J. Prosser[1]; Jack D Henion[1]; *[1]Advion Inc., Ithaca, NY*

TP 393 **Biomolecule Sequencing and Quantification with Atmospheric-Pressure Ionization and Fragmentation *via* Solution-Cathode Glow Discharge Mass Spectrometry**; Courtney Walton[1]; Judy Wu[1]; Andrew J Schwartz[2]; Jacob T Shelley[1]; *[1]Rensselaer Polytechnic Institute, Troy, NY; [2]SUNY, at Buffalo, Buffalo, NY*

TP 394 **Matrix Assisted Ionization in Vacuum for Fast Analysis Directly from Biological or Synthetic Environments**; Ellen D. Inutan[1]; Anil Kumar Meher[1]; Srinivas B. Narayan[2];

Sarah Trimpin[1, 2]; *[1]Department of Chemistry, Wayne State University, Detroit, MI; [2]Detroit Medical Center: Detroit Hospital, Detroit, Michigan (MI)*

TP 395 **Evaluation of the Micro Flow Ion Source with Cartridge Columns in LC-MS/MS Bioanalysis**; Tomasz Bieńkowski[1, 2]; Konrad Piotr Kowalski[1, 2]; Michał Książkiewicz[1]; Irmina Tomaszewska[1]; *[1]MS Ekspert Sp. z o.o., Gdańsk, Poland; [2]Masdiag Sp. z o.o., Warszawa, Poland*

TP 396 **A Cooled Inlet System to Enable the Accurate Mass Measurement of a Volatile Compound by EI Sector MS**; Alan T. Taylor[1]; G. John Langley[2]; C.Logan Mackay[3]; *[1]University of Edinburgh, Edinburgh, UK; [2]Southampton university, Southampton, UK; [3]Edinburgh University, Edinburgh, UK*

TP 397 **A New Platform for High-Throughput Mass Spectrometry: Acoustic Droplet Ejection with an Open Port Probe Sampling Interface**; Lucien Ghislain[1]; Chang Liu[2]; Don Arnold[3]; Sammy Datwani[4]; *[1]Labcyte Inc, Sunnyvale, CA; [2]SCIEX, Concord, ON, Canada; [3]Verstad, LLC, Livermore, CA; [4]Labcyte, San Jose, CA*

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TP 398 **Analysis of Polysorbates in Biopharmaceuticals by Liquid Chromatography-Ion Mobility Mass Spectrometry**; Asha Hewarathna[1]; Kui Yang[1]; Connie Ruzicka[1]; David Keire[1]; *[1]US FDA, St. Louis, MO*

TP 399 **Combining Cryogenic Ion Mobility Spectrometry and Cryogenic Vibrational Spectroscopy for Use in Analytical Workflows**; Stephan Warnke[1]; Ahmed Ben Faleh[1]; Chiara Masellis[1]; Valeriu Scutelnic[1]; Thomas Rizzo[1]; *[1]Ecole Polytechnique Fédérale de Lausanne, Ch-1015 Lausanne, Switzerland*

TP 400 **Supramolecular Coordination Complexes as Ion Thermometers: Observations in Ion Cooling for Ion Mobility-Mass Spectrometry Instrumentation**; Christopher Mallis[1]; Manik Lal Saha[2]; Peter J. Stang[2]; David H. Russell[1]; *[1]Texas A&M University, College Station, TX; [2]University of Utah, Salt Lake City, UT*

TP 401 **The Figura4 Electrospray Ion Mobility Spectrometer for Intact Singly Charged Biomacromolecules**; Henry Benner[1]; Mike Bogan[1]; *[1]Ion Dx, Monterey, CA*

TP 402 **The Generation of Large-Scale CCS Database to Support Ion Mobility – Mass Spectrometry based Metabolomics and Lipidomics**; Zhiwei Zhou[1]; Jia Tu[1]; Zhengjiang Zhu[1]; *[1]Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai, China*

TP 403 **High-Throughput Robotic Nanoliter Sample Manipulation with SLIM IM-MS Analysis**; Christopher D. Chouinard[1]; Gabe Nagy[1]; Maowei Dou[1]; Isaac K. Attah[1]; Ian K. Webb[1]; Ying Zhu[1]; Tujin Shi[1]; Tao Liu[1]; Andre V. Liyu[1]; Spencer A. Prost[1]; Erin S. Baker[1]; Ryan T. Kelly[1]; Yehia M. Ibrahim[1]; Richard D. Smith[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

TP 404 **Ion Mobility Mass Spectrometry of Human Adult Hippocampus Gangliosides**; Mirela Sarbu[1]; *Željka Vukelić[2]*; David E. Clemmer[3]; Alina D. Zamfir[1]; *[1]National Institute for Research and Development in Electrochemistry and Condensed Matter, Timisoara, Romania; [2]Department of Chemistry and Biochemistry, University of Zagreb Medical School, Zagreb, Croatia; [3]Department of Chemistry, Indiana University, Bloomington, Indiana*

TP 405 **Characterization of Kaempferol Glycoside Isomers with Drift Tube Ion Mobility Mass Spectrometry and MOBCAL Calculations**; David McCaskill[1]; Nick X Wang[1]; John O'Brien[2]; Jeffrey Gilbert[1]; *[1]Dow-DuPont, Indianapolis, IN; [2]Dow-DuPont, Lake Jackson, TX*

TP 406 **Investigation of 3-Carboxy-5-Nitrophenyl-Boronic Acid Derivatized Mono- and Disaccharides Using a Q-ToF Fitted with a Cyclic IMS Mobility Separator**; Li Li[1]; Kristin R. McKenna[1]; Andy Baker[2]; Jakub Ujma[3]; Ramanarayanan Krishnamurthy[4]; Charles Liotta[1]; Facundo M. Fernandez[1]; *[1]Georgia Institute of Technology, Atlanta, GA; [2]Waters Corporation, Pleasanton, California; [3]Waters Corporation, Wilmslow, UK; [4]The Scripps Research Institute, La Jolla, CA*

TP 407 **Combining Collision-Induced Unfolding and H/D Exchange to Study Structure Difference of Apo- and Partially Metalated Metallothioneins**; Shiyu Dong[1]; David H. Russell[1]; *[1]Texas A&M University, College Station, TX*

TP 408 **Short Liquid Chromatography -Differential Mobility Spectrometry-Mass Spectrometry for Monitoring Oxidative Stress Markers in Human Whole Blood**; Sophie Bravo-Veyrat[1]; Gérard Hopfgartner[1]; *[1]University of Geneva, Life Sciences Mass Spectrometry, Department of Inorganic and Analytical Chemistry, 24 Quai Ernest-Ansermet, CH-1211 Genève 4, Switzerland, Geneva, Switzerland*

TP 409 **Group I Metal Cation Adduct Effects on Polyester Oligomers: Ion Mobility – Mass Spectrometry**; Tiffany M Crescentini[1]; Jody C. May[1]; John A. McLean[1]; David M. Hercules[1]; *[1]Vanderbilt University, Nashville, TN*

TP 410 **Separation of Noncovalently-Labeled Disaccharide Isobars by Traveling Wave and Frequency-Modulated Drift Tube Ion Mobility-Mass Spectrometry**; Kristin R. McKenna[1]; Li Li[1]; Kelsey A. Morrison[2]; Brian H. Clowers[2]; Facundo M. Fernandez[1]; *[1]Georgia Institute of Technology, Atlanta, GA; [2]Washington State University, Pullman, WA*

TP 411 **Withdrawn**

TP 412 **Nano Electrospray Differential Mobility Analysis of Adeno-Associated Viruses as Gene Therapy Platform**; Samuele Zoratto[1]; Victor U. Weiss[1]; Gernot Friedbacher[1]; Carsten Buengener[2]; Alexandra Foettinger-Vacha[2]; Ernst Boehm[2]; Michael Graninger[2]; Guenter Allmaier[1]; *[1]TU Wien, Wien, Austria; [2]Shire, Vienna, Austria*

TP 413 **Evaluation and Optimization of Rapid DDA and DIA Screening Methods for Yeast Sub-Metabolome Analysis on a High-Resolution IM-QTOF Mass Spectrometer**; Teresa Mairinger[1]; Ruwan T. Kurulugama[2]; Tim Causon[1]; George Stafford[2]; John Fjeldsted[2]; Stephan Hann[1]; *[1]Division of Analytical Chemistry, Department of Chemistry, University of Natural Resources and Life Sciences (BOKU), Vienna, Austria; [2]Agilent Technologies, Inc., Santa Clara, CA*

TP 414 **Manipulation of Protomer, or Deprotomer Ratios of Multifunctional Gaseous Ions: A Survey by Ion Mobility Mass Spectrometry**; Athula B. Attygalle; *Stevens Institute of Technology, Hoboken, NJ*

TP 415 **Revisiting Protomers of Aniline By High-Resolution Ion Mobility Spectrometry, Capillary Electrophoresis-Mass Spectrometry, and Ab-Initio Calculations**; Christopher Kune[1]; Cédric Delvaux[1]; Jean R. N. Haler[1]; Edwin De Pauw[1]; Johann Far[1]; *[1]Mass Spectrometry Laboratory, University of Liège, Liège, Belgium*

TP 416 **Resolving Poly(oxazoline) Side Chain Isomers Using Tandem Mass Spectrometry and Ion Mobility-Mass Spectrometry**; Jean R. N. Haler[1]; Victor R. de la Rosa[2]; Philippe Massonnet[1]; Richard Hoogenboom[2]; Johann Far[1]; Edwin A De Pauw[1]; *[1]Liege University, Liege, Belgium; [2]Ghent University, Ghent, Belgium*

TP 417 **Rapid, Parallelized Collision Induced Unfolding of Intact Antibodies: The Influence of Excipients on Antibody Charge Stripping**; Daniel D Vallejo[1]; Daniel A Polasky[1]; Jukyung Kang[2]; Anna Schwendeman[2, 3]; Brandon T Ruotolo[1]; *[1]University of Michigan, Ann Arbor, MI; [2]Department of Pharmaceutical Sciences, University of Michigan, Ann Arbor, MI; [3]Biointerfaces Institute, University of Michigan, Ann Arbor, MI*

TP 418 **Analysis of Protein-Ligand Complexes with Collisional Induced Unfolding**; Neil Quebbemann[1]; Michael Nshanian[1]; Joseph A Loo[1]; *[1]University of California Los Angeles, Los Angeles, CA*

TP 419 **Analysis of Dissolved Organic Matter from Subtropical Wetlands Using Tandem Trapped Ion Mobility Spectrometry and FT-ICR MS**; Lilian Tose[1, 2]; Paolo Benigni[1]; Dennys Leyva[1]; Abigail Sundberg[1]; Cesar E. Ramirez[1]; Mark E. Ridgeway[3]; Melvin A. Park[3]; Rudolf Jaffé[1]; Francisco Fernandez-Lima[1]; *[1]Florida International University, Miami, FL; [2]UFES, Vitória, Brazil; [3]Bruker Daltonics Inc., Billerica, MA*

TP 420 **High-Resolution Ion Mobility-Mass Spectrometry of Isobaric Ribonucleotides Variants**; Reza Nemati[1]; Andrew Baker[2]; Jakub Ujma[3]; Christopher DeMott[4]; Lucas Davison[1]; Kathleen McDonough[4]; Maksim Royzen[1]; Daniele Fabris[1]; *[1]University at Albany, Albany, NY; [2]Waters Corporation, Pleasanton, California; [3]Waters Corporation, Wilmslow, UK; [4]Wadsworth Center/New York State Department Of Health, Albany, NY*

TP 421 **Ion Mobility Collision Cross Section as a Proxy for Elucidating Structural Uniqueness in Support of Natural Product Discovery**; Andrzej Balinski[1]; Jody C May[1]; Berkley M. Ellis[1]; John A McLean[1, 2]; *[1]Vanderbilt University, Nashville, TN; [2]Center for Innovative Technology, Vanderbilt University, Nashville, TN*

TP 422 **Rapid Protein Structural Characterization Using Collision Induced Unfolding and Techniques Coupled with High Resolution IM-Q-TOF Mass Spectrometry**; Ruwan T. Kurulugama[1]; Daniel A. Polasky[2]; Brandon T. Ruotolo[2]; John C. Fjeldsted[1]; *[1]Agilent Technologies, Inc., Santa Clara, CA; [2]University of Michigan, Ann Arbor, MI*

TP 423 **Study of Ion Helical Propensity in the Gas Phase Using Ion Mobility Spectrometry - Mass Spectrometry and Molecular Dynamics Simulations**; Ahmad Kiani Karanji[1]; Stephen J Valentine[1]; *[1]West Virginia University, Morgantown, WV*

TP 424 **From Solution Additives to Gas-Phase Dopants: Effect of the Molecular Environment on the Conformational Space of Heme Proteins**; David Butcher[1]; Jaroslava Miksovska[1, 2]; Francisco Fernandez-Lima[1, 2]; *[1]Department of Chemistry & Biochemistry, Florida International University, Miami, FL; [2]Biomolecular Sciences Institute, Florida International University, Miami, FL*

TP 425 **Gas-Phase Unfolding Reveals Stability Shifts in Substrate-Bound Modular Polyketide Synthases**; Chunyi Zhao[1]; Andrew N. Lowell[2]; Jennifer J. Schmidt[2]; Kinshuk Srivastava[2]; Nicholas B. Borotto[1]; Kristina Hakansson[1]; David H. Sherman[1, 2]; Brandon T. Ruotolo[1]; *[1]Department of Chemistry, University of Michigan, Ann Arbor, MI; [2]Life Sciences Institute, University of Michigan, Ann Arbor, MI*

TP 426 **Using Differential Mobility Spectrometry and Machine Learning-Based Modelling to Predict Physicochemical Properties of Molecules**; J. Larry Campbell[1]; W. Scott Hopkins[2]; Zack Bowman[2]; J.C. Yves Leblanc[1]; Bradley B. Schneider[1]; *[1]SCIEX, Concord, ON, Canada; [2]University of Waterloo, Waterloo, ON, Canada*

TP 427 **Large-Scale, High Precision Collision Cross Section Measurements Methods in Support of Metabolomics**; Charles M Nichols[1]; James N. Dodds[1]; Jody C. May[1]; Stacy D. Sherrod[1]; John A. McLean[1]; *[1]Vanderbilt University, Nashville, TN*

TP 428 **Ion Mobility-Mass Spectrometry Based Characterization of MOAG-4: An Intrinsically Disordered Protein Implicated in Neurodegenerative Disease**; Varun V. Gadkari[1]; Ben Meinen[1]; James C. Bardwell[1]; Brandon T. Ruotolo[1]; *[1]University of Michigan, Ann Arbor, MI*

TP 429 **Separation of Saccharide Isomers Using High Performance Ion Mobility Spectrometry for an Orbitrap Mass Spectrometer**; Julia Kaszycki[1]; Aurelio La Rotta[1]; Ching Wu[1]; *[1]Excellims Corporation, Acton, MA*

TP 430 **Evaluating the Influence of Ion Mobility Techniques on Conformer Interconversion for Routine Quantitation of 25-Hydroxyvitamin D3**; Nicholas Oranzi[1]; Michael Wei[1]; Nicolas C Polfer[1]; Richard A. Yost[1]; *[1]University of Florida, Gainesville, FL*

TP 431 **Achieving Highly Accurate CCS Measurements in LC-IM-MS Analyses**; Ruwan T. Kurulugama[1]; Tim Causon[2]; Julia Klein[3]; Sarah M. Stow[1]; George Stafford[1]; Aaron Boice[1]; Oliver J. Schmitz[3]; Stephan Hann[2]; John Fjeldsted[1]; *[1]Agilent Technologies, Inc., Santa Clara, CA; [2]Division of Analytical Chemistry, Department of Chemistry, University of Natural Resources and Life Sciences (BOKU), Vienna, Austria; [3]University Duisburg-Essen, Essen, Germany*

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TP 432 **Shotgun Analysis of Neutral Lipids Enabled by Thiol-Ene Click Chemistry**; Sarju Adhikari[1, 2]; Wenpeng Zhang[1, 2]; Qinhua Chen[3]; Yu Xia[1, 2]; *[1]Purdue University, West Lafayette, IN; [2]Tsinghua University, Beijing, China; [3]Affiliated Dongfeng Hospital, Hubei University of Medicine, Shiyan, China*

TP 433 **A Monophasic Extraction for Simultaneous Analysis of Polar and Non-Polar Lipids in Brain Sample by Liquid Chromatography – Mass Spectrometry**; Spiro Khoury[1]; Stéphanie Cabaret[1]; Elodie A.Y. Masson[1]; Olivier Berdeaux[1]; *[1]CSGA, INRA, Dijon, France*

TP 434 **Analysis of Gangliosides in Biological Samples by Hydrophilic Interaction Liquid Chromatography Coupled with Electrospray Ionization Tandem Mass Spectrometry**; Spiro Khoury[1]; Stéphanie Cabaret[1]; Elodie A.Y. Masson[1]; Olivier Berdeaux[1]; *[1]CSGA, INRA, Dijon, France*

TP 435 **An Integrated Software Package for High-Confidence Lipid Identification**; Paul Hutchins[1, 2]; Jason D. Russell[2, 3]; Joshua Coon[1, 2, 3, 4]; *[1]Department of Chemistry, University of Wisconsin–Madison, Madison, WI; [2]Genome Center of Wisconsin, Madison, WI; [3]Morgridge Institute for Research, Madison, WI; [4]Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI*

TP 436 **Quantitative Glycolipid Tissue and Plasma Analysis by Broadband and Scanning Quadrupole Data Independent LC-MS Analysis**; Mina Mirzaian[1]; Lee A Gethings[2]; Ningombam Sanjib Meitei[3]; Maria J Ferraz[1]; Kassiani Kytidou[1]; Johannes P.C Vissers[2]; Johannes M.F.G Aerts[1]; *[1]Department of Biochemistry, Leiden Institute of Chemistry, University of Leiden, Netherlands; [2]Waters Corporation, Wilmslow, UK; [3]PREMIER Biosoft, Palo Alto, CA*

TP 437 **Analysis of Lipoprotein Metabolism in Atherosclerotic Cardiovascular Disease Based on Lipidomics and Targeted Proteomics Combined Approach**; Hiroaki Takeda[1]; Yoshihiro Izumi[1]; Kohta Nakatani[1]; Kosuke Hata[1]; Tomonari Koike[2, 3]; Ying Yu[2, 3]; Fumio Matsuda[4]; Masaki Matsumoto[1]; Masashi Shiomi[3]; Takeshi Bamba[1]; *[1]Medical Institute of Bioregulation, Kyushu University, Fukuoka-shi, Japan; [2]University of Michigan Medical Center, Ann Arbor, MI; [3]Kobe University Graduate School of Medicine, Kobe-shi, Japan; [4]Graduate School of Information Science and Technology, Osaka University, Suita-Shi, Japan*

TP 438 **Development of Absolute Quantitative Lipidomics to Study the Dysregulated Lipid Metabolism in Colorectal Cancer**; Jia Tu[1]; Yandong Yin[1]; Zheng-Jiang Zhu[1]; *[1]Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai, China*

TP 439 **Lipidomics of Spinal Cord Injury: High sensitivity Analysis of Small Volumes of Biological Fluids by NanoLC-MS**; Adriana Zardini Buzatto[1]; Brian Kwon[2]; Liang Li[1]; *[1]University of Alberta, Edmonton, AB, Canada; [2]University of British Columbia, Vancouver, BC, Canada*

TP 440 **Lipidomics For Host-Pathogen Relationship Investigation of Leishmaniasis**; Fernanda Negrao[1]; Célio Fernando Figueiredo Angolini[1]; Selma Giorgio[1]; Marcos Nogueira Eberlin[1]; *[1]UNICAMP, Campinas, Brazil*

TP 441 **Applying Trapped Ion Mobility Separation (TIMS) in Combination with Parallel Accumulation Serial Fragmentation (PASEF) for Analysis of Lipidomics Samples**; Sebastian Götz[1]; Sven W Meyer[1]; Ulrike Schweiger-Hufnagel[1]; Aiko Barsch[1]; Ningombam Sanjib Meitei[2]; *[1]Bruker, Bremen, Germany; [2]PREMIER Biosoft, Indore, India*

TP 442 **Uncovering New Pathways of Sterol Metabolism in Man: Clues from In-Born Errors of Metabolism**; William James Griffiths[1]; Yuqin Wang[1]; Eylan Yutuc[1]; *[1]Swansea University, Swansea, UK*

TP 443 **Unusual Novel Ether-Linked Phosphatidylinositol Specie as Biomarker of Acanthamoeba Castellanii Infection**; Marta Palusinska-Szysz[1]; Rosmarie Süß[2]; Beate Fuchs[3]; *[1]Maria Curie-Sklodowska University, Lublin, Poland; [2]Universität Leipzig, Leipzig, Germany; [3]Leibniz-Institut für Nutztierbiologie (FBN), Rostock-Dummerstorf, Germany*

TP 444 **Effects of Lipid Aggregation in Analysis of Stratum Corneum Lipids *via* HILIC-MS/MS**; William LaFon[1]; Chad Herrman[1]; *[1]Unilever, Trumbull, CT*

TP 445 **A Follow-Up to the NIST Interlaboratory Comparison Exercise for Lipidomics**; John Bowden; *NIST, Charleston, SC*

TP 446 **High Resolution Selected Reaction Monitoring Based Quantification of Phospholipids Using Unit Mass SWATH® Acquisition and Targeted Data Processing**; Michel Raetz[1]; Eva Duchoslav[2]; Ron Bonner[3]; Gérard Hopfgartner[1]; *[1]Life Sciences Mass Spectrometry, University of Geneva, Geneva, Switzerland; [2]SCIEX, Concord, ON, Canada; [3]Ron Bonner Consulting, Newmarket, ON, Canada*

TP 447 **The Analysis of Archaeological Lipids Using UHPSFC-MS**; Julie Herniman[1]; Placido Franco[2]; G. John Langley[1]; George Attard[1]; Aldo Roda[2]; *[1]University of Southampton, Southampton, UK; [2]University of Bologna, Bologna, Italy*

TP 448 **Rapid Analysis of Lipids in Foods by PESI-MS**; Kenta Terashima; *Shimadzu Corporation, Kyoto, Japan*

TP 449 **Comprehensive Metabolomics, Lipidomics and 13C Metabolic Flux Analysis of Cancer Cell Response to Metformin Treatment**; Juan Liu[1]; Xiaojing Liu[1]; Jason Locasale[1]; *[1]Duke University, Durham, NC*

TP 450 **Hepatic Lipid Analysis in an Experimental Model of Chronic Alcohol Exposure Using of MALDI-TOF and MALDI-FT-ICR Mass Spectrometry**; Jeremy J. Wolff[1]; Emine Bihter Yalcin[2]; Suzanne M. de la Monte[3]; *[1]Bruker Daltonics, Billerica, MA; [2]Alpert Medical School of Brown University, Providence, RI; [3]Warren Alpert Medical School of Brown University, Providence, RI*

TP 451 **High pH Mobile Phase for LC-MS Global Lipidomics Profiling with Quadrupole Orbitrap Mass Spectrometer Detection**; Josef Ruzicka[1]; David A. Peake[2]; *[1]Thermo Fisher Scientific, Somerset, NJ; [2]Thermo Fisher Scientific, San Jose, CA*

TP 452 **Lipidomic Analysis of Viral Infection Leads to the Identification of New Lipids Very Long Chain Fatty Acid Tails**; John Purdy[1]; Lisa Wise[1]; Yuecheng Xi[1]; Elizabeth Dahlmann[1]; Sam Harwood[1]; *[1]University of Arizona, Tucson, AZ*

TP 453 **Optimization of Sample Diluent and Chromatography for the Detection of Hydrophilic and Hydrophobic Lipids in a Single Reverse-Phase LC-MS/MS Method**; Tobias Marcus Maile[1]; Bryson Bennett[1]; *[1]Calico LLC, South San Francisco, CA*

TP 454 **Analysis of Isotopically Modified Glycosphingolipids on Cancer Cell Membranes**; Maurice Wong[1]; Gege Xu[2]; Mariana Barboza[1]; Carlito B. Lebrilla[1]; *[1]University of California Davis, Davis, CA; [2]University of California Davis, Davis, CA*

TP 455 **Comprehensive Lipidomics Workflow Using Automated Flow Injection Analysis for Data Independent Acquisition of Lipids Generated after Activation of Human Platelets**; Sheher Bano Mohsin[1]; Federico Tesio Torta[2, 3]; Ningombam Sanjib Meitei[4]; Bo Burla[2, 5]; Michael Woodman[6]; Markus R. Wenk[3]; *[1]Agilent Technologies, Wood Dale, IL-Illinois; [2]National University of Singapore, Singapore; [3]Singapore Lipidomics Incubator (SLING), Department of Biochemistry, YLL School of Medicine, National University of Singapore, Singapore; [4]PREMIER Biosoft, Palo Alto, CA; [5]Singapore Lipidomics Incubator (SLING), Life Sciences Institute, National University of Singapore, Singapore; [6]Agilent Technologies, Inc., Wood Dale, IL*

TP 456 **De Novo Lipogenesis in Fractionated and Unfractionated Plasma Lipids Using Stable-Isotope GC/MS-MIDA Methodology, Variable Tracer Administration and LC-MS/MS Triglyceride Profiling**; Sergiu P. Palii[1]; Grace M. Jones[1]; Aruna Souri[1]; Moises Velasco-Alin[1]; Zachary Woodward[1]; Yasamin Taghikhan[1]; Ewan F. Sinclair[1]; Souad Hamade[1]; Jean-Marc Schwarz[1, 2]; *[1]Touro University California, Vallejo, CA; [2]University of California San Francisco, San Francisco, CA*

TP 457 **Metabolites of Lipoxin A4 and Their Role in Modulating Inflammation**; Marina C Sarcinella[1]; Gregory J Buchan[1]; Bhupinder Singh[1]; Crystal E Uvalle[1]; Sonia R Salvatore[1]; Steven R Woodcock[1]; Bruce A Freeman[1]; Stacy Gelhaus Wendell[1]; *[1]Department of Pharmacology and Chemical Biology, University of Pittsburgh, Pittsburgh, PA*

TP 458 **In Situ TrEnDi: Enhancing the Sensitivity and Safety of MS-Based Quantitative Lipidomics Analyses *via* Novel Chemistry on a New Device**; Samuel W. J. Shields[1]; Peter J. Pallister[1]; Christian Rosales[1]; Carlos R. Canez[1]; Karl V. Wasslen[1]; Jeffrey M. Manthorpe[1]; Jeffrey C. Smith[1]; *[1]Carleton University, Ottawa, ON, Canada*

TP 459 **Defining the LOS-TLR4 Structure-Activity Relationship Using Rationally Designed LOS Variants**; Alison J Scott[1]; Benjamin L Oyler[2]; Erin M Harberts[1]; Belita N Opene[1]; David R Goodlett[3]; Robert K. Ernst[1]; *[1]Department of Microbial Pathogenesis, School of Dentistry, University of Maryland Baltimore, Baltimore, MD; [2]School of Medicine, University of Maryland Balitmore, Baltimore, MD; [3]School of Pharmacy, University of Maryland Baltimore, Baltimore, MD*

TP 460 **Expression, Purification, and Structural Determination of Intact Lipooligosaccharides for TLR4 Structure-Activity Relationship Definition**; Graham Goodlett[1]; Alison J Scott[1]; Benjamin L. Oyler[2]; Erin M Harberts[1]; Belita N Opene[1]; David R Goodlett[3]; Robert K Ernst[1]; *[1]Department of Microbial Pathogenesis, School of Dentistry, University of Maryland Baltimore, Baltimore, MD; [2]School of Medicine, University of Maryland Baltimore, Baltimore, MD; [3]School of Pharmacy, University of Maryland Baltimore, Baltimore, MD*

TP 461 **Lipidomics Analysis of Butanol-Producing *Escherichia coli*.**; Amaury Cazenave-Gassiot[1, 2]; Nikolay Berezhnoy[3]; Thomas William Saviour[3]; Jamie Hinks[3]; Staffan Kjelleberg[3]; Markus R. Wenk[1, 2]; *[1]Department of Biochemistry, Yong Loo Lin School of Medicine, National University of Singapore, Singapore; [2]Singapore Lipidomics Incubator (SLING), Life Sciences Institute, National University of Singapore, Singapore; [3]Singapore Center for Environmental Life Sciences Engineering (SCELSE), Nanyang Technological University, Singapore*

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TP 462 **Rapid Evaporative Ionization Mass Spectrometry (REIMS) Analysis of the Mucosal Lipidome to Distinguish Adenomas and Early Colorectal Cancer**; Petra Paizs[1]; Eftychios Manoli[1]; Sam E Mason[1]; James Alexander[1]; Zsolt Bodai[1]; Emma White[1]; Afeez Adebesin[1]; Julia Balog[2]; Steven D Pringle[2, 3]; Ara Darzi[1]; Jonathan Hoare[1]; Robert Goldin[1]; James M Kinross[1]; Zoltan Takats[1];

[1]Imperial College London, London, UK; [2]Waters Research Centre, Budapest, Hungary; [3]Waters Corporation, Wilmslow, UK

TP 463 **Mass Spectrometry Analysis of Non-Adherent Single Cancer Cells: Towards Studies of Patient Cells Obtained from Liquid Biopsy**; Devon H Colby[1]; Shawna J Standke[1]; Naga Rama Kothapalli[1]; Anthony W. G. Burgett[1]; Zhibo Yang[1]; [1]University of Oklahoma, Norman, OK

TP 464 **Utilizing Microfluidic Devices to Evaluate Cellular Metabolism of Therapeutics with Online Mass Spectrometric Detection**; Campbell B Mousseau[1]; Amanda B. Hummon[1]; Chengpeng Chen[2]; Scott Martin[2]; [1]The Ohio State University, Columbus, OH; [2]Saint Louis University, St. Louis, MO

TP 465 **A Multi-Omic Investigation of the Role of APOE Genotype in Alzheimer's Disease**; Xueyun Zheng[1]; Kristin E. Burnum-Johnson[1]; Carrie D. Nicora[1]; Kelly G. Stratton[1]; Kent J. Bloodsworth[1]; Catriona A. Mclean[2, 3]; Jennifer E. Kyle[1]; Richard D. Smith[1]; Blaine R. Roberts[2]; Erin S. Baker[1]; [1]Pacific Northwest National Laboratory, Richland, WA; [2]Florey Institute of Neuroscience and Mental Health, U. of Melbourne, Parkville, Australia; [3]Department of Anatomical Pathology, Alfred Hospital, Prahran, Australia

TP 466 **Identification of Key Lipids Critical for Platelet Activation by Comprehensive Analysis of the Platelet Lipidome**; Bing Peng[1]; Sascha Geue[2]; Cristina Coman[1]; Dominik Kopczynski[1]; Patrick Münzer[2]; Albert Sickmann[1]; Meinrad Gawaz[2]; Oliver Borst[2]; Robert Ahrends[1]; [1]ISAS, Dortmund, Germany; [2]Department of Cardiology and Cardiovascular Medicine, Tuebingen, Germany

TP 467 **Quantitative Analysis of Chemically Derivatized Short Chain Fatty Acids in Biological Samples by LC-MS/MS**; Jaeman Byun[1]; Adil Jadoon[1]; Anna V. Mathew[1]; Farsad Afshinnia[1]; Subramaniam Pennathur[1]; [1]University of Michigan, Ann Arbor, MI

TP 468 **Phenotyping Multidrug-Resistant Pseudomonas Aeruginosa Strains by Mass Spectrometry**; Sigmund J. Haidacher[1, 2]; Jennifer K. Spinler[1, 2]; Kathleen Hoch[1, 2]; Ruth Ann Luna[1, 2]; Anthony M. Haag[1, 2]; [1]Baylor College of Medicine, Houston, TX; [2]Texas Children's Hospital, Houston, Texas

TP 469 **Untargeted Metabolomic Analysis of Omega-3 Ethyl Ester Supplementation Identifies the Novel Metabolite 3-Carboxy-4-Methyl-5-Propyl-2-Furanpropanoic Acid (CMPF)**; Stacy Wendell[1]; Sonia R Salvatore[1]; Carsten Skarke[2]; Francisco Schopfer[1]; [1]University of Pittsburgh School of Medicine, Pittsburgh, PA; [2]University of Pennsylvania School of Medicine, Philadelphia, PA

TP 470 **Identifying Rheumatoid Arthritis Patients Unresponsive to Methotrexate Using Metabolomics**; Francis Brière[1]; Nancy Boucher[2]; Pier-Luc Plante[1, 2, 3]; Paul R. Fortin[1]; Gilles Boire[4]; Jacques Corbeil[1, 2, 3]; [1]Universite Laval, Quebec, QC, Canada; [2]Infectious Disease Research Center, Québec, QC, Canada; [3]Universite Laval Big Data Research Center, Québec, QC, Canada; [4]Université Sherbrooke, Sherbrooke, QC, Canada

TP 471 **Integrated Analysis of Proteomics and Metabolomics Data in ER- and ER+ Breast Cancer Tissues**; Bei Gao[1]; Dinesh Barupal[1]; Jan Budzies[2]; Carsten Denkert[2]; Oliver Fiehn[1]; [1]UC Davis, Davis, CA; [2]University Clinics Charite, Berlin, Germany

TP 472 **Automated MALDI Magnetic Resonance Mass Spectrometry (MRMS) and NMR for Biomarker Based Determination of Diabetes During Pregnancy**; Franklin E. Leach III[1]; Christopher J Thompson[2]; Jeremy J Wolff[2]; Jacquelyn Welko[1]; Anushka Chelliah[3]; Maureen Keller-Wood[3]; Gary Kruppa[2]; Aruthur S Edison[1]; [1]University of Georgia, Athens, GA; [2]Bruker Daltonics Inc., Billerica, MA; [3]University of Florida, Gainesville, FL

TP 473 **The Development, Validation & Clinical Application of a LC – MS/MS Method for Absolute Quantification of Anti-Epileptic Drugs in Serum**; Don Davis[1]; Randi L. Gant-Branum[1]; Stacy D. Sherrod[1]; Jennifer Colby[2]; John A. McLean[1]; [1]Vanderbilt University, Nashville, TN; [2]Vanderbilt University Medical Center, Nashville, TN

TP 474 **Quantitation of Glycocholic Acid and Unconjugated Bilirubin in Human Bile for Gall Bladder Diseases by Flow-Injection MS/MS Using Standard Addition**; Raghavi Kakarla[1]; Ramakrishna Reddy Voggu[1]; Janet Donaldson[2]; Baochuan Guo[1]; [1]Cleveland State University, Cleveland, OH; [2]Mississippi State University, Starkville, MS

TP 475 **Untargeted LC-MS Metabolomics of Skin Samples from Kidney Transplant Recipients**; Emmanuel O. Elijah[1]; Alan K. Jarmusch[1]; Krizia del Rosario[1]; Jeremiah D. Momper[1]; Shirley M. Tsunoda[1]; Pieter C. Dorrestein[1]; [1]Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California, San Diego, La Jolla, California

TP 476 **Development of an LC-MS/MS Method for the Quantitation of Metanephrines from Human Plasma and Dried Blood Spots**; Vincent R. Richard[1]; Andre LeBlanc[1]; Rene Zahedi[1]; Shaun Eintracht[2]; Christoph H. Borchers[1, 3, 4, 5]; [1]Jewish General Hospital Proteomics Centre, McGill University, Montreal, QC, Canada; [2]Department of Diagnostic Medicine, Sir Mortimer B. Davis Jewish General Hospital, Montreal, QC, Canada; [3]Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC, Canada; [4]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [5]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada

TP 477 **Simple Quantitative Analysis of Total and Fractionated Bile Acids in Serum using LC-MS/MS**; Rory M Doyle[1]; Andrew Harron[2]; [1]Thermo Fisher Scientific, Somerset, NJ; [2]Thermo Fisher Scientific, West Palm Beach, Fl

TP 478 **Quantitative Analysis of Organic Acids in Urine by LC-MS/MS and Comparison with GC-MS and IC-MS**; RORY M DOYLE[1]; Susan S Bird[2]; Suresh Seethapathy[1]; [1]Thermo Fisher Scientific, Somerset, NJ; [2]Thermo Fisher Scientific, Boston, MA

TP 479 **DESI-MSI as a Tool for Molecular Mapping of Colorectal Tissue Samples**; Anna Mroz[1]; Renata Soares[1]; James McKenzie[1]; James Alexander[1]; Liam Poynter[1]; Robert Goldin[1]; Zoltan Takats[1]; [1]Imperial College London, London, UK

TP 480 **Exploring the Linkage Between Behavior Changes and the Gut Microbiome and Metabolome in C57BL/6 Mice**; Young-Mo Kim[1]; Antoine M. Snijders[2]; Colin J. Brislawn[1]; Erika M. Zink[1]; Sarah F. Fansler[1]; Galya Orr[1]; Thomas O. Metz[1]; Jian-Hua Mao[2]; Janet K. Jansson[1]; [1]Pacific Northwest National Laboratory, Richland, WA; [2]Lawrence Berkeley Laboratory, Berkeley, CA

TP 481 **Express Screening of Cervical Neoplasia Metabolome Alteration by Direct Spray from Cervical Cytology Brush**; Vitaliy Chagovets[1]; Maria Nekrasova[1]; Alisa Tokareva[2]; Natalia Starodubtseva[1]; Alexey Kononikhin[1]; Niso Nazarova[1]; Vladimir Frankevich[1]; [1]Research Center for Obstetrics, Gynecology and Perinatology of the Ministry of Healthcare of the Russian Federation, Moscow, Russia; [2]Moscow Institute of Physics and Technology, Moscow, Russia

TP 482 **Quality Control for Global Metabolomic LC-MS/MS Analysis in the Clinical Laboratory**; Lisa Ford[1]; Adam Kennedy[1]; Kirk Pappan[1]; Jacob Wulff[1]; Douglas Toal[1]; [1]Metabolon, Inc., Research Triangle Park, NC

TP 483 **Urine Metabolomics Profile of Adolescents with Chronic Kidney Disease**; Levy Anderson Cesar Alves[1]; Taciana Mara Couto da Silva[1]; Rafael Celestino Sousa[1]; Meriellen Dias[2]; Maria Anita Mendes[2]; Ana Lidia Ciamponi[1]; [1]Dental School , University of São Paulo, São Paulo, São

Paulo, Brazil; [2]Dempster MS Lab - Chemical Engineering Department of Polytechnic School of University of São Paulo –São Paulo, Brazil

TP 484 **Days to Hours: Harnessing Mass Spectrometry for Rapid Detection of Blood Stream Infections**; Thomas Rydzak[1]; Ryan A Groves[1]; Heather Semeniuk[1]; Rajnigandha Pushpker[1]; Dan Gregson[1, 2]; Deirdre Church[1, 2]; Ian A Lewis[1]; *[1]University of Calgary, Calgary, AB, Canada; [2]Calgary Laboratory Services, Alberta Health Services, Calgary, AB, Canada*

TP 485 **Microbial Metabolites of Tryptophan Metabolism Predicts Inflammation in Amniotic Fluid**; Eliska Cechova[1]; Tereza Pavlova[2]; Julie Bienertova-Vasku[2]; Marian Kacerovsky[3, 4]; Jana Klanova[2]; Zdenek Spacil[2]; *[1]Masaryk University, Brno, Czech Republic; [2]Masaryk University, Brno, Czech Republic; [3]Charles University, Faculty of Medicine, Hradec Kralove, Czech Republic; [4]University Hospital Hradec Kralove, Biomedical Research Center, Hradec Kralove, Czech Republic*

TP 486 **Expanding Human Metabolic Phenotypes in Urines from Black Raspberry Food Interventions**; Ken Riedl[1]; Kristen M Roberts[1]; Elizabeth M Grainger[2]; Jennifer M Thomas-Ahner[2]; Junnan Gu[2]; Yael Vodovotz[2]; Steven J Schwartz[2]; Steven K Clinton[2]; *[1]Ohio State University, Columbus, OH; [2]Ohio State University, Columbus, OH*

TP 487 **Prebiotic Fiber Supplementation Alters Metabolic Profile Including Improvements in Markers for Cardiovascular Disease**; Brittany Lee-McMullen[1]; Kevin Contrepois[2]; Charles Abbott[2]; Wenyu Zhao[1]; Dalia Perelman[2]; Michael Snyder[1]; *[1]Stanford University, Palo Alto, CA; [2]Stanford University, Palo Alto, CA*

TP 488 **Serial Quantification Using Isotope Dilution (SQUID): A Rapid Diagnostic Method Applying Targeted LC-MS Metabolomics**; Ryan A Groves[1]; Spencer Dylan Wildman[1]; Heather Semeniuk[2]; Dan Gregson[1, 2]; Ian A Lewis[1]; *[1]University of Calgary, Calgary, AB, Canada; [2]Calgary Laboratory Services, Alberta Health Services, Calgary, AB, Canada*

TP 489 **Characterizing Amino Acid Biosignatures amongst Individuals with Schizophrenia: A Case-Control Study**; Bing Cao[1]; Dongfang Wang[1]; Lailai Yan[1]; Elisa Brietzke[2, 3]; Roger S. McIntyre[2, 4]; Xiaoyu Sun[1]; Jingjing Yan[1]; Jingyu Wang[1]; *[1]Peking University, Beijing, China; [2]University Health Network, Toronto, ON, Canada; [3]Federal University of São Paulo, Sao Paulo, Brazil; [4]Brain and Cognition Discovery Foundation, Toronto, ON, Canada*

TP 490 **Evidence for a Systemic Antimicrobial Influence on the Metabolome of Pre-Term Infants Following Topical Coconut Oil Application**; Joel P.A Gummer[1, 2]; Andrew Currie[3]; Robert D Trengove[1, 2]; Tobias Strunk[4]; *[1]Murdoch University, Murdoch, Australia; [2]Metabolomics Australia, Western Australia Node, Perth, Australia; [3]School of Veterinary and Life Sciences, Murdoch University, Perth, Australia; [4]Neonatal Directorate, King Edward Memorial Hospital for Women, Perth, Australia*

TP 491 **A Framework for Ultrafast Metabolic Phenotyping Utilizing Isotopic Fine Structure and Ultra-High Resolution Magnetic Resonance Mass Spectrometry**; Matthew R Lewis[1]; Matthias Witt[2]; Nikolas Kessler[2]; Mark E Ridgeway[3]; Aiko Barsch[2]; Christopher Thompson[3]; Jeremy K Nicholson[1]; *[1]Imperial College London, London, UK; [2]Bruker Daltonik GmbH, Bremen, Germany; [3]Bruker Daltonics Inc., Billerica, MA*

TP 492 **Comparative Analysis of Lipid Composition of Peritoneal Fluid and Blood Plasma in Patients with Endometriosis and Uterine Myoma**; Vladimir Frankevich[1]; Vitaly Chagovets[1]; Anna Borisova[1]; Alexey Kononikhin[1]; Natalia Starodubtseva[1]; *[1]Research Center for Obstetrics, Gynecology and Perinatology, Moscow, Russia*

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TP 493 **Metabolomic Analysis of Live Single Cancer Stem Cells Using Mass spectrometry**; Mei Sun; *University of Oklahoma, Norman, OK*

TP 494 **An Infusion "Shotgun" Approach for High-Throughput Untargeted Metabolomics**; Mariateresa Maldini[1]; Baljit K. Ubhi[2]; *[1]SCIEX, Milano, Italy; [2]SCIEX, Redwood City, CA*

TP 495 **A Liquid Chromatography-High Resolution Mass Spectrometry Metabolomics Study of Fecal Matter from Parkinsonian Mice Treated with a Novel Vaccine Therapy**; Emily L. Gill[1]; Jeremy P. Koelmel[1]; Laurel Meke[2]; Richard A. Yost[1]; Michael S. Okun[3]; Timothy J. Garrett[2]; Vinata Vedam-Mai[4]; *[1]University of Florida Department of Chemistry, Gainesville, FL; [2]University of Florida, Department of Pathology, Immunology and Laboratory Medicine, Gainesville, FL; [3]University of Florida, Department of Neurology, Gainesville, FL; [4]University of Florida, Department of Neurosurgery, Gainesville, FL*

TP 496 **Metabolomics-Based Characterization of Functional Microbiota Changes in a Parasitic Disease**; Laura-Isobel McCall[1]; Anupriya Tripathi[2]; Fernando Vargas[2]; Rob Knight[2]; Pieter C. Dorrestein[2]; Jair L. Siqueira-Neto[2]; *[1]*University of Oklahoma, Norman, OK; [2]University of California, San Diego, La Jolla, CA*

TP 497 **Standardization and Harmonization of LC-MS Bioanalysis Using Certified Reference Materials and Libraries of Recurrent Mass Spectra**; Yamil Simón-Manso[1]; Xinjian Yan[1]; Kelly H. Telu[1]; Yuri Mirokhin[1]; Yuxue Liang[1]; Stephen E. Stein[1]; *[1]NIST, Gaithersburg, MD*

TP 498 **LCMS-Based Untargeted Metabolomics Highlights Differences in Perilymph Metabolome with and without a Posteriori Hydrogen Gas Administration Following Loud Noise Exposure**; Kristian Pirttilä[1, 2, 3]; Annette E Fransson[4]; Jakob Haglöf[2]; Mikael Engskog[2]; Pernilla Videhult Pierre[5]; Göran Laurell[6]; Curt Pettersson[2]; Torbjörn Arvidsson[2]; *[1]Uppsala University, Uppsala, Sweden; [2]Department of Medicinal Chemistry, Faculty of Pharmacy, Uppsala University, Uppsala, Sweden; [3]Department of Medicinal Chemistry, Faculty of Pharmacy, Uppsala University, Uppsala, Uppsala, Sweden; [4]Department of Surgical Science, Uppsala University, Uppsala, Sweden, Uppsala, Sweden; [5]Division of Audiology, Department of Clinical Science, Intervention and Technology, Karolinska Institutet, Stockholm, Sweden; [6]Department of Surgical Science, Uppsala University, Uppsala, Sweden*

TP 499 **Automated in-situ Double Derivatization Strategy Coupled to SWATH-MS Data Acquisition for Broad Range Metabolite Coverage**; David Ruskic[1]; Maria Fernanda Cifuentes Girard[1]; Renzo Picenoni[2]; Guenter Boehm[2]; Gérard Hopfgartner[1]; *[1]Life Sciences Mass Spectrometry, University of Geneva, Geneve, Switzerland; [2]CTC Analytics AG, Zwingen, Switzerland*

TP 500 **Mining the Human Microbiome for Microbial Metabolites Using LC-MS/MS and GNPS**; William J Comstock[1]; Robert A Quinn[1]; Pieter C. Dorrestein[1]; *[1]University of California, San Diego, La Jolla, CA*

TP 501 **Metabolomic Profiling of *Caenorhabditis elegans* Using Capillary Electrophoresis Mass Spectrometry (CE-MS)**; Brianna M Garcia[1, 2]; Patience Sanderson[1]; Franklin E. Leach III[1]; Arthur Edison[2]; I. Jonathan Amster[1]; *[1]University of Georgia, Athens, GA; [2]Complex Carbohydrate Research Center, University of Georgia, Athens, GA*

TP 502 **Gradient Boosting Feature Selection and Classification of Metabolomic Signatures in Urine from Renal Cell Carcinoma Patients**; David A. Gaul[1]; Harsh Shrivastava[1]; Srinivas Aluru[1]; Rebecca S. Arnold[2]; John A. Petros[2]; Facundo M. Fernandez[1]; *[1]Georgia Institute of Technology, Atlanta, GA; [2]Emory University, Atlanta, GA*

TP 503 **Towards standardization: A Robust Workflow to Optimize HILIC and RPLC Methods for Untargeted Metabolomics**; Fuad J Naser[1]; Nathaniel G Mahieu[1]; Jonathan L Spalding[1]; Lingjue Wang[1]; Stephen L Johnson[1]; Gary J Patti[1]; *[1]Washington University in St. Louis, St. Louis, MO*

TP 504 **Digging Deeper: Exometabolomics by Nano-RP/HILIC-ESI-HRMS/MS Reveals Complex Variability of Small Molecules with Depth and by Vegetation Type in Arctic Soils**; Mallory P. Ladd[1, 2]; Colleen M. Iversen[1, 3]; Stan D. Wullschleger[3, 4]; Robert L. Hettich[1, 2]; *[1]Bredesen Center for Interdisciplinary Research and Graduate Education, University of Tennessee, Knoxville, TN; [2]Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN; [3]Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN; [4]Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN*

TP 505 **Using Mass-Spectrometry Based Tools to Optimize Production of Molecules of Industrial Interest in the Microorganism Pseudomonas Putida**; Nathalie Munoz[1]; Young-Mo Kim[1]; Swarnendu Tripathi[1]; Christopher Johnson[2]; Davinia Salvachua[2]; Sandra Notonier[2]; Peter St Johns[2]; Jamie Meadows[3]; Jeremy Zucker[1]; Kristin E. Burnum-Johnson[1]; Carrie D. Nicora[1]; Mark Butcher[1]; John Gladden[3]; Gregg Beckham[2]; Jon Magnuson[1]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]National Renewable Energy Laboratory, Golden, CO; [3]Lawrence Berkeley Laboratory, Berkeley, CA*

TP 506 **Integration of Metabolomic Data with Genome-Based Metabolic Model of *Citrobacter sedlakii***; Ellen Kuang[1]; Matthew Marney[2]; Mikayla Marrin[3]; Robert Edwards[4]; Erica M Forsberg[1]; *[1]San Diego State University, Department of Chemistry and Biochemistry, San Diego, CA; [2]San Diego State University, Biological and Medical Informatics, San Diego, CA; [3]San Diego State University, Department of Biology, San Diego, CA; [4]San Diego State University, Computer Science, San Diego, CA*

TP 507 **In-Depth Characterization of Chemical Differences Between Heat-Not-Burn Tobacco Products and Cigarettes Using LC-HRAM-MS-Based Non-Targeted Differential Screening (NTDS)**; Daniel Arndt[1]; Christian Wachsmuth[1]; Christoph Buchholz[1]; Mark Bentley[1]; *[1]PMI R&D, Philip Morris Products S.A., Neuchâtel, Switzerland*

TP 508 **Development of a Tissue Extraction Protocol Coupled with Chemical Isotope Labeling LC-MS for Metabolite Biomarker Discovery of Alzheimer's Disease**; Xiaohang Wang[1]; Jing Yang[1]; David Westaway[1]; Liang Li[1]; *[1]University of Alberta, Edmonton, AB, Canada*

TP 509 **Development of a Human Urine Experimental Metabolome Database Using Chemical Isotope Labeling and High-Resolution LC-MS**; Tran Tran[1]; Tao Huan[1]; Wei Han[1]; Yunong Li[1]; Liang Li[1]; *[1]University of Alberta, Edmonton, AB, Canada*

TP 510 **Development of High-Performance Chemical Isotope Labeling LC-MS for Profiling the Carboxylic Acid Submetabolome Using Dansylhydrazine**; Shuang Zhao[1]; Liang Li[1]; *[1]University of Alberta, Edmonton, AB, Canada*

TP 511 **Understanding Synthetic Biology Using the Q Exactive™ GC Orbitrap and A High Resolution Accurate Mass Metabolomics Library for Untargeted Metabolomics**; Cristian Cojocariu[1]; Maria Vinaxia[2]; Mark Dunstan[3]; Adrian J Jervis[3]; Paul Silcock[1]; Deven Shinholt[4]; Nicolas J W Rattray[5]; *[1]Thermo Fisher Scientific, Runcorn, NA; [2]University of Manchester, Manchester, UK; [3]The University of Manchester, Manchester, UK; [4]Thermo Fisher Scientific, Ausitn, TX; [5]University of Manchester, Manchester, UK*

TP 512 **Bioavailabilty and Metabolomic Studies of Crocus-Derived Bioactive Compounds Following i.p. Administration In Mice**; Anthony Tsarbopoulos[1, 2]; Evangelia Karkoula[1, 2]; Evagelos Gikas[3]; Nikolaos Kokras[4]; Christina Dalla[1]; Alexios-Leandros Skaltsounis[3]; *[1]National and Kapodistrian University of Athens Medical School, Department of Pharmacology, Athens, Greece; [2]The Goulandris Natural History Museum, Kifissia, Greece; [3]National and Kapodistrian University of Athens, Department of Pharmacy, Athens, Greece; [4]National and Kapodistrian University of Athens Medical School, First Department of Psychiatry, Athens, Greece*

TP 513 **Metabolomics Study of Hyper-IgE Syndrome (HIES) Serum and Cell-Line Samples Using Chemical Isotope Labeling LC-MS**; Minnie Jacob[1]; Xinyun Gu[2]; Xian Luo[2]; Rand Arnaout[1]; Bandar AlSaud[1]; Hamoud Al-Mousa[1]; Andreas Lopata[3]; Majed Dasouki[1]; Liang Li[2]; Anas Abdel Rahman[1, 4, 5]; *[1]King Faisal Specialist Hospital and Research Center, Riyadh, Saudi Arabia; [2]University of Alberta, Edmonton, AB, Canada; [3]James Cook University, Townsville, Australia; [4]Al Faisal University, Riyadh, Saudi Arabia; [5]Memorial University of Newfoundland, St John's, NL, Canada*

TP 514 **Scrutinizing Feature Selection in Untargeted Metabolomics**; Yasin El Abiead[1, 2, 3]; Michaela Schwaiger[1]; Gerrit Hermann[1, 4]; Gunda Koellensperger[1, 2, 3]; *[1]University of Vienna, Department of Analytical Chemistry, Vienna, Austria; [2]Vienna Metabolomics Center (VIME), University of Vienna, Vienna, Austria; [3]Chemistry Meets Microbiology, Vienna, Austria; [4]ISOtopic Solutions, Vienna, Austria*

MICROORGANISMS: IDENTIFICATION AND CHARACTERIZATION II
515-534

TP 515 **Kidney Stones and the Intestinal Microbiome: A Metabolomic Characterization of Oxalate Degraders by UHPLC-HRMS**; Casey A. Chamberlain[1]; Cory A. Leonard[1]; Marguerite Hatch[1]; Timothy J. Garrett[1]; *[1]University of Florida, Gainesville, FL*

TP 516 **Infection Kinetics and Mass Spectrometry/Scanning Electron Microscopy Image Fusion in a Rat Model of Experimental Aspergillosis**; Tomas Pluhacek[1]; Anton Skriba[1]; Milos Petrik[2]; Dominika Luptakova[1]; Jiri Novak[1]; Andrea Palyzova[1]; Oldrich Benada[1]; Tereza Jurikova[1]; Karel Lemr[1]; Vladimir Havlicek[1]; *[1]Institute of Microbiology, Prague 4, Czech Republic; [2]Institute of Molecular and Translational Medicine, Olomouc, Czech Republic*

TP 517 **Selection of Salmonella Taxon-Specific Peptide Markers for Identification to the Serovar Level by Mass Spectrometry**; Shu-Hua Chen[1]; Christine Parker[1]; Timothy Croley[1]; Melinda McFarland[1]; *[1]FDA, College Park, MD*

TP 518 **Determination of 42 Chiral Amino Acids in Biological Samples Using High-Throughput and Comprehensive LC-MS/MS: D-Amino Acids Produced by Intestinal Microbiota**; Akihiro Kunisawa[1, 2]; Takanari Hattori[1, 2]; Shuichi Kawana[1]; Shinichi Kawano[1, 2]; Yoshihiro Hayakawa[1]; Junko Iida[1, 2]; Eiichiro Fukusaki[2, 3]; Mitsuharu Matsumoto[4]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]Osaka University Shimadzu Analytical Innovation Research Laboratory, Osaka University, Osaka, Japan; [3]Graduate School of Engineering, Osaka University, Osaka, Japan; [4]Kyodo Milk Industry Co. Ltd., Tokyo, Japan*

TP 519 **MALDI-TOF MS and GC-VUV for the Identification of Bacteria and their Responses to Environmental Stressors**; Ines C. Santos[1, 2]; Misty S. Martin[1]; Michelle L. Reyes[1]; Doug D. Carlton[1, 2]; Jonathan Smuts[3]; Woo-Sik Choi[4]; Younghoon Kim[4]; Seoung Bum Kim[4]; Kristina Withworth[5]; Paula Stigler-Granados[5]; Zacariah L.

Hildenbrand[2, 6]; Kevin A. Schug[1, 2]; *[1]University of Texas, Arlington, Arlington, TX; [2]Affiliate of the Collaborative Laboratories for Environmental Analysis and Remediation, The University of Texas at Arlington, Arlington, Tx; [3]VUV Analytics, Inc., Austin, TX; [4]Department of Industrial Management Engineering, Korea University, Seoul, South Korea; [5]University of Texas School of Public Health, San Antonio Regional Campus, San Antonio, TX; [6]Inform Environmental, LLC, Dallas, TX*

TP 520 **Development of Liquid Extraction Surface Analysis Mass Spectrometry for Identification of ESKAPE Pathogens**; Jana Havlikova[1, 2]; Klaudia I. Kocurek[2]; Willem van Schaik[2]; Robin C. May[2]; Iain B. Styles[3]; Helen J. Cooper[2]; *[1]EPSRC Centre for Doctoral Training in Physical Sciences for Health, University of Birmingham, Birmingham, UK; [2]School of Biosciences, University of Birmingham, Birmingham, UK; [3]School of Computer Science, University of Birmingham, Birmingham, UK*

TP 521 **Lipid Signatures Associated with Glycopeptide, Lipopeptide and Lipoglycopeptide Cross-Resistance and the β-Lactam "Seesaw Effect" in MRSA**; Kelly M. Hines[1]; Tianwei Shen[1]; Adam Waalkes[2]; Kelsi Penewit[2]; Elizabeth A. Holmes[2]; Stephen J. Salipante[2]; Brian J. Werth[3]; Libin Xu[1]; *[1]Department of Medicinal Chemistry, University of Washington, Seattle, WA; [2]Department of Laboratory Medicine, University of Washington, Seattle, WA; [3]Department of Pharmacy, University of Washington, Seattle, WA*

TP 522 **MALDI-MS Proteotyping for Phylogenetic Classification of Yeasts**; Kanae Teramoto[1]; Yoshihiro Yamada[1]; Sadanori Sekiya[1]; Shinichi Iwamoto[1]; Hiroyasu Onaka[2]; Koichi Tanaka[1]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]The University of Tokyo, Bunkyo, Japan*

TP 523 **A Novel Software for the Characterization of Microorganisms Using Lipid Phenotyping and Statistical Analysis of MALDI-MS Data**; Gema Méndez-Cervantes[1]; Luis Mancera[1]; Gerald Stübiger[2]; *[1]Clover Bioanalytical Software, Granada, Spain; [2]Medical University of Vienna, Vienna, Austria*

TP 524 **Quantitative Proteomic Analysis of Viable *Bacillus pumilus* SAFR-032 Exposed to Space**; Abby J Chiang[1]; Ganesh Babu Malli Mohan[2]; Nitin K Singh[2]; Gerda Horneck[3]; Kasthuri Venkateswaran[2]; Markus Kalkum[1]; *[1]City of Hope, Duarte, CA; [2]Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA; [3]Institute of Aerospace Medicine, German Aerospace Center, Cologne, Germany*

TP 525 **MS-Based Proteomics Reveals Details of How Cellulosome Modification in Clostridium Thermocellum Leads to Enhanced Cellulose Solubilization of Plant Biomass**; Payal Chirania[1, 2]; Suresh Poudel[1, 2]; Richard J. Giannone[2]; Robert L. Hettich[1, 2]; *[1]University of Tennessee, Knoxville, TN; [2]Oak Ridge National Laboratory, Oak Ridge, TN*

TP 526 **Investigation of an Additional Protease in B-9 Strain Collected from Freshwater Using LC/MS**; Kaya Ueno[1]; Haiyan Jin[1]; Yosuga Kokubo[1]; Kotomi Kawashima[1]; Rina Hirayanagi[1]; Andrea R.J. Anas[1]; Kiyomi Tsuji[2]; Susumu Y. Imanishi[1]; Ken-ichi Harada[1]; *[1]Meijo University, Nagoya, Japan; [2]Kanagawa Prefectural Institute of Public Health, Chigasaki, Japan*

TP 527 **A Novel Bioinformatics Pipeline to Treat Metaproteomic Data Derived from Ocean Bacterioplankton Communities**; Keqiang Yan[1, 2]; Yan Ren[1]; Siqi Liu[1, 2]; *[1]BGI-Shenzhen, Shenzhen, China; [2]Beijing Institute of Genomics, Chinese Academy of Sciences, Beijing, China*

TP 528 **Laser-Assisted Rapid Evaporative Ionization Mass Spectrometry (REIMS): An Automated and High-Throughput Platform for Direct Analysis of Microorganisms and Clinical Samples**; Simon Cameron[1]; Alvaro Perdones-Montero[1]; Richard Schaffer[2]; Daniel Simon[2]; Frances Bolt[1]; Kate Hardiman[1]; Adam Burke[1]; Alireza Abdosarousoli[1, 3]; Monica Rebec[3]; Tamas Karancsi[2]; Zoltan Takats[1]; *[1]Imperial College London, London, UK; [2]Waters Research Centre, Budapest, Hungary; [3]Imperial College Healthcare NHS Trust, London, UK*

TP 529 **Quantitative LC-MS/MS-Based Metaproteomics Analysis of the Vaginal Microbiome**; Zameera H Hassan[1]; Myrna G Serrano[1]; Jennifer M Fettweis[1]; Kimberly K Jefferson[1]; Gregory A Buck[1]; Adam M Hawkridge[1]; *[1]Virginia Commonwealth University, Richmond, VA*

TP 530 **iMetaLab: A Web Platform for Metaproteomics Data Analysis**; Bo Liao[1]; Zhibin Ning[1]; Kai cheng[1]; xu zhang[1]; Leyuan Li[1]; Daniel Figeys[1]; *[1]University of Ottawa, Ottawa*

TP 531 **Impact of Resistant Starch in the Mouse Model of Chronic Kidney Disease: Metaproteomics of the Gut Content**; Oleg Karaduta[1]; John Arthur[1]; Alan J. Tackett[1]; Taylor McElroy[1]; Samuel Mackintosh[1]; Lisa Orr[1]; Boris Zybailov[1]; *[1]University of Arkansas for Medical Sciences, Little Rock, AR*

TP 532 **A Novel Approach to High-Throughput LC-MS Analysis of Human Stool Samples for Gut Metaproteomics Study**; Joanne Y Chan[1]; Lihua Jiang[1]; Ruiqi Jian[1]; Wenyu Zhou[1]; Michael Snyder[1]; *[1]Stanford University, Palo Alto, CA*

TP 533 **ProteoStorm: An Ultrafast Metaproteomics Database Search Framework**; Miin S. Lin[1]; Doruk Beyter[2]; Yanbao Yu[3]; Rembert Pieper[3]; Vineet Bafna[2]; *[1]Bioinformatics and Systems Biology Graduate Program, University of California San Diego, La Jolla, CA; [2]Computer Science and Engineering, University of California, San Diego, La Jolla, CA; [3]The J. Craig Venter Institute, Rockville, MD*

TP 534 **Systematic Assessment of Metaproteomic Sample Preparation, MS Measurement and Data Analysis Applied to Mouse Models of Neurodevelopmental Disorders**; Tariq Ahmad Ganief[1]; Nicolas Nalpas[1]; Viktoria Anselm[1]; Irina Droste-Borel[1]; Laura Martinez-Gili[2]; Lesley Hoyles[2]; Patricia Bermudez Martin[3]; Cristina Grau[4]; Laetitia Davidovic[3]; Xavier Altafaj[4]; Marc-Emmanuel Dumas[2]; Boris Macek[1]; *[1]Proteome Centre Tuebingen, Tubingen, Germany; [2]Department of Surgery & Cancer, Imperial College, London, UK; [3]Université Côte d'Azur, Nice, France; [4]IDIBEL - Neuropharmacology Unit, Barcelona, Spain*

NUCLEIC ACIDS AND OLIGONUCLEOTIDES I
535-554

TP 535 **Investigating the Physiochemical Parameters of Organic Base Mobile-Phase Additives on Cation Adduction in Electrospray Desorption Ionization for Oligonucleotides**; James Michael Sutton[1]; Michael G Bartlett[1]; *[1]University of Georgia, Athens, GA*

TP 536 **Enhancing the Mass Spectrometry Sensitivity for Oligonucleotides Detection by Organic Vapor Assisted Electrospray**; Guofeng Weng[1, 2]; Fangjun Wang[2]; Yuanjiang Pan[1]; *[1]Zhejiang University, Hangzhou, China; [2]Dalian Institute of Chemical Physics, Dalian, China*

TP 537 **Full Characterization and Confirmation of Diverse Oligonucleotides by Ion Pairing-Liquid Chromatography Coupled with the Q ExactiveTMHF-X HRMS**; Stephanie N. Samra[1]; Tanya Porras-Yakushi[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

TP 538 **Detection and Mapping of Post-Transcriptional tRNA Modifications in the Radioresistant Bacterium Deinococcus Radiodurans**; Ruoxia Zhao[1]; Manasses Jora[1]; Peter Lobue[1]; Patrick A Limbach[1]; *[1]University of Cincinnati Chemistry Dept, Cincinnati, OH*

TP 539 **Cytotoxic and Mutagenic Properties of Alkylphosphotriester Lesions in *Escherichia coli***; Jiabin Wu[1]; Pengcheng Wang[2]; Yinsheng Wang[2]; *[1]Environmental Toxicology Graduate Program, University of California,*

Riverside, Riverside, California; [2]Department of Chemistry, University of California, Riverside, Riverside, CA

TP 540 **Aptamer Gas-Phase Structures Studied by Ion Mobility Spectrometry: Comparison Between Free and Bound Cocaine Binding Aptamers**; Stefano Piccolo[1]; Valérie Gabelica[1]; *[1]INSERM, CNRS & University of Bordeaux (ARNA laboratory), Pessac, France*

TP 541 **Sequence Mapping and SNP Detection in Large mRNA Therapeutics by Orthogonal Enzymatic Digestions and LC-MS/MS**; Tao Jiang[1]; Ningxi Yu[2]; John-Ross Murgo[1]; Mildred Kissai[1]; Kanchana Ravichandran[1]; Ed Miracco[1]; Serenus Hua[1]; *[1]Moderna Therapeutics, Cambridge, MA; [2]University of Cincinnati, Cincinnati, OH*

TP 542 **New Tools for RNA Epigenetics: An Open-Source Approach to RNA Modification Analysis**; Samuel Wein[1]; Byron Andrews[2]; Timo Sachsenberg[3]; Helena Santos-Rosa[4]; Tony Kouzarides[4]; Benjamin A. Garcia[1]; Hendrik Weisser[2]; *[1]Epigenetics Program, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA; [2]STORM Therapeutics Limited, Cambridge, UK; [3]Applied Bioinformatics, Department for Computer Science, University of Tuebingen, Tuebingen, Germany; [4]Gurdon Institute, University of Cambridge, Cambridge, UK*

TP 543 **LC-MS/MS for the Quantitative Measurements of N-Methylated Nucleosides in DNA**; Jiekai Yin[1]; Yuxiang Cui[1]; Yang Yu[1]; Pengcheng Wang[1]; Jun Wu[1]; Yinsheng Wang[1]; *[1]University of California, Riverside, Riverside, CA*

TP 544 **Utilizing Ion Mobility Spectrometry - Mass Spectrometry and Coarse-Grain Molecular Dynamics to Support Rational Design of Nucleic Acid Nanotechnology**; Rebecca D'Esposito[1]; Thomas Kenderdine[1]; Botros Toro[1]; Srivathsan Ranganathan[2]; Pan Li[2]; Daniel Fabris[2]; *[1]University at Albany, Albany, NY; [2]RNA Institute, University at Albany, Albany, NY*

TP 545 **Electro-Elution Chromatography of RNA Oligonucleotides: A Novel Paradigm in RNA Analysis by LC-MS/MS**; Richard Lauman[1]; Samuel Wein[1]; Kevin Janssen[1]; Benjamin A. Garcia[1]; *[1]University of Pennsylvania School of Medicine, Philadelphia, PA*

TP 546 **Transcriptional Inhibition and Repair Mechanism of Alkyl Phosphotriester DNA Adducts In Mammalian Cells**; Ying Tan[1]; Jiabin Wu[1]; Yinsheng Wang[1]; *[1]UC Riverside, Riverside, CA*

TP 547 **Evaluation of the Binding of Novel Thiazole Orange Derivatives to G-Quadruplex DNA by Electrospray Ionization Mass Spectrometry**; Siwen Wang[1]; Dazhou Yang[1]; Ryan Hekman[1]; Zhihan Ye[2]; Craig Vierra[1]; Liang Xue[1]; *[1]University of the Pacific, Stockton, CA; [2]University of Melbourne, Victoria, Australia*

TP 548 **LC-MS Based Determination of Pseudouridine at a Single Nucleotide Resolution in Mammalian Small Nuclear and Nucleolar RNAs**; Yuka Yamaki[1]; Yuko Nobe[1]; Hiroshi Nakayama[2]; Yoshio Yamauchi[1]; Keiichi Izumikawa[3]; Nobuhiro Takahashi[3]; Toshiaki Isobe[1]; Masato Taoka[1]; *[1]Tokyo Metropolitan University, Tokyo, Japan; [2]RIKEN Center for Sustainable Resource Science, Wako, Japan; [3]Tokyo University of Agriculture and Technology, Fuchu, Japan*

TP 549 **Negative-Ion Mode Mass Spectrometry for Revealing Interaction Sites within RNA-Protein Complexes by Selective Infrared Multiphoton Dissociation of RNA-Peptide Crosslinked Species**; Kevin M Ileka[1]; Carolina Rojas Ramirez[1]; Kristina Hakansson[1]; *[1]University of Michigan, Ann Arbor, MI*

TP 550 **Using Glutaraldehyde Stabilization to Determine the System Architectures of Nucleoprotein Complexes**; Erica Jacobs[1]; Peter C Fridy[1]; Roman I Subbotin[2]; Michael P. Rout[1]; Brian T. Chait[1]; *[1]Rockefeller University, New York, NY; [2]iBio CMO, Bryan/College Station, TX*

TP 551 **Semi-Quantitative Determination of Oligonucleotide Drug Impurities: Main and Co-Eluting Species**; Stilianos G. Roussis[1]; Claus Renteal[1]; *[1]Ionis Pharmaceuticals, Inc., Carlsbad, CA*

TP 552 **Genotyping Bloodborne HBV with PCR and MALDI-TOF**; Jun Xu[1]; Jun J Hu[2]; Yunxuan Bu[2]; Yi Zhao[3]; hongji Zhu[3]; *[1]Suzhou Central Blood Center, Suzhou, China; [2]Ningbo University, Ningbo, China; [3]Cold Spring Harbor Asia DNA Learning Center, Suzhou, China*

TP 553 **RNA Modification Mapping of UVR-Induced Effects on Escherichia Coli tRNA by LC-MS**; Congliang Sun[1]; Patrick A Limbach[1]; Balasubrahmanyam Addepalli[1]; *[1]University of Cincinnati, Cincinnati, OH*

TP 554 **Qualitative and Quantitative Analysis of RNA Modifications in Ribosomes from Bacteria and Human Cells**; Anna Popova[1]; Luigi D'Ascenzo[1]; James R. Williamson, Ph.D. [2]; *[1]The Scripps Research Institute, La Jolla, CA; [2]The Scripps Research Institute, La Jolla, CA*

PEPTIDES: PTM IDENTIFICATION I
555-570

TP 555 **The PASEF Method on a TIMS-QTOF Mass Spectrometer for High Sensitivity Phosphoproteomics**; Heiner Koch[1]; Thomas Kosinski[1]; Matt Willets[2]; Robert Fezatte[2]; Scarlet Koch[1]; Markus Lubeck[1]; Oliver Raether[1]; Gary Kruppa[2]; *[1]Bruker Daltonik GmbH, Bremen, Germany; [2]Bruker Daltonics, Billerica, MA*

TP 556 **Rate of Asparagine Deamidation and Aspartic Acid Isomerization in Immunoglobulin (IgG) Peptides during Trypsin Digestion**; David Fischler[1]; Ron Orlando[1]; *[1]Complex Carbohydrate Research Center, UGA, Athens, GA*

TP 557 **Kinase Assay Linked to Phosphoproteomics Provides Novel Insights into the Kinase Specificity of CDKL5**; J Sebastian Paez[1]; Justine V Arrington[1]; Chuan-Chih Hsu[1]; Anton B Iliuk[1]; Barbara Terzic[2]; Zhaolan Zhou[2]; Andy W. Tao[1]; *[1]Purdue University, West Lafayette, IN; [2]University of Pennsylvania School of Medicine, Philadelphia, PA*

TP 558 **Positive Ion Mode Detection and Discovery of Tyrosine Sulfation *via* Alkylamine Adduction**; Nicholas B. Borotto[1]; Phillip J. McClory[1]; Brent R. Martin[1]; Kristina Hakansson[1]; *[1]University of Michigan, Ann Arbor, MI*

TP 559 **Mass Spectrometry-Based Assessment of the Impact Of Manufacturing Changes on the PTM Profile of the Recombinant Vaccine Carrier ExoProtein A**; Martin Burkhardt[1]; Karine Reiter[1]; Vu Nguyen[1]; Motoshi Suzuki[2]; Lisa R Olano[2]; Richard Shimp, Jr[1]; David L. Narum[1]; *[1]Laboratory of Malaria Immunology and Vaccinology, NIAID, NIH, Rockville, MD; [2]Research Technologies Branch, NIAID, NIH, Rockville, MD*

TP 560 **Orthogonal Extension of Enzymatic Digestion Repertoire in Glycoproteomic Workflow Increases Glycoprotein Coverage in a Leukemia T Cell Line**; David M Hoi[1]; Johannes Stadlmann[2]; Jasmin Taubenschmid[2]; Karl Mechtler[1, 2]; Josef M Penninger[2]; *[1]Institute of Molecular Pathology (IMP), Vienna, Austria; [2]IMBA - Institute of Molecular Biotechnology of the Austrian Academy of Sciences, Vienna, Austria*

TP 561 **Identification of Mono- and Poly-Phosphorylated Peptides by Solid Phase Beta-Elimination and Michael Addition**; Bih Fang Pan[1]; Chuan Fen Wu[1]; Sue-Hwa Lin[1]; Jian Kuang[1]; David Hawke[1]; *[1]UT- M.D. Anderson Cancer Center, Houston, TX*

TP 562 **Glycopeptide Fragmentation Optimization and Quantitation by Multi Collision Energy Ramp Scanning Quadrupole Data Independent Acquisition**; Lee A Gethings[1]; Christopher Hughes[1]; YiJu Chen[2]; David Heywood[1]; YuJu Chen[2]; Johannes P.C Vissers[1]; *[1]Waters Corporation, Wilmslow, UK; [2]Academia Sinica, Taipei, Taiwan*

TP 563 **Investigation of a Multiply Post-Translationally Modified Brain Protein by Capillary Electrophoresis-Mass Spectrometry (CE-MS)**; Bettina Sarg[1]; Klaus Faserl[2]; Herbert Lindner[2]; *[1]Div. of Clin. Biochemistry, Biocenter Innsbruck, Innsbruck, Austria; [2]Div. of Clin. Biochemistry, Biocenter Innsbruck, Innsbruck, Austria*

TP 564 **Identification of Tyrosine Phosphorylation Sites on Cardiac Myosin Binding Protein-C *via* In-gel Tryptic Digestion Followed by UPLC-MS/MS**; Amanda Pearson[1]; Sanjib Mukherjee[2]; Paola C Rosas[2]; Carl W Tong[2, 3]; Elyssia S Gallagher[1]; *[1]Department of Chemistry and Biochemistry, Baylor University, Waco, TX; [2]Department of Medical Physiology, Texas A&M University College of Medicine, Temple, TX; [3]Division of Cardiology, Baylor Scott & White Health, Temple, TX*

TP 565 **Characterizing and Comparing Modification Profiles in Large-Scale Shotgun Proteomics Using PTM-Shepherd**; Andy Kong[1]; Daniel Geiszler[1]; Dmitry M. Avtonomov[1]; Felipe da Veiga Leprevost[1]; Hui-Yin Chang[1]; Alexey I. Nesvizhskii[1]; *[1]University of Michigan, Ann Arbor, MI*

TP 566 **Mass Spectrometry Based Method to Improve the Enrichment and Identification of Palmitoylated Peptides**; Nina Nguyen[1]; Zixiang Fang[1]; Saiful Chowdhury[2]; *[1]University of Texas Arlington, Arlington, TX; [2]Univerisity of Texas at Arlington, Arlington, TX*

TP 567 **Retention Time Prediction for Phosphorylated Peptides in Reversed-Phase Chromatography**; Haley Neustaeter[1]; Victor Spicer[2]; Oleg V. Krokhin[1]; *[1]University of Manitoba, Winnipeg, MB, Canada; [2]Manitoba Centre for Proteomics and Systems Biology, Winnipeg, MB, Canada*

TP 568 **Identification of Isomerized Aspartate Residues in Peptides by MALDI-PSD and ESI-HCD**; John Hui[1]; Andrew Dykstra[1]; Michael D Bartberger[1]; Tawnya Flick[1]; Iain D. G. Campuzano[1]; Joseph A Loo[2]; *[1]Amgen Inc., Thousand Oaks, CA; [2]University of California Los Angeles, Los Angeles, CA*

TP 569 **Identification of the Sites of Ubiquitinated Proteins Using Stable Isotope Labeling Integrated with nanoLC-ESI-MS/MS**; Yueh Ying Lin[1]; He-Hsuan Hsiao[1]; *[1]National Chung Hsing University, Department of Chemistry, Taichung City, Taiwan*

TP 570 **Online Porous Graphic Carbon Chromatography-Mass Spectrometry for Post-Translational Modification Analysis**; Rui Chen[1]; Jacek Stupak[2]; Sam William[2]; Susan Twine[2]; Jianjun Li[2]; *[1]National Research Council Canada, Ottawa, ON, Canada; [2]National Research Council, Ottawa, ON, Canada*

POLYMERS
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TP 571 **Evaluating the Potential of DESI-Ion Mobility-Mass Spectrometry for Polymer Aging and Stability Studies**; Eleanor Riches[1]; Philippa J. Hart[1]; Baiba Cabovska[2]; *[1]Waters Corporation, Wilmslow, UK; [2]Waters Corporation, Milford, MA*

TP 572 **Chemical Analysis of Medical Device Materials to Probe Material Equivalency**; Berk Oktem[1]; Keaton Nahan[1]; Li Yang[1]; Eric Sussman[1]; Irada Isayeva[1]; Samanthi I Wickramasekara[1]; *[1]US-FDA, Silver Spring, MD*

TP 573 **Extractables and Leachables Analyses to Support Biocompatibility Evaluation of Additive Manufacturing Products**; Samanthi I Wickramasekara[1]; Keaton Nahan[1]; Berk Oktem[1]; Lester Schultheis[2]; Eric Sussman[1]; *[1]US Food and Drug Administration, Silver Spring, MD; [2]University of Maryland, College Park, MD*

TP 574 **Molecular Structure Study of Polyether Polyols by UPLC-QTOF MS**; Junyan Liu[1]; Liyan Jiang[1]; *[1]Sinopec Shanghai Research Institute of Petrochemical Technology, Shanghai, China*

TP 575 **"Je T'aime, Moi Non Plus": The Love-Hate Relationship of Charge States and Mass Defects of Polymer Ions**; Thierry Nicolas Jean Fouquet[1]; Robert B. Cody[2]; Takaya Satoh[3]; Hiroaki Sato[1]; *[1]AIST, Tsukuba, Japan; [2]JEOL USA, Inc., Peabody, MA; [3]JEOL Ltd., Akishima, Tokyo, Japan*

TP 576 **Reverse Engineering Polyurethane Foams by Thermal Degradation Methods**; Evan Larson[1]; Junghyun Lee[2]; Young-Jin Lee[3]; *[1]Iowa State University, Ames; [2]Hyundai Motor Company, Seoul, South Korea; [3]Iowa State University, Ames, IA*

TP 577 **Analysis of Poly(butyl acrylate) by Py-GC/MS, MALDI-MS and Thermal Desorption and Pyrolysis Combined with DART-MS**; Chikako Takei[1]; Kenichi Yoshizawa[1]; Toshiji Kudo[2]; Hajime Ohtani[3]; *[1]BioChromato, Inc., Fujisawa, Japan; [2]Bruker Japan K.K., Yokohama, Japan; [3]Nagoya Institute of Technology, Nagoya, Japan*

TP 578 **Coupling Gel Permeation Chromatography to Charge Reduction Mass Spectrometry and Ion Mobility for the Analysis of Synthetic Polymers**; John Stutzman[1]; John P O'Brein[2]; Miroslav Janco[3]; James N Alexander III[3]; Binghe Gu[1]; *[1]The Dow Chemical Company, Midland, MI; [2]The Dow Chemical Company, Lake Jackson, TX; [3]The Dow Chemical Company, Collegeville, PA*

TP 579 **Analysis of Polyglycerol Fatty Acid Esters *via* Liquid Chromatography Coupled to Ion Mobility Mass Spectrometry**; Jason Michael O'Neill; *The University of Akron, Akron, OH*

TP 580 **Comprehensive Extractable Analysis of Semi-Permeable FilterUsing LC-HRMS, GC-MS, and ICP-MS**; Mike Ludlow[1]; Abigale Marcus[2]; Kate Comstock[3]; Ekong Bassy[4]; John Schmelzel[3]; *[1]LGC, Fordham, UK; [2]LGC Biosearch Technologies, Petaluma, California; [3]Thermo Fisher Scientific, San Jose, CA; [4]Thermo Scientific, San Jose, CA*

TP 581 **Surface-Layer Matrix-Assisted Laser Desorption Ionization Mass Spectrometry (SL-MALDI-MS) of Synthetic Materials**; Kevin J. Endres[1]; Jacob A. Hill[1]; Mark D. Foster[1]; Chrys Wesdemiotis[1]; *[1]The University of Akron, Akron, OH*

PROTEINS: COMPLEXES/NON-COVALENT INTERACTIONS II
582-606

TP 582 **Supercharging Stabilizes Membrane Protein Nanodiscs for Native MS**; James E Keener[1]; Deseree J Reid[1]; Dane Evan Zambrano[1]; Michael Thomas Marty[1]; *[1]University of Arizona, Tucson, AZ*

TP 583 **Mass Spectrometry Behavior of Heterogeneous Lipid Nanodiscs Under Charge Reducing and Supercharging Conditions**; Guozhi Zhang[1]; Dane Evan Zambrano[1]; James E. Keener[1]; Michael T. Marty[1]; *[1]University of Arizona, Tucson, AZ*

TP 584 **An Ion Mobility-Orbitrap Mass Spectrometer for Analyzing Intact Protein Complexes**; Michael Poltash[1]; John W Patrick[2]; Arthur Laganowsky[2]; David H. Russell[2]; *[1]Texas A&M University, College Station; [2]Texas A&M, College Station, TX*

TP 585 **Determination of Site-specific Calcium Binding Affinities and Binding Order of Human Calprotectin Protein Using HDX, PLIMSTEX and Native Mass Spectrometry**; Jagat Adhikari[1]; Jules R. Stephan[2]; Don L. Rempel[1]; Elizabeth M. Nolan[2]; Michael L. Gross[1]; *[1]Washington University St Louis, St. Louis, MO; [2]Massachusetts Institute of Technology, Cambridge, MA*

TP 586 **Collision-Induced Dissociation of Multi-Protein Complexes: Molecular Dynamics Simulations Using a Refined Mobile Proton Model**; Justin H Lee[1]; Katja Pollert[1]; Lars Konermann[1]; *[1]University of Western Ontario, London, ON, Canada*

TP 587 **Post-Acquisition Targeted Searches for Novel Peptides in Big Mass Spectrometry Data Sets**; Yu Gao[1]; Jiao Ma[2]; Alan Saghatelian[2]; John R. Yates[1]; *[1]The Scripps Research Institute, La Jolla, CA; [2]Salk Institute, La Jolla, CA*

TP 588 **Structural Evaluation of Protein-Metal Complexes *via* Ultraviolet Photodissociation and Native Mass Spectrometry**; Christopher M Crittenden[1]; Elisa T Novelli[1]; Gulan N Xu[1]; Whitney A Fies[1]; Lauren J Webb[1]; Jennifer S Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX*

TP 589 **Identifying Protein-Protein Interactions in the Synapse by Chemical Cross-Linking Mass Spectrometry**; Iwan Parfentev[1]; Momchil Ninov[2]; Reinhard Jahn[3]; Henning Urlaub[3]; *[1]MPI for Biophysical Chemistry, Goettingen, Germany; [2]MPI for biophysical Chemistry, Goettingen, Germany; [3]Max-Planck-Institute for Biophysical Chemistry, Goettingen, Germany*

TP 590 **Higher-Energy Surface Induced Dissociation on an Orbitrap Platform: Applications to Native MS**; Zachary VanAernum[1]; Joshua D. Gilbert[1]; Alexander Makarov[2]; Stevan R. Horning[2]; Vicki H. Wysocki[1]; *[1]The Ohio State University, Columbus, OH; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

TP 591 **The Utility of Improved Dynamic Range in the Quantitative Study of Protein-Protein Interactions**; Julia Hülsmann[1]; Bojana Kravic[1]; Matthias Weith[1]; Matthias Gstaiger[2]; Ruedi Aebersold[2, 3]; Hemmo Meyer[1]; Ben Collins[4]; *[1]University of Duisburg-Essen, Essen, Germany; [2]ETH Zurich, Zurich, Switzerland; [3]University of Zurich, Zurich, Switzerland; [4]ETH Zurich, Zurich, Switzerland*

TP 592 **Identification and Affinity Determination of Antibody Epitopes against the Chemokine CXCL8 by High-Pressure Proteolytic Excision Mass Spectrometry and Biosensor Analysis**; Pascal Wiegand[1, 2]; Nico Hüttmann[3]; Julia Wack[2]; Loredana Lupu[3]; Alexander Lazarev[4]; Katja Schmitz[2]; Michael Przybylski[3]; *[1]Steinbeis Centre for Biopolymer Analysis and Biomedical Mass Spectrometry, Rüsselsheim am Main, Germany; [2]TU Darmstadt, Darmstadt, Germany; [3]Steinbeis Centre for Biopolymer Analysis and Biomedical Mass Spectrometry, Rüsselsheim am Main, Germany; [4]Pressure Bioscience Inc., South Easton, MA*

TP 593 **Allosteric Modulation of Protein-Protein Interactions by Individual Lipid Binding Events**; Yang Liu[1, 2]; Xiao Cong[1]; Wen Liu[1]; Xiaowen Liang[1]; Arthur Laganowsky[2]; *[1]Institute of Biosciences and Technology, Texas A&M Health Science Center, Houston, TX; [2]Department of Chemistry, Texas A&M University, College Station, TX*

TP 594 **Monitoring the Conformational States of Pre-Amyloid Protein Oligomers Using Collision-Induced Dissociation and Ion Mobility Mass Spectrometry**; Tyler Marcinko[1]; Richard W. Vachet[1]; *[1]Department of Chemistry, University of Massachusetts Amherst, Amherst, MA*

TP 595 **Global and Unbiased Identification of RNA-binding Protein Regions in Mammalian Tissue Using High-Resolution Mass Spectrometry**; Meeli Mullari[1]; Niels H. Skotte[1]; Michael L. Nielsen[1]; *[1]NNF CPR, Copenhagen, Denmark*

TP 596 **Native FTICR Mass Spectrometry, Electron Microscopy, and Synchrotron Spectromicroscopy Provide Detailed Insight into Amyloid Beta Aggregation and Amyloid-Metal Interaction**; Frederik Lermyte[1]; James Everett[2]; Jake Brooks[1]; Yuko P.Y. Lam[1]; Christopher A. Wootton[1]; Mark P. Barrow[1]; Peter J. Sadler[1]; Neil D. Telling[2]; Peter B. O'Connor[1]; Joanna F. Collingwood[1]; *[1]University of Warwick, Coventry, UK; [2]Keele University, Stoke-on-Trent, UK*

TP 597 **Label-Free Differential Mass Spectrometry for Identification of Proteasomal Substrates**; Xuemei Zeng[1]; Megan E. Yates[2]; Pamela S. Cantrell[1]; Jeffrey L. Brodsky[3]; Nathan A Yates[1, 4]; *[1]Biomedical Mass Spectrometry Center, University of Pittsburgh Schools of the Health Sciences, Pittsburgh, PA; [2]Department of Biological Sciences, University of Pittsburgh, Pittsburgh, PA; [3]Department of Biological Sciences, University of Pittsburgh, Pittsburgh, PA; [4]Department of Cell Biology, University of Pittsburgh School of Medicine, Pittsburgh, PA*

TP 598 **Native and Top-Down MS Characterization of Noncovalent Complex between ISD11 and Mitochondrial ACP Tethered with Intermediate Acyl-Chains**; Xidong Feng[1]; Alain Martelli[2]; Joseph Nabhan[2]; Jaimeen Majmudar[2]; Nicholas Fox[3]; Wyatt W Yue[3]; Christine Bulawa[2]; *[1]Pfizer Worldwide Research, Groton, CT; [2]Pfizer Worldwide Research, Cambridge, MA; [3]University of Oxford, Oxford, UK*

TP 599 **Structural Characterization of Bifurcating [FeFe] Hydrogenase Purified from Strictly Anaerobic Hyperthermophilic Bacterium Thermotoga Maritima.**; Monika Tokmina-Lukaszewska[1]; Oleg A. Zadvornyy[2]; Angela Patterson[1]; Gerrit J. Schut[3]; Diep Nguyen[3]; Simone Raugei[4]; Mike W.W. Adams[3]; John W. Peters[2]; Brian Bothner[1]; *[1]Montana State University, Bozeman, MT; [2]Washington State University, Pullman, WA; [3]University of Georgia, Athens, GA; [4]Pacific Northwest National Laboratory, Richland, WA*

TP 600 **Neoglycolipids for Protein-Glycolipid Binding Studies Using ESI-MS and Model Membranes**; Ling Han[1, 2]; Xiaochao Xue[1, 2]; Elena N. Kitova[1, 2]; Todd L. Lowary[1, 2]; John S. Klassen[1, 2]; *[1]University of Alberta, Edmonton, AB, Canada; [2]Alberta Glycomics Centre, Edmonton, Alberta, Canada*

TP 601 **Detecting Protein-Glycolipid Interactions Using Passively-loaded Model Membranes and CaR-ESI-MS**; Jun Li[1, 2]; Ling Han[1, 2]; Jianing Li[1, 2]; Elena N. Kitova[1, 2]; John S. Klassen[1, 2]; *[1]University of Alberta, Edmonton, AB, Canada; [2]Alberta Glycomics Centre, Edmonton, AB, Canada*

TP 602 **Quantifying the Influence of Labeling On Glycan Binding Profiles of Glycan-Binding Proteins**; Elena N. Kitova[1, 2]; Ling Han[1, 2]; Daniel Vinals[1, 2]; Ratmir Derda[1, 2]; John S. Klassen[1, 2]; *[1]University of Alberta, Edmonton, AB, Canada; [2]Alberta Glycomics Centre, Edmonton, AB, Canada*

TP 603 **Detection of Protein-Protein Interactions Using a 2-Dimensional Chemical Crosslinking Activity Correlated Proteomics Platform (2D-XL-ACPP)**; Morgan W Mann[1]; Hongyan Ma[1]; Zhe Wang[1]; Si Wu[1]; *[1]University of Oklahoma, Norman, OK*

TP 604 **Identifying Specific Lipids that Stabilise Membrane Protein Interfaces Using Native Mass Spectrometry and Surface Induced Dissociation**; Denis Shutin[1]; Joseph Gault[1]; Jakub Ujma[2]; Kevin Giles[2]; Carol V Robinson[1]; *[1]University Of Oxford, Oxford, UK; [2]Waters Corporation, Wilmslow, UK*

TP 605 **Native Top-Down MS Clarifies Metal Binding by the Methanobactin Biosynthetic Complex**; Luis F. Schachner[1]; Grace Kenney[1]; Owen Skinner[2]; Amy C Rosenzweig[1]; Neil Kelleher[1]; *[1]Northwestern University, Evanston, IL; [2]Harvard Medical School, Boston, MA*

TP 606 **Bag-1 Isoforms Interact Differentially with Cell Survival Pathway and Protein Homeostasis Regulators to Modulate Cancer Progression in Breast Cancer Cells**; Nisan Can[1]; Tugba Kizilboga[1]; Sevilay Acar[1]; Ezgi Basturk[1]; Ozge Tatlı[1]; Baran Dingiloglu[1]; Gizem Dinler Doganay[1]; *[1]Istanbul Technical University, Istanbul, Turkey*

PROTEINS: CONFORMATION ANALYSIS AND STRUCTURAL BIOLOGY II
607-621

TP 607 **Energy Barriers to the Pre-amyloid Structural Change of β-2-Microglobulin Under Amyloid Forming Conditions Studied by Covalent Labeling and Mass Spectrometry**; Blaise Arden[1]; Nicholas B. Borotto[1]; Richard W. Vachet[1]; *[1]University of Massachusetts Amherst, Amherst, MA*

TP 608 **From IDP to Fibril: Effect of Small Drug-Like Molecules and Metal Ions on α-Synuclein Conformation and Aggregation**; Rani Moons[1]; Albert Konijnenberg[1]; Frank Sobott[1, 2, 3]; *[1]University of Antwerp, Antwerp, Belgium; [2]Astbury Centre for Structural Molecular Biology, Leeds, UK; [3]School of Molecular and Cellular Biology, Leeds, UK*

TP 609 **Surface Induced Dissociation to Shed Light on the Mechanism of *Transthyretin amyloidosis***; Mehdi Shirzadeh[1]; Christopher D. Boone[1]; Arthur Laganowsky[1]; David H. Russell[1]; *[1]Texas A&M, College Station, TX*

TP 610 **Proteome-Wide Characterization of Phosphorylation-Induced Conformational Changes in Breast Cancer**; He Meng[1]; Michael C. Fitzgerald[1]; *[1]Duke University, Durham, NC*

TP 611 **Top-Down Investigations of Oxidative Modifications Using CID-IMS-MS/MS: Probing the Role of Cytochrome c in Apoptosis**; Victor Yin[1]; Lars Konermann[1]; *[1]University of Western Ontario, London, ON, Canada*

TP 612 **Comparison of Gas-Phase and Solution Conformations of Roundabout 1 – Effect of Heparan Binding**; Robert Williams[1]; Yujie Zhao[1]; Alexander Eletsky[1]; Jeong Yeh Yang[1]; Pradeep Prabhakar[1]; Kelley Moremen[1]; James H. Prestegard[1]; I. Jonathan Amster[1]; *[1]University of Georgia, Athens, GA*

TP 613 **Structural Proteomics of an Organelle-Sized Assembly**; Yi Shi[1]; Seung Joong Kim[2]; Javier Fernandez-Martinez[3]; Ilona Nudelman[3]; Wenzhu Zhang[4]; Barak Raveh[2]; Martin F Jarrold[5]; Andrej Sali[2]; Michael P Rout[3]; Brian T. Chait[4]; *[1]University of Pittsburgh School of Medicine, Pittsburgh, PA; [2]UCSF, San Francisco, CA; [3]Laboratory of Cellular and Structural Biology, Rockefeller University, New York, NY; [4]Laboratory of Mass Spectrometry and Gaseous Ion Chemistry, Rockefeller University, New York, NY; [5]Department of Chemistry, Indiana University, Bloomington, IN*

TP 614 **Coupling Gas-Phase HDX to IMS Reveals Structural Transitions as Proteins Leave their Native State**; Shane A Chandler[1]; Timothy M. Allison[1, 2]; George Wright[1]; Ulrik H. Mistarz[3]; Joana Costeira-Paulo[4]; Todd H. Mize[1]; Erik G. Marklund[4]; Kasper D. Rand[3]; Mike R. Morris[5]; Justin L.P. Benesch[1]; *[1]University Of Oxford, Oxford, UK; [2]University of Canterbury, Christchurch, New Zealand; [3]University of Copenhagen, Copenhagen, Denmark; [4]Uppsala University, Uppsala, Sweden; [5]Waters Corporation, Wilmslow, UK*

TP 615 **Relative Quantification of TMT-labeled, Cross-Linked Proteins Using XlinkX Node in Proteome Discoverer Software**; Rosa Viner[1]; Kai Fritzemeier[2]; Berg Frank[2]; Torsten Ueckert[2]; Ryan Bomgarden[3]; Richard A Scheltema[4]; Albert J.R. Heck[4]; Clinton Yu[5]; Lan Huang[5]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Bremen, Germany; [3]Thermo Fisher Scientific, Rockford, IL; [4]Utrecht University, Utrecht, Netherlands; [5]University of California, Irvine, CA*

TP 616 **Ion Mobility Mass Spectrometry Reveals Protein and Lipid Interactions in Protein Misfolding**; Tara L Pukala[1]; Blagojce Jovcevski[1]; Henry Sanders[1]; Denise Tran[1]; *[1]University of Adelaide, Adelaide, Australia*

TP 617 **Orienting the Ultra-Large DNA-PK Homodimer with Crosslinking Mass Spectrometry**; Morgan Hepburn[1]; Yaping Yu[1]; Susan P Lees-Miller[1]; David Schriemer[1]; *[1]University of Calgary, Calgary, AB, Canada*

TP 618 **Integrative Structural Proteomic Analysis of the V-ATPase-RAVE complex**; Zhuolun Shen[1, 2]; Yi Shi[2]; *[1]School of Medicine, Tsinghua University, Beijing, China; [2]Department of Cell Biology, University of Pittsburgh School of Medicine, Pittsburgh, PA*

TP 619 **The Molecular Organization of *Salmonella* T3SS sorting Platform Unraveled by Native MS, SAXS and Computational Modeling**; Johannes Heidemann[1]; Ivonne Bernal[2, 3, 4]; Jonathan Börnicke[2, 3, 4]; Dmitri Svergun[5]; Anne Tuukkanen[5]; Charlotte Uetrecht[1, 6]; Michael Kolbe[2, 3, 4, 7]; *[1]Heinrich Pette Institute, Hamburg, Germany; [2]Center for Structural Systems Biology, Hamburg, Germany; [3]Helmholtz Centre for Infection Research, Braunschweig, Germany; [4]Max Planck Institute for Infection Biology, Berlin, Germany; [5]EMBL, European Molecular Biology Laboratory, Hamburg, Germany; [6]European XFEL, Schenefeld, Germany; [7]University of Hamburg, Hamburg, Germany*

TP 620 **A Fast and Accurate Trajectory Method for Macromolecular CCS-calculations**; Erik Gustav Marklund[1]; Joana Costeira-Paulo[1]; *[1]Department of Chemistry - BMC, Uppsala University, Uppsala, Sweden*

TP 621 **Native Protein Top-Down Electron Capture Dissociation as a Structural Tool: Insights from the Analysis of Library of Carbonic Anhydrase Variants**; Sam Hughes[1]; C.Logan Mackay[1]; David J Clarke[1]; *[1]EaStChem School of Chemistry, University of Edinburgh, Edinburgh, UK*

PROTEINS: PTMS I
622-651

TP 622 **Utilizing Mass Spectrometry to Study Phosphorylation Patterns in Ion Channels and Their Roles in Neurodegeneration and Neuroprotection**; Thu T. A. Nguyen[1]; Wenping Li[1]; Vince G. Amoroso[1]; Liang-Wei Gong[1]; Thomas J. Park[1]; Stephanie M. Cologna[1]; *[1]University of Illinois at Chicago, Chicago, IL*

TP 623 **Characterization of RNA Binding Motif 20 Phosphorylation by Middle-Down Mass Spectrometry**; Yutong Jin[1]; Mingming Sun[2]; Chaoqun Zhu[2]; Wei Guo[2]; Ying Ge[1]; *[1]University of Wisconsin, Madison, Madison, WI; [2]University of Wyoming, Laramie, WY*

TP 624 **Avoiding Method Induced Heterogeneity in the Analysis of Heterogeneity of Monoclonal Antibodies Using Mass Spectrometry after Single Site Proteolysis**; Gideon Oudgenoeg[1]; Anja Boumeester[2]; Peter van Maurik[2]; Jeroen de Keijzer[2]; Emile van Corven[2]; *[1]Bioceros, Utrecht, Netherlands; [2]Bioceros, Utrecht, Netherlands*

TP 625 **Proteome-Wide Effects of Singlet Oxygen Produced by Next Generation Iridium Anti-Cancer Metallodrugs**; Cookson K. C. Chiu[1]; Pingyu Zhang[1]; Yuko P. Y. Lam[1]; Christopher A. Wootton[1]; Mark P. Barrow[1]; Peter J. Sadler[1]; Peter B. O'Connor[1]; *[1]University of Warwick, Coventry, UK*

TP 626 **Towards Elucidation of Protein-Protein Cross-Links in Food and Fibers**; Evelyne Maes[1]; Jolon M. Dyer[1, 2, 3, 4]; Santanu Deb-Choudhury[1]; Stefan Clerens[1, 2]; *[1]AgResearch Ltd., Christchurch, New Zealand; [2]Biomolecular Interaction Centre, University of Canterbury, Christchurch, New Zealand; [3]Riddet Institute, Massey University, Palmerston North, New Zealand; [4]Wine, Food & Molecular Biosciences, Lincoln University, Lincoln, New Zealand*

TP 627 **Identification of the 3-Hydroxyproline Isomer at the Xaa Position in Collagen by MS3.**; Nick Van Huizen[1]; Peter C Burgers[1]; Christoph Stingl[1]; Jan N.M. IJzermans[1]; Theo M. Luider[1]; *[1]Erasmus University Medical Center, Rotterdam, Netherlands*

TP 628 **Combination of Trypsin and Lys-C Can Improve the Phosphoproteomic Identifications in Testis**; Yiwei Cheng[1]; Fangjuan Liu[1]; Yueshuai Guo[1]; Zuomin Zhou[1]; Jiahao Sha[1]; Xuejiang Guo[1]; *[1]State Key Laboratory of Reproductive Medicine, Nanjing Medical University, Nanjing, China*

TP 629 **Characterization of Ubiquitination during NOD2 Signaling**; Anita Izrael-Tomasevic[1]; Tatiana Goncharov[2]; Melinda Mulvihill[2]; Surinder Jeet[2]; Anna Fedorova[2]; Celine Eidenschenk[2]; Andrey Shaw[2]; Wayne Fairbrother[2]; Domagoj Vucic[2]; Donald Kirkpatrick[2]; Kebing Yu[2]; *[1]Genentech, Inc., South San Francisco, CA; [2]Genentech Inc., South San Francisco, CA*

TP 630 **Proteomic Profiling of Protein Tyrosine Phosphorylation in Mouse Testis**; Yiwei Cheng[1]; Xiaofei Liu[1]; Yueshuai Guo[1]; Zuomin Zhou[1]; Jiahao Sha[1]; Xuejiang Guo[1]; *[1]Nanjing Medical University, Nanjing, China*

TP 631 **Global Analysis of Ubiquitinome, Acetylome and Phosphoproteome Dynamics Reveals Post-Translational Regulatory Events in T-Cell Activation**; Albert Casanovas[1, 2]; Oscar Gallardo[1]; Joaquin Abian[1, 2]; Montserrat Carrascal[1]; *[1]Proteomics Laboratory CSIC/UAB, IIBB-CSIC, Barcelona, Spain; [2]Autonomous University of Barcelona, Bellaterra, Spain*

TP 632 **Proteome Wide PTM-PTM Interaction Network Partner Identification by the Julienne Method**; Thomas Clark[1]; Greg Stacey[1]; Ryan Riley[1]; Nikolay Stoynov[1]; Leonard Foster[1]; *[1]UBC, Vancouver, BC, Canada*

TP 633 **Deep Profiling of the Human Protein Arginine Methyl-Transferase Enzyme Class Interactome**; Jeremy D. O'Connell[1]; Marcus Kelly[1]; Nancie A Mooney[1]; Janos Demeter[1]; Peter K. Jackson[1]; *[1]Stanford Medical School, Palo Alto, CA*

TP 634 **Identification of O3-Derived Oxysterol-Protein Adducts and Site-Mapping of Modifications in Human Bronchial Epithelial Cells**; Hye-Young H. Kim[1]; Adam M. Speen[2]; Ilona Jaspers[3]; Ned A. Porter[4]; *[1]Department of Chemistry and Vanderbilt Institue of Chemical Biology, Vanderbilt University, Nashville, TN; [2]Curriculum in Toxicology, University of North Carolina, Chapel Hill, NC; [3]Curriculum in Toxicology, Department of Pediatrics, University of North Carolina, Chapel Hill, NC; [4]Department of Chemistry, Vanderbilt Institute of Chemical Biology, Department of Psychiatry and Kennedy Center for Reserach of Human Development, Vanderbilt Univeristy, Nashville, TN*

TP 635 **Quantitative Proteomic Approach Reveals the Role of p300-Mediated Lysine 2-Hydroxyisobutyrylation in Glycolysis**; He Huang[1]; Shuang Tang[2]; Ming Ji[2]; Xiaojing Liu[3]; Yejing Weng[1]; Jason W. Locasale[3]; Yingming Zhao[1]; Xiaoling Li[2]; *[1]University of Chicago, Chicago, IL; [2]National Institute of Environmental Health Sciences, Durham, NC; [3]Duke University School of Medicine, Durham, NC*

TP 636 **Development of Mass Spectrometry-Based Analysis of Blood Protein Glycation in Birds**; Agnes Hovasse[1]; Christine Schaeffer-Reiss[1]; Alain Van Dorsselaer[1]; Francois Criscuolo[2]; Fabrice Bertile[1]; *[1]IPHC, CNRS, LSMBO, Université de Strasbourg, Strasbourg, France; [2]IPHC, CNRS, DEPE, Université de Strasbourg, Strasbourg, France*

TP 637 **Comparing the Performance of ETD and HCD for Confident Localization of Peptide ADP-Ribosylation Sites**; Sara C Larsen[1]; Ivo Hendriks[1]; Michael L. Nielsen[1]; *[1]University of Copenhagen NNF CPR, Copenhagen N, Denmark*

TP 638 **Evaluation of Combined IEX and RP Chromatography Mass Spectrometry Analysis of Intact Antibodies as an Alternative to Peptide Mapping**; Gang Xiao[1]; Pavel Bondarenko[2]; Andrew Nichols[3]; Aaron O. Bailey[4]; *[1]AMGEN, Thousand Oaks, CA; [2]Amgen, Inc., Thousand Oaks, CA; [3]Protein Metrics Inc., San Carlos, CA; [4]ThermoFisher, San Jose, CA*

TP 639 **An Optimized Strategy for Detection of Ubiquitylation Events upon DNA Stresses in Xenopusegg Extracts on a Q Exactive HF-X**; Camilla S. Colding-Christensen[1]; Julien P. Duxin[1]; Michael L. Nielsen[1]; *[1]University of Copenhagen NNF CPR, København N, Denmark*

TP 640 **Improved Identification of Multiple Phosphorylation Sites Using CESI-MS in Comparison to Conventional Nano LC-MS System**; Faraz Rashid[1]; Dipankar Malakar[1]; Prashant Dour[1]; Manoj Pillai[1]; Stephen Lock[2]; Anindita Paul[3]; Dipanjan Chakrabarti[3]; Maitrayee DasGupta[3]; *[1]SCIEX, Gurgaon, India; [2]SCIEX, Cheshire UK; [3]Department of Biochemistry, University of Calcutta, Kolkata, India*

TP 641 **Discovery Proteomics Uncovered Damaged Proteins in TCA Cycle Induced Bioenergetic Decline in Aging Mice**; Xue Guo[1]; Jung Eun Park[1]; Gallart Palau Xavier Ramon[1]; Siu Kwan Sze[1]; *[1]Nanyang Technological University, Singapore, Singapore*

TP 642 **Serum Protein Termini Modifications in the Analysis of Septic Patients**; Katelyn Ludwig[1, 2]; Bridget A Moroney[1]; Amanda B. Hummon[2]; Matthew M Champion[1]; *[1]University of Notre Dame, Notre Dame, IN; [2]The Ohio State University, Columbus, OH*

TP 643 **Characterizing Lysine Acylations in a Syntrophic Bacterium**; John Muroski[1]; Hong H Nguyen[1]; Michael J Mclnerney[2]; Rachel R Ogorzalek Loo[1]; Joseph A Loo[1]; *[1]UCLA, Los Angeles, CA; [2]University of Oklahoma, Norman, OK*

TP 644 **Characterisation of the Phagosome Ubiquitinome of Activated Macrophages Reveals a Novel Role for RNF115 in Innate Immunity**; Orsolya Bilkei-Gorzo[1]; Julien Peltier[2]; Anetta Hartlova[2]; Matthias Trost[2]; *[1]MRC PPU, University of Dundee, Dundee, UK; [2]Newcastle University, Newcastle-upon-Tyne, UK*

TP 645 **Mapping the Modification Sites of Ubiquitin-Like Proteins (UBLs) in Fission Yeast**; Guang-Can Shao[1]; Shan Lu[1]; Le-Mei Jia[2]; Mei-Qing Zuo[1]; Zhen-Lin Chen[3]; Si-Min He[4]; Li-Lin Du[1]; Meng-Qiu Dong[1]; *[1]National Institute of Biological Sciences, Beijing, China; [2]Tsinghua University, Beijing, China; [3]Chinese Academy of Sciences, Beijing, China; [4]Chinese Academy of Sciences, Beijing, China*

TP 646 **Quantitative Interactome Analysis Revealed Novel Roles of Proline Hydroxylation in Brd4-mediated Transcriptional Activities**; Luke Erber[1]; Ang Luo[1]; Yue Chen[1]; *[1]University of Minnesota, Minneapolis, MN*

TP 647 **Approaches for Environmental Phosphoproteomics: Measuring, Validating and Interpreting a "Metaphosphoproteome"**; Noelle Held[1, 2]; Matthew McIlvin[1]; Jacyln Saunders[1]; Joe Futrelle[1]; Claire Mahaffey[3]; Maeve Lohan[4]; Malcolm Woodward[5]; Mak Saito[1]; *[1]Woods Hole Oceanographic Institution, Woods Hole; [2]Massachusetts Institute of Technology, Cambridge, MA; [3]University of Liverpool, Liverpool, UK; [4]University of Southampton, Southampton, UK; [5]Plymouth Marine Laboratory, Plymouth, UK*

TP 648 **No Signaling by a Soluble Guanylyl Cyclase-Thioredoxin Transnitrosation Complex**; Hong Li[1]; 'changgong Wu[1]; Annie Beuve[1]; *[1]Rutgers New Jersey Medical School, Newark, NJ*

TP 649 **Characterization of a Tubulin Glycylase TTLL3 Using X-Ray Crystallography and Mass Spectrometry**; Christopher P. Garnham[1]; Ian Yu[1]; Yan Li[2]; Antonina Roll-Mecak[1, 3]; *[1]Cell Biology and Biophysics Unit, Porter Neuroscience Research Center, National Institute of Neurological Disorders and Stroke, Bethesda, MD; [2]Protein/peptide Sequencing Facility, National Institute of Neurological Disorders and Stroke, Bethesda, MD, United States, Bethesda, MD; [3]National Heart, Lung, and Blood Institute, Bethesda, MD*

TP 650 **Ancient Regulatory Role of Lysine Acetylation Revealed by Phyloproteomics**; Ernesto S Nakayasu[1]; Meagan C Burnet[1]; Hanna E Walukiewicz[2]; Anil K. Shukla[1]; Shelby Brooks[1]; Matthew J Plutz[2]; Brady D Lee[1]; Birgit Schilling[3]; Alan J Wolfe[4]; Susanne Mueller[5]; John R Kirby[5]; Christopher V Rao[2]; John R Cort[1]; Sam Payne[6]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]University of Illinois at Urbana-Champaign, Urbana, IL; [3]Buck Institute for Research on Aging, Novato, CA; [4]Loyola University Chicago, Maywood, IL; [5]Medical College of Wisconsin, Milwaukee, WI; [6]Pacific Northwest National Lab, Richland, WA*

TP 651 **Heart Proteomics and Oxidation Status after Myocardial Infarction**; Aleksandra Binek[1]; Celia Castans[1]; Rodrigo Fernández-Jiménez[1, 2, 3]; Carlos Galán-Arriola[1, 2];

Inmaculada Jorge[1, 2]; Borja Ibáñez[1, 2, 4]; Jesús Vázquez[1, 2]; *[1]CNIC – Fundación Centro Nacional de Investigaciones Cardiovasculares Carlos III, Madrid, Spain; [2]CIBERCV - Centro de Investicación Biomédica en Red, Madrid, Spain; [3]The Zena and Michael A. Wiener CVI, Icahn School of Medicine at Mount Sinai, New York, NY; [4]IIS - Fundación Jiménez Díaz Hospital, Madrid, Spain*

PROTEOMICS: NEW APPROACHES (I & II)
652-713

TP 652 **Fully Automated Sample Treatment Method for High Throughput Proteome Analysis**; Huiming Yuan; *Dalian Institute of Chemical physics, The Chinese Academy of Sciences, Dalian, China*

TP 653 **Identification of GHB-Binding Proteins by Photoaffinity Labeling Coupled to Quantitative Mass Spectrometry**; Ulrike Leurs[1]; Bente Frølund[1]; Rasmus P. Clausen[1]; Christian D. Kelstrup[2]; Jesper V. Olsen[2]; Petrine Wellendorph[1]; *[1]Department of Drug Design and Pharmacology, Faculty of Health and Medical Sciences, University of Copenhagen, Copenhagen, Denmark; [2]Proteomics Program, Faculty of Health and Medical Sciences, Novo Nordisk Foundation Center for Protein Research, University of Copenhagen, Copenhagen, Denmark*

TP 654 **Tracking Host Cell Proteins while Biopharmaceutical Manufacturing: Advanced Methodologies to Improve Product Quality**; Stefanie Wohlrab[1]; Regina Kufer[2]; Michael Wiedmann[2]; Martina Suessmair[2]; Ingo Lindner[2]; Don Walker[3]; Christopher Yu[4]; Markus Haindl[2]; *[1]Roche Diagnostic GmbH, Penzberg, Germany; [2]Roche Diagnostic GmbH, Penzberg, Germany; [3]Genentech Inc., South San Francisco, CA; [4]Genentech, South San Francisco, CA*

TP 655 **Nanowell-Mediated Two-Dimensional Liquid Chromatography Enables In-Depth Proteome Profiling of Low-Nanogram Samples**; Maowei Dou[1]; Ying Zhu[1]; Andrey Liyu[1]; Yiran Liang[1]; Paul D. Piehowski[1]; Rui Zhao[1]; Ronald J. Moore[1]; Weijun Qian[1]; Ryan T. Kelly[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

TP 656 **In-Depth Quantification of Protein Expression in Single Mammalian Cells by Nanodroplet Sample Processing and Ultrasensitive LC-MS**; Ying Zhu[1]; Geremy C. Clair[1]; William B. Chrisler[1]; Yufeng Shen[1]; Rui Zhao[1]; Anil K. Shukla[1]; Ronald J. Moore[1]; Richard D. Smith[1]; Charles K. Ansong[1]; Ryan T. Kelly[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

TP 657 **In-Situ Click Reaction Coupled with Proteomics Techniques for Identification of Protein Targets of Catechol Estrogens and Binding Strength Classification**; Shu-Hui Chen; *National Cheng Kung University, Tainan, Taiwan*

TP 658 **Bead Assisted Mass Spectrometry (BAMS): A Robust, Affinity Capture MALDI TOF MS Method for Multiplexed Biomarker Profiling**; Sergey Mamaev[1]; Jeffrey C. Silva[1]; Camilla Worsfold[1]; Matthew P. Stokes[2]; Kimberly A. Lee[2]; Morty Razavi[3]; N. Leigh Anderson[3]; Vladislav B Bergo[1]; *[1]ADEPTRIX CORP., Beverly, MA; [2]Cell Signaling Technology, Danvers, MA; [3]SISCAPA Assay Technologies, Victoria, BC, Canada*

TP 659 **Application of Human Immunodepletion Reagents, Isobaric Tagging and Offline Fractionation for Quantitative Discovery Proteomic Analysis of Swine Plasma**; Daryl Bulloch[1]; Matthew Rardin[1]; Bradford W Gibson[1]; James R Turk[2]; *[1]Amgen, South San Francisco, CA; [2]Amgen, Thousand Oaks, CA*

TP 660 **Fast Algorithms for Clustering Tandem Mass Spectra**; Lei Wang[1]; Sujun Li[1]; Haixu Tang[1]; *[1]Indiana University Bloomington, Bloomington, IN*

TP 661 **Optimizing and Validating the Julienne Method for Maximum Proteoform Coverage**; Leonard Foster[1]; Thomas Clark[1]; Richard G Stacey[1]; *[1]University of British Columbia, Vancouver, BC, Canada*

TP 662 **Laser Microdissection Coupled Nano-Proteomic Characterization of Functional Dysregulation in Pancreatic Islets of Pre-Type 1 Diabetic Patients**; Adam Swensen[1]; Paul D. Piehowski[1]; Jing Chen[2]; Ercument Dirice[3]; Vladislav Petyuk[1]; Lian Yi[1]; Ronald J. Moore[1]; Martha Campbell-Thompson[2]; Mark A Atkinson[2]; Clayton E Mathews[2]; Rohit N Kulkarni[3]; Weijun Qian[1]; *[1]Battelle - PNNL, Richland, WA; [2]University of Florida, Department of Pathology, Immunology and Laboratory Medicine, Gainesville, FL; [3]Harvard Medical School, Boston, MA*

TP 663 **In-solution Isoelectric Focusing Device for pI-Code Sample Multiplexing in Proteome Analysis**; Juan Astorga-Wells[1]; Thorleif Lavold[2]; Roman Zubarev[3]; *[1]Karolinska Institutet, Stockholm, Sweden; [2]Biomotif AB, Stockholm, Sweden; [3]Karolinska Institutet, Stockholm, Sweden*

TP 664 **Magnetic HILIC: A Versatile, Enabling Tool for Robust Automated MS Sample Preparation Workflows**; Stoyan Stoychev[1]; Previn Naicker[1]; Sindisiwe Buthelezi[1]; Isak Gerber[1]; Chris van der Westhuyzen[1]; Justin Jordaan[2, 3]; *[1]CSIR, Pretoria, South Africa; [2]Rhodes University, Grahamstown, South Africa; [3]ReSyn BioSciences, Johannesburg, South Africa*

TP 665 **Effects of Copper on Chlorella Protothecoides (UTEX 256)Microalgae: Proteomic Changes Due to the Presence of Copper**; Lidiane Maria de Andrade[1, 2]; Meriellen Dias[1]; Cristiano José Andrade[1]; Maria Anita Mendes[1]; Jorge Alberto Soares Tenório[2]; Claudio Augusto Oller do Nascimento[1]; *[1]Dempster MS Lab - Chemical Engineering Department of Polytechnic School of University of São Paulo – Brazil, São Paulo, Brazil; [2]LAREX - Laboratory of Recycling, Waste Treatment and Extraction - Chemical Engineering Department of Polytechnic School of University of São Paulo –São Paulo, Brazil*

TP 666 **Functional Proteomics of FANCA: Identifying Novel Molecular Functions of FA Proteins in the Endocrine Pancreas**; Dragana Lagundžin[1]; Nicholas T Woods[1]; *[1]University of Nebraska Medical Center, Omaha, NE*

TP 667 **Protein Chromatography for Bottom-Up Proteomics to Extend the Proteome Coverage**; Kosuke Ogata[1]; Michio Funahashi[1]; Hsin-Yi Chang[1]; Naoyuki Sugiyama[1]; Yasushi Ishihama[1]; *[1]Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, Japan*

TP 668 **Evaluation of TIMS-MS and MS/MS Data for Targeted Proteomics**; Markus Lubeck[1]; Heiner Koch[2]; Scarlet Koch[1]; Oliver Raether[1]; Schmit Pierre-Olivier[3]; Gary Kruppa[4]; *[1]Bruker Daltonik GmbH, Bremen, Germany; [2]Bruker Daltonik GmbH, Bremen, Germany, Bremen, Germany; [3]Bruker Daltonique S.A., Wissembourg, France; [4]Bruker Daltonics Inc., Billerica, MA*

TP 669 **LC-MS/MS Assessment of Monoclonal Antibody Stability: Monitoring Tryptophan and Methionine Oxidation**; Ravi Kumar Krovvidi; *Syngene International Ltd, Bangalore, India*

TP 670 **Factors Affecting Digestion Efficiency and Adventitious Modifications during Trypsinization of Plasma Proteins for Bottom-Up Proteomics**; Sarah R Rains[1]; Matthew Foster[1]; J. Will Thompson[1]; M. Arthur Moseley[1]; *[1]Duke University School of Medicine, Durham, NC*

TP 671 **Rapid Isobaric Peptide Classification by Trapped Ion Mobility Spectrometry**; Ryan D Leib[1]; Christopher M Adams[1]; Kratika Singhal[1]; Allis S Chien[1]; *[1]Stanford University, Stanford, CA*

TP 672 **Strong Cation Exchange-Reversed Phase Liquid Chromatography-Capillary Zone Electrophoresis-Tandem Mass Spectrometry Platform with High Peak Capacity for Deep Bottom-Up Proteomics**; Daoyang Chen[1]; Liangliang Sun[1]; *[1]Michigan State University, East Lansing, MI*

TP 673 **Bacterial Proteotyping Using Machine Learning Defined Peptide Signatures and Validation on Q Exactive HF-X Coupled to Capillary Flow Liquid Chromatography**; Florence Roux-Dalvai[1]; Clarisse Gotti-Barban[1]; Mickael Leclercq[1]; Frédéric Fournier[1]; Marie-Claude Hélie[2]; Judith Marcoux[1]; Tabiwang N. Arrey[3]; Julie Bestman-Smith[4]; Claire Dauly[5]; Maurice Boissinot[2]; Michel G. Bergeron[2]; Arnaud Droit[1]; *[1]Proteomics Plateform, CHU Quebec - Laval University, Quebec, QC, Canada; [2]Infectiology Research Center, , CHU Quebec - Laval University, Quebec, QC, Canada; [3]Thermo Fisher Scientific, Bremen, Germany; [4]Enfant-Jesus Hospital, CHU Quebec - Laval University, Quebec, QC, Canada; [5]Thermo Fisher Scientific, Paris, France*

TP 674 **Quantitative Cancer Proteomics Atlas: Pathway-Scale Functional Profiling of Cell Signaling Using Quantitative Targeted Mass Spectrometry**; Paolo Cifani[1]; Alex Kentsis[1, 2]; *[1]Memorial Sloan Kettering Cancer Center, New York, NY; [2]Weill Cornell Medical College, New York, NY*

TP 675 **Optimized DDA+ and HR-DIA Workflows for Standardized, Reproducible, Precise and Robust Label-Free Quantitation of Proteomes**; Aaron Gajadhar[1]; Oleksandr Boychenko[2]; Xin Zhang[3]; Yue Xuan[4]; Andreas Huhmer[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Germering, Germany; [3]Thermo Fisher Scientific, Sunnyvale, CA; [4]Thermo Fisher Scientific, Bremen, Germany*

TP 676 **Development of an Improved CHO HCP Detection System Utilizing SWATH MS**; Shannon L Hayes[1]; Jennifer P Nelson[1]; Jeremy Woods[1]; Mindy Wan[1]; Michael Nold[1]; *[1]KBI Biopharma, Durham, NC*

TP 677 **Analysis of Specific Synaptic Proteomes in Rodent Models of Autism Spectrum Disorder**; Yi-Zhi Wang[1]; Samuel N. Smukowski[1]; Kira A. Cozzolino[1]; Jeffrey N. Savas[1]; *[1]Northwestern University, Chicago, IL*

TP 678 **Establishing a Robust Cross-linking Mass Spectrometry (XL-MS) Platform for Dissecting Protein Interaction Landscapes at the Proteome Scale**; Andrew Wheat[1]; xiaorong Wang[1]; Clinton Yu[1]; Anthony Burke[1]; Robyn M. Kaake[2]; Scott Rychnovsky[1]; Jing Yang[3]; Lan Huang[1]; *[1]University of California, Irvine, CA; [2]University of California San Francisco, San Francisco, CA; [3]Vanderbilt University Medical Center, Nashville, TN*

TP 679 **Fast Algorithms for Searching Peptides from Massive Mass Spectra**; Lei Wang[1]; Kaiyuan Liu[1]; Sujun li[1]; Haixu Tang[1]; *[1]Indiana University Bloomington, Bloomington, IN*

TP 680 **Hands-Free Sample Preparation for Proteomics Using Universal Chemistry and a Microfluidic Benchtop Instrument**; Greg Foster[1]; Aaron Robitaille[1]; Michael Krawitzky[1]; Daniel Lopez-Ferrer[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

TP 681 **Defining the Liver Polysome-Associated Proteome**; Dylan Harney[1]; Harunori Yoshikawa[2]; Angus Lamond[2]; Mark Larance[1]; *[1]The University of Sydney, Camperdown, Australia; [2]University of Dundee, Dundee, UK*

TP 682 **EVOSEP One Enables Robust Deep Proteome Coverage in Half the Time of Nano-LC Metholds**; Jonathan R. Krieger[1]; Lasse Falkenby[2]; Paul Taylor[1]; Nicolai Bache[2]; Jiefei Tong[3]; Michael F Moran[3]; *[1]SPARC Biocentre, The Hospital for Sick Children, Toronto, ON, Canada; [2]Evosep, Odense, Denmark; [3]Program in Cell Biology, The Hospital for Sick Children, Toronto, ON, Canada*

TP 683 **Universal and Standardized Workflow for Sample Preparation in Proteomics**; Aaron Robitaille[1]; Michael Krawitzky[2]; Greg Foster[2]; Gina Tan[1]; Ryan Bomgarden[3]; Sergei Snovida[3]; Daniel Lopez-Ferrer[1]; *[1]Thermo Scientific, San Jose, CA; [2]Thermo Fisher Scientific, San Jose, CA; [3]ThermoFisher Scientific Inc., Rockford, IL*

TP 684 **Rapid and Comprehensive Proteome Analysis Using LC-FAIMS-MS/MS**; Alexander S Hebert[1]; Satendra Prasad[2]; Michael W Belford[2]; Derek J Bailey[2]; Susan E Abbatiello[2]; Romain Huguet[2]; Graeme C McAlister[2]; Eloy R Wouters[2]; Jean-Jacques Dunyach[2]; Michael S Westphall[1]; Joshua J Coon[1, 3, 4, 5]; *[1]Genome Center of Wisconsin, Madison, WI; [2]Thermo Fisher Scientific, San Jose, CA; [3]Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI; [4]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [5]Morgridge Institute for Research, Madison, WI*

TP 685 **Maximized Throughput and Analytical Depth for Shotgun Proteomics Using PASEF on a TIMS Equipped QTOF and a Novel LC System**; Thomas Kosinski[1]; Scarlet Koch[1]; Markus Lubeck[1]; Nicolai Bache[2]; Ole Bjeld Horning[2]; Lasse Falkenby[2]; Heiner Koch[1]; *[1]Bruker Daltonik GmbH, Bremen, Germany; [2]Evosep, Odense, Denmark*

TP 686 **Immobilised Enzymatic on Customised Micro Solid-Phase Extraction Cartridges for Automated Protein Digestion**; Karen Doung[1]; Simin D. Maleknia[2]; Andrew Minett[3]; Philip Doble[1]; *[1]School of Mathematical and Physical Sciences, University of Technology Sydney, Sydney, Australia; [2]University of Technology Sydney, Sydney, Australia; [3]Eprep Pty Ltd, Mulgrave, Australia*

TP 687 **Systematic Study of Nonspecific Trypsin Cleavages Leads to an Optimal2-hr Trypsin Digestion Protocol**; Zhilong Lin[1]; Yan Ren[1]; Piliang Hao[2]; *[1]BGI-Shenzhen, Shenzhen, China; [2]ShanghaiTech University, Shanghai, China*

TP 688 **Antibody-Assisted Target Identification of Covalent Kinase Inhibitor Afatinib by Mass Spectrometry**; Chi-Chi Chou[1, 2]; Cheng-Han Yu[3]; Geen-Dong Chang[3]; Kay-Hooi Khoo[2, 3]; *[1]Taiwan Protein Project, Academia Sinica, Taipei, Taiwan; [2]Institute of Biological Chemistry, Academia Sinica, Taipei, Taiwan; [3]Institute of Biological Chemistry, National Taiwan University, Taipei, Taiwan*

TP 689 **Development of a Method to Profile Specific Interactions Between Proteins and Antisense Oligonucleotides**; Helene Meistermann[1, 2]; Sabrina Golling[1, 2]; Balazs Banfai[1, 2]; Erich Koller[1, 2]; Sabine Sewing[1, 2]; Stefan Kustermann[1, 2]; Tom Dunkley[1, 2]; *[1]Roche Pharma Research and Early Development, Roche Innovation Center Basel, Hoffmann-La Roche Ltd, Basel, Switzerland; [2]Pharmaceutical Sciences, Basel, Switzerland*

TP 690 **Protease Cleavage Site Profilling by Label Free In-Gel Degradomics**; Robert Vidmar[1]; Matej Vizovisek[1]; Dusan Turk[1]; Boris Turk[1]; Marko Fonovic[1]; *[1]Jozef Stefan Institute, Ljubljana, Slovenia*

TP 691 **Investigations of the Cleavage Specificity of the ClpXP Protease and Its Potential Use in Proteomics Experiments**; Catherine Tremblay[1]; Robert H. Vass[1]; Peter C. Chien[1]; Richard W. Vachet[1]; *[1]University of Massachusetts Amherst, Amherst, MA*

TP 692 **Identification of a Protein Target Highly Specific to 2-Nitroimidazole-Indocyanine Green for Imaging Tumor Hypoxia**; Lei Wang[1]; Christopher Dietz[1]; Feifei Zhou[2]; Mohsen Erfanzadeh[2]; Bin Deng[3]; Quing Zhu[2, 4]; Michael Smith[1]; Xudong Yao[1]; *[1]Department of Chemistry, University of Connecticut, Storrs, CT; [2]Department of Electrical and Computer Engineering, University of Connecticut, Storrs, CT; [3]Department of Biology, University of Vermont, Burlington, VT; [4]Department of Biomedical Engineering, Washington University in St. Louis, St. Louis, MO*

TP 693 **Proteomic Analysis of *Aspergillus niger* Fungus Isolated From Mine Environment: Screening for Protein Biomarkers Induced by Copper**; Meriellen Dias[1]; José Thalles Jocelino Gomes de Lacerda[2]; Lidiane Maria de Andrade[1]; Enrique Eduardo Rozas Sanchez[1]; Maria Anita Mendes[1]; *[1]Dempster MS Lab- Poli-USP, Sao Paulo, Brazil; [2]Federal University of São Paulo, Sao Paulo, Brazil*

TP 694 **Optimization of SWATH Proteome Coverage through Two-Dimensional Fractionation for Peptide Ion Library**

Building; Liang Jin[1]; Chenqi Hu[1]; shichen Shen[2]; Xue Wang[2]; Edit Tarcsa[1]; Jun Qu[2]; Yu Tian[1]; *[1]AbbVie, Worcester, MA; [2]University at Buffalo, Buffalo, NY*

TP 695 **The Concept of "Protein Digestibility Profile" Using the MELD Approach**; Gabriel Mazzucchelli[1]; Denis Morsa[1]; Dominique Baiwir[2]; Nicolas Smargiasso[2]; Marie-Alice Meuwis[3, 4]; Rémi Longuespée[5]; Elodie Grifnée[1]; Tyler A Zimmerman[6]; Edwin De Pauw[2]; *[1]University of Liege, MS Lab - GIGA, MolSys Research Unit, Liege, Belgium; [2]Univeristy of Liege, MS Lab - GIGA, MolSys Research Unit, Liege, Belgium; [3]University of Liege, Translationnal Gastroenterology unit, GIGA-R, Liege, Belgium; [4]Hepato-Gastroenterology and Digestive Oncology, CHU, Liege, Belgium; [5]University of Heidelberg, Institute of Pathology, Heidelberg, Germany; [6]UTC Aerospace Systems, Pomona, CA*

TP 696 **TMT-MATRIX: A Global Unbiased Methodology for the Exploration of Dynamic Changes in Translation**; Jonathan R Krieger[1]; J. J. David Ho[2]; Paul Taylor[1]; Michael F. Moran[1, 3]; *[1]SPARC Biocentre, The Hospital for Sick Children, Toronto, ON, Canada; [2]Department of Biochemistry and Molecular Biology, Miller School of Medicine, University of Miami, Miami, FL; [3]Program in Cell Biology, The Hospital for Sick Children, Toronto, ON, Canada*

TP 697 **Results As Soon As Possible (rASAP): 2 Hours from Lysis to Label Free Quantification of Cells and Tissues Using Subtilisin**; Humberto Gonczarowska-Jorge[1, 2]; Stefan Loroch[1]; Margherita Dell'Aica[1, 3]; Albert Sickmann[1, 4, 5]; Christoph H. Borchers[3, 6, 7]; Kristina Lorenz[8, 9]; Andreas Roos[1]; René Zahedi[10]; *[1]Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Dortmund, Germany; [2]CAPES Foundation, Brasília, Brazil; [3]Jewish General Hospital Proteomics Centre, McGill University, Montreal, QC, Canada; [4]Medizinisches Proteom-Center, Ruhr-Universität, Bochum, Germany; [5]Department of Chemistry, University of Aberdeen, Aberdeen, UK; [6]Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC, Canada; [7]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [8]Leibniz-Institut für Analytische Wissenschaften-ISAS-e.V., Dortmund, Germany; [9]Comprehensive Heart Failure Center, University of Wuerzburg, Wuerzburg, Germany; [10]JGH Proteomics Centre, McGill University, Montreal, QC, Canada*

TP 698 **TMT Multiplexing with a Carrier/Reference Increases Coverage for 1.0 Nanogram Samples**; Nicholas J. Carruthers[1]; Zhijing Tan[2]; David M. Lubman[2]; Joseph A. Caruso[3]; Paul M. Stemmer[3]; *[1]Wayne State University, Detroit, MI; [2]University of Michigan, Ann Arbor, MI; [3]Wayne State University, Detroit , MI*

TP 699 **Global Analysis of Protein Stability by Chemical Oxidation and Mass Spectrometry**; Ethan J Walker[1]; Sina Ghaemmaghami[1]; Jennifer Hryhorenko[2]; Kevin Welle[2]; *[1]University of Rochester, Rochester, NY; [2]University of Rochester Mass Spectrometry Resource Laboratory, Rochester, NY*

TP 700 **Identification of Potential Protein Targets of ML404 (a mitoPTP Inhibitor) Using Photoaffinity Labeling and Chemical Proteomics**; Rong-Fang Gu[1]; Ceren Korkut[1]; Benbo Gao[1]; Patrick Faloon[1]; Jeffrey Vessels[1]; Kevin Guckian[1]; Brigitte Pettmann[1]; Peter Juhasz[1]; Ru Wei[1]; *[1]Biogen, Cambridge, MA*

TP 701 **Mechanism of Protein Immobilization by Aggregation and Its Application for Target Identification**; Tanveer Singh Batth[1]; Christian D. Kelstrup[1]; Jesper V. Olsen[1]; *[1]Novo Nordisk Foundation Center for Protein Research, University of Copenhagen, Copenhagen, Denmark*

TP 702 **A Metabolic Labeling Approach for Deep Proteome Quantification that Enables Alternative Digestion Methods**; Christoph Schräder[1]; Shaun Moore[1]; Gareth J. Williams[1]; Aaron A. Goodarzi[1]; David C. Schriemer[1]; *[1]University of Calgary, Calgary, AB, Canada*

TP 703 **Meltome Atlas – Proteome-Wide Analysis of Protein Thermostability**; Anna Jarzab[1]; Thomas Hopf[2]; Hannes Hahne[2]; Nils Kurzawa[3]; Matthias Moerch[4]; Angel Angelov[4]; Niels Leijten[5]; Julia Mergner[1]; Britta Spanier[6]; Simone Lemeer[5]; Mikhail Savitski[3]; Wolfgang Liebl[4]; Bernhard Kuster[1]; *[1]Chair of Proteomics and Bioanalytics, Technical University of Munich (TUM), Freising, Germany; [2]OmicScouts GmbH, Freising, Germany; [3]Genome Biology Unit, EMBL, Heidelberg, Germany; [4]Department of Microbiology, Technical University of Munich, Freising, Germany; [5]Netherlands Proteomics Center, Utrecht, Netherlands; [6]Molecular Nutrition Unit, Technical University of Munich, Freising, Germany*

TP 704 **Site-Specific Proteomic Profiling Using a Novel Chemical Probe Identifies New Members in the Deubiquitinase Family**; Taylur Ma[1]; David Hewings[1]; Johanna Heideker[1]; Andrew Ah Young[1]; Farid El Oualid[2]; Alessia Amore[2]; Gregory Costakes[2]; Daniel Kirchhofer[1]; Bradley Brasher[3]; Thomas Pillow[1]; Nataliya Popovych[1]; Till Maurer[1]; Carsten Schwerdtfeger[3]; William Forrest[1]; John Flygare[1]; Matthew Bogyo[4]; Ingrid Wertz[1]; Kebing Yu[1]; *[1]Genentech, Inc., South San Francisco, CA; [2]UbiQ Bio BV, Amsterdam, Netherlands; [3]Boston Biochem Inc., Cambridge, MA; [4]Stanford University, Palo Alto, CA*

TP 705 **Quantifying Proteoform Thermal Stability Using Peptide-Level Readouts**; Kyle N Hess[1, 2]; Ian R Smith[2]; Ricard A Rodriguez-Mias[2]; Ariadna Llovet[2]; Judit Villén[2]; *[1]Molecular and Cellular Biology Program, University of Washington, Seattle, WA; [2]University of Washington Genome Sciences, Seattle, WA*

TP 706 **Improving BioID: Molecularly Engineered Ligases for More Efficient Proximity Labeling in Living Cells and Organisms**; Tanya Svinkina[1]; Tess C Branon[2, 3, 4]; Justin A Bosch[5]; Ariana D Sanchez[4]; Namrata D Udeshi[1]; Steven A Carr[1]; Jessica L Feldman[4]; Norbert Perrimon[5, 6]; Alice Y Ting[2, 3, 4, 7]; *[1]Broad Institute, Cambridge, MA; [2]Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA; [3]Departments of Genetics and Chemistry, Stanford University, Palo Alto, CA; [4]Department of Biology, Stanford University, Palo Alto, CA; [5]Department of Genetics, Harvard Medical School, Boston, MA; [6]Howard Hughes Medical Institute, Boston, MA; [7]Chan Zuckerberg Biohub, San Francisco, CA*

TP 707 **Automated TMT Labeling Using Solid Phase Micro Extraction Cartridges**; Michael Krawitzky[1]; Julian Saba[2]; Greg Foster[1]; Aaron Robitaille[1]; Daniel Lopez-Ferrer[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Mississauga, ON, Canada*

TP 708 **Protein Identification by Limited Trypsin Digestion and Mass Spectrometry**; Feifei Zhao[1]; Eric Dziekonski[2]; Scott A McLuckey[1]; *[1]Purdue University, West Lafayette, IN; [2]SCIEX, Concord, ON, Canada*

TP 709 **Allele Specific Turnover (pAST) Reveals Preferential Protein Usage in a Yeast Hybrid**; Danielle A Faivre[1]; Miguel Martin-Perez[1]; Judit Villen[1]; *[1]University of Washington Genome Sciences, Seattle, WA*

TP 710 **Broad-Spectrum Kinase Profiling in Live Cells with Lysine-Targeted Sulfonyl Fluoride Probes**; Qian Zhao[1]; Xiaohu Ouyang[2]; Xiaobo Wan[2]; Alma L. Burlingame[2]; Jack Taunton[2]; *[1]Hong Kong Polytechnic Univeristy, Hong Kong, Hong Kong; [2]University of California San Francisco, San Francisco, CA*

TP 711 **Differentiation of Blood Group Oligosaccharides in Lectins by Determination of Epitope Ligands Using Proteolytic Excision Mass Spectrometry**; Yannick Baschung[1]; Loredana Mirela Lupu[1]; Adrian Moise[2]; Stefan Rawer[3]; Alexander Lazarev[4]; Michael Przybylski[1];

[1]Steinbeis Centre for Biopolymer Analysis and Biomedical Mass Spectrometry, Rüsselsheim am Main, Germany; [2]Department of Chemistry, University of Konstanz, Konstanz, Germany; [3]ThermoFisher Scientific, Darmstadt, Germany; [4]Pressure Bioscience Inc., South Easton, MA

TP 712 **Effect of Metagenome on Stable-Isotope-Enabled Metaproteomic Analyses of Soil Microbial Communities**; Sneha P Couvillion[1]; Samuel O. Purvine[1]; Carrie D. Nicora[1]; Anil K. Shukla[1]; Evan Starr[2]; Erin Nuccio[3]; Kateryna Zhalnina[4]; Eoin L. Brodie[4]; Ulas Karaoz[4]; Jillian F. Banfield[2]; Jennifer Pett-Ridge[3]; Mary K. Firestone[2]; Mary S. Lipton[1]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]University of California Berkeley, Berkeley, California; [3]Lawrence Livermore National Laboratory, Livermore, CA; [4]Lawrence Berkeley Laboratory, Berkeley, CA*

TP 713 **Direct Linkage of Post-translational Modification Status with Subcellular Localization**; Daniel N Itzhak[1]; Sophia Doll[1]; Jürgen Cox[1]; Florian Gnad[2]; Georg H. H. Borner[1]; *[1]Max Planck Institute of Biochemistry, Martinsried, Germany; [2]Cell Signaling Technology, Danvers, MA*

PROTEOMICS: QUANTITATIVE II
714-739

TP 714 **Quantification of Membrane Proteins for Quality Control of Extracellular Vesicles Isolation**; Tingting Wang[1, 2]; Kyle W. Anderson[1, 2]; Illarion V. Turko[1, 2]; *[1]Institute for Bioscience and Biotechnology Researc, Rockville, MD; [2]National Institute of Standards and Technology, Gaithersburg, MD*

TP 715 **Profiling the Phosphotyrosine Interactome of Receptor Tyrosine Kinases by Affinity Purification-Mass Spectrometry**; Runsheng Zheng[1]; Chen Meng[1]; Bernhard Kuster[1, 2, 3]; *[1]Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; [2]Bavarian Biomolecular Mass Spectrometry Center, Technical University of Munich, Freising, Germany; [3]Partner Site of the German Cancer Consortium, Freising, Germany*

TP 716 **Multiplexing Quantification of Mass-limited Yeast Digest using Capillary Electrophoresis ESI-HRMS**; Vi Quach[1]; Camille Lombard-Banek[1]; Peter Nemes[1]; *[1]University of Maryland, College Park, MD*

TP 717 **Quantitative Proteomic Analysis of Intestinal and Diffuse Types of Gastric Cancer Using a New Peff-Oriented Pipeline by Patternlab for Proteomics**; Helisa Helena Wippel[1, 2]; Marlon Dias Mariano Santos[2]; Milan Avila Clasen[2]; Louise Ulrich Kurt[2]; Fabio Cesar Sousa Nogueira[3]; Thaís Messias McCormick[4]; Guilherme Pinto Bravo Neto[5]; Lysangela Ronalte Alves[6]; Maria da Gloria da Costa Carvalho[4]; Paulo Costa Carvalho[2]; Juliana de S. da G. Fischer Carvalho[1, 2]; *[1]Laboratory of Proteomics and Protein Engineering, Carlos Chagas Institute, Fiocruz, Curitiba, Brazil; [2]Computational Mass Spectrometry & Proteomics Group, Curitiba, Brazil; [3]Laboratory of Protein Chemistry, Proteomic Unit, Institute of Chemistry, Federal University of Rio de Janeiro, Rio de Janeiro, Brazil; [4]Pathology Service of the Clementino Fraga Filho University Hospital, Rio de Janeiro, Brazil; [5]Division of Esophageal and Gastric Surgery, General Surgery Service, Rio de Janeiro, Brazil; [6]Laboratory of Gene Expression Regulation, Carlos Chagas Institute, Curitiba, Brazil*

TP 718 **The Proteome of Human Mesenchymal Stem Cells Conditioned by Hypoxia and the Pro-Inflammatory Cytokine Interferon-Gamma**; Holly M. Wobma[1]; Shahar Goeta[1]; Fereshteh Zandkarimi[1]; Lewis Brown[1]; Gordana Vunjak-Novakovic[1]; *[1]Columbia University, New York, NY*

TP 719 **The Effects of Cathepsin D Knockout on Global Protein Expression**; Lie Min[1]; Jongyoun Baik[1]; Kelvin H. Lee[1]; *[1]Department of Chemical and Biomolecular Engineering and Delaware Biotechnology Institute, University of Delaware, Newark, DE*

TP 720 **Characterizing the Inducible Degradation of Mutant PIK3CA**; Lilian Phu[1]; Kyle A Edgar[1]; Kyung Song[1]; William Forrest[1]; Lori Friedman[1]; Donald S Kirkpatrick[1]; *[1]Genentech, South San Francisco, CA*

TP 721 **Temporal Proteomic Analysis of Pancreatic β-Cells in Response to Lipotoxicity and Glucolipotoxicity**; Zonghong Li[1, 2]; Hongyang Liu[3]; Zhangjing Niu[2]; Wen Zhong[2, 4]; Yifang Zhou[1]; Tao Xu[2, 3]; Junjie Hou[2]; *[1]Northeast Normal University, CHANGCHUN, China; [2]Institute of Biophysics, Chinese Academy of Sciences, Beijing, China; [3]University of Chinese Academy of Sciences, Beijing, China; [4]HuaZhong University of Science and Technology, Wuhan, China*

TP 722 **Identification of DNA-Protein Interaction Partners of ALOX5-Promoter Using Quantitative Proteomics**; Katharina Melanie Schlag[1]; Bernd Sorg[1]; Michael Karas[1]; *[1]Goethe University, Institute of Pharmaceutical Chemistry, Frankfurt, Germany*

TP 723 **Towards Elucidation of Muscle-Specific Receptor Tyrosine Kinase (MuSK) Signaling Pathway**; Hanna Budayeva[1]; Arundhati Sengupta Ghosh[1]; Lilian Phu[1]; Gai Ayalon[1]; Donald S Kirkpatrick[1]; *[1]Genentech Inc., South San Francisco, CA*

TP 724 **MRM-MS with Stable-Isotope Labelled Internal Standards for Multiplexed Quantitation of Proteins in Dried Blood Spots**; Azad Eshghi[1]; Adam J. Pistawka[1]; Nicholas J.T. Sinclair[1]; Darryl B. Hardie[1]; Monica Elliott[1]; Rachael Newman[1]; Christoph H. Borchers[1, 2, 3, 4]; *[1]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [2]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada; [3]Jewish General Hospital Proteomics Centre, McGill University, Montreal, QC, Canada; [4]Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC, Canada*

TP 725 **Develop of a Robust and Reproducible Global Plasma Proteome Profiling Workflow**; Scott Peterman[1]; David Sarracino[1]; Emily Chen[1]; Amol Prakash[2]; Ken Miller[3]; *[1]Thermo Fisher Scientific, Cambridge, MA; [2]Optys Technologies, Boston, MA; [3]Thermo Fisher Scientific, San Jose, CA*

TP 726 **Proteomic Investigation of Protein Synthesis during Aging in *Drosophila***; Lu Yang[1]; Jing Zhao[1]; Nan Liu[1]; Yaoyang Zhang[1]; *[1]Interdisciplinary Research Center on Biology and Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, 26 Qiuyue Rd., Pudong, Shanghai, China*

TP 727 **Integration of Chemical Proteomics and Metabolomics Reveals Direct Cellular Targets of PFOA**; Xiaojian SHAO[1]; Qian ZHAO[2]; Zongwei Cai[1]; *[1]State Key Laboratory of Environmental and Biological Analysis, Department of Chemistry, Hong Kong Baptist University, Hong Kong, China; [2]Department of Applied Biology and Chemical Technology, The Hong Kong Polytechnic University, Hong Kong, China*

TP 728 **A Streamlined Workflow for High-Throughput, Precise, and Comprehensive Large-Scale Quantitative Proteomics Analysis**; Yue Xuan[1, 2]; Yue Zhou[3]; Sebastien Gallien[1, 4]; Pedro Navarro[2]; Oleksandr Boychenko[5]; Joshua J. Nicklay[6]; Jenny Ho[7]; Scott Peterman[8]; Emily Chen[8]; Ken Miller[9]; *[1]Thermo Fisher Scientific, Precision Medicine Science Center, Cambridge, MA; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [3]Thermo Fisher Scientific, Shanghai, China; [4]Thermo Fisher Scientific, Paris, France; [5]Thermo Fisher Scientific, Germering, Germany; [6]Thermo Fisher Scientific, Somerset, NJ; [7]Thermo Fisher Scientific, Hemel Hempstead, UK; [8]Thermo Fisher Scientific, Precision Medicine Science Center, Cambridge, MA; [9]Thermo Fisher Scientific, San Jose, CA*

TP 729 **ArgC-like Digestion and Quantification through Chemical Labelling of Lysines with Propionic Anhydride**; Vahid Golghalyani[1]; Yannik Lewin[1]; Michael Karas[1]; *[1]Goethe University, Institute of Pharmaceutical Chemistry, Frankfurt am Main, Germany*

TP 730 **Proteomics Based Analysis of the Nicotine Catabolism in Paenarthrobacter Nicotinovorans pAO1**; Devika Channaveerappa[1]; Marius Mihasan[2]; Cornelia Babii[2]; Roshanak Aslebagh[1]; Emmalyn Dupree[1]; Costel C. Darie[1]; *[1]Clarkson University, Potsdam, NY; [2]Alexandru Ioan Cuza University, Iaşi, Romania*

TP 731 **Evaluation of Cross-Instrument Data for SWATH Peptide Library Construction and Quantification**; Xiaomin Song[1]; Robert J.A. Goode[2]; Thiri Zaw[1]; Jemma Wu[1]; Dana Pascovici[1]; William Klare[3]; Stuart Cordwell[3]; Ralf B Schittenhelm[2]; Mark P Molloy[1]; *[1]Australian Proteome Analysis Facility, Macquarie University, Sydney, Australia; [2]Monash Biomedical Proteomics Facility, Monash University, Melbourne, Australia; [3]Charles Perkins Centre, University of Sydney, Sydney, Australia*

TP 732 **Protein Turnover Experiments Using Skyline**; Nicholas Shulman[1]; Natan Basisty[2]; Birgit Schilling[2]; Michael J MacCoss[1]; Brendan MacLean[1]; *[1]University of Washington Genome Sciences, Seattle, WA; [2]Buck Institute for Research on Aging, Novato, CA*

TP 733 **Applying sMRMhr Strategy for Glycolysis Enzyme Quantitation Based on SCIEX TripleTOF® 5600+ system**; Chen Chen[1]; Ji Luo[1]; Lihai Guo[1]; Wenhai Jin[1]; *[1]SCIEX, Shanghai, China*

TP 734 **Semi-Micro-Scale UHPLC-MS Proteomics Enables High-Throughput and Robust Quantitation of Biomarker Candidates in Clinical Samples**; Kiyonaga Fujii[1]; Tomoyo Nakano[2]; Akio Kori[3]; Takashi Kondo[3]; Yasuhiko Bando[2]; Fumihiko Usui[2]; Hirotaka Koizumi[1]; Hisashi Saji[1]; Masayuki Takagi[1]; Haruhiko Nakamura[1]; Toshihide Nishimura[1]; *[1]St. Marianna University School of Medicine, Kawasaki, Japan; [2]AMR Inc., Meguro-ku, Japan; [3]Agilent Technologies Japan, Ltd, Hachioji, Japan*

TP 735 **Absolute Membrane Quantification – A Mass Spectrometry-Based Proteomics Approach**; Minia Antelo[1]; Jürgen Bartel[1]; Thomas Sura[1]; Andreas Otto[1]; Becher Dörte[1]; *[1]Institute for Microbiology University of Greifswald, Greifswald, Germany*

TP 736 **A Combined Pulsed SILAC-TMT Strategy Enables Peptide Level Turnover Measurements and the Study Of Proteoform Dynamics**; Jana Zecha[1, 2, 3]; Chen Meng[1]; Daniel Paul Zolg[1]; Patroklos Samaras[1]; Mathias Wilhelm[1]; Bernhard Kuster[1, 2, 3, 4]; *[1]Chair of Proteomics and Bioanalytics, Technical University of Munich (TUM), Freising, Germany; [2]German Cancer Consortium (DKTK), Heidelberg, Germany; [3]German Cancer Research Center (DKFZ), Heidelberg, Germany; [4]Bavarian Biomolecular Mass Spectrometry Center, Technical University of Munich, Freising, Germany*

TP 737 **High-Throughput Proteomics Quantification Enabled by Fast LC Separation and Advanced PRM Acquisition**; Sebastien Gallien[1, 2]; Aaron Gajadhar[3]; Bhavin Patel[4]; Tabiwang Arrey[5]; David Sarracino[1]; Yue Xuan[1, 5]; Emily Chen[1]; *[1]Thermo Fisher Scientific, Precision Medicine Science Center, Cambridge, MA; [2]Thermo Fisher Scientific, Paris, France; [3]Thermo Fisher Scientific, San Jose, CA; [4]Thermo Fisher Scientific, Rockford, IL; [5]Thermo Fisher Scientific, Bremen, Germany*

TP 738 **21-plex DiLeu Isobaric Tags for High-Throughput Quantitative Proteomics**; Dustin Frost[1]; Yu Feng[1]; Lingjun Li[1]; *[1]University of Wisconsin–Madison, Madison, WI*

TP 739 **Annexin A2 is Upregulated in Fast Moving Gliomas**; Emmanuel Ojefua[1]; Vincent Chen[1]; *[1]Brandon University, Brandon, MB, Canada*

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TP 740 **Effect of Supercharging Reagents in Protein Identification**; Faraz Rashid[1]; Dipankar Malakar[1]; Amit Kumar Dey[2]; Bhoj Kumar[2]; Tushar Kanti Maity[2]; Manoj Pillai[1]; *[1]SCIEX, 121, Udyog Vihar, Phase IV, Gurgaon, India; [2]Regional Centre for Biotechnology, Faridabad, India*

TP 741 **Improved Top-Down Sequence Coverage on a Tribrid Mass Spectrometer by Ion-Ion Proton Transfer (IIPT) Reactions Subsequent to ETD and UVPD**; Christopher Mullen[1]; Jae C. Schwartz[2]; John E. P. Syka[2]; Lee Earley[2]; A. Michelle English[3]; Jeffrey Shabanowitz[4]; Donald F. Hunt[4]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]ThermoFisher, San Jose, CA; [3]Pfizer, Cambridge, MA; [4]University of Virginia, Charlottesville, VA*

TP 742 **Top-Down Mass Spectrometry with Multiple MS/MS Strategies to Identify Age-Related Proteoform Changes in Tear Fluid**; Daniel Lopez-Ferrer[1]; Romain Huguet[2]; David Horn[1]; Michael Krawitzky[1]; Peter PM Raus[3]; Vlad Zabrouskov[1]; Andreas Huhmer[1]; Peter Verhaert[4]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Scientific, San Jose, CA; [3]Miro Center, Geel, Belgium; [4]ProteoFormiX, Beerse, Belgium*

TP 743 **An Isotope Depletion Strategy for Intact Protein Mass Spectrometry and Top-Down Fragmentation**; Kelly J Gallagher[1]; Michael Palasser[2]; Sam Hughes[1]; C.Logan Mackay[1]; Clinton G.L Veale[3]; David P. A. Kilgour[4]; David J Clarke[1]; *[1]EaStChem School of Chemistry, University of Edinburgh, Edinburgh, UK; [2]Institut für Organische Chemie and Center for Molecular Biosciences Innsbruck (CMBI), Innsbruck, Austria; [3]School of Chemistry and Physics, University of KwaZulu-Natal, Pietermaritzburg, South Africa; [4]Nottingham Trent University, Nottingham, UK*

TP 744 **Identification of Low pH-Induced Auto-Proteolytic Cleavage Sites of Human Bocavirus1 Using Top-Down Sequencing**; Kari B. Green[1]; Mengxiao Luo[1]; Mavis Agbandje-McKenna[1]; *[1]University of Florida, Gainesville, FL*

TP 745 **Optimization of Single-Shot Capillary Zone Electrophoresis Mass Spectrometry for Sensitive Analysis of Intact Proteins**; Rachele Lubeckyj; *Michigan State University, East Lansing, MI*

TP 746 **Intact Protein Quantitation in Complex Samples Using Protein-Level TMT Labeling and Top-down Mass Spectrometry**; Dahang Yu[1]; Zhe Wang[1]; Hongyan Ma[1]; Qiang Kou[2]; Xiaowen Liu[2]; Si Wu[1]; *[1]University of Oklahoma, Norman, OK; [2]Indiana University, Purdue University-Indianapolis, Indianapolis, IN*

TP 747 **Top-Down Analysis of Histone Proteoforms Following Tazemetostat Exposure**; Aaron J Storey[1]; Brian S Koss[2]; Alan J Tackett[1]; Ricky D Edmondson[1]; *[1]University of Arkansas for Medical Sciences, Little Rock, AR; [2]University of Arkansas for Medical Sciences, Little Rock, Arkansas*

TP 748 **Characterizing Cysteine Modifications in β-lactoglobulin by Top-down Mass Spectrometry**; Jianzhong Chen; *University of Alabama at Birmingham, Birmingham, AL*

TP 749 **Informatic Roadmap for a Cell-Based Proteoform Atlas**; Richard LeDuc[1]; Ryan T. Fellers[2]; Paul Martin Thomas[2]; Neil L. Kelleher[2]; *[1]Northwestern University, Bloomington, IN; [2]Northwestern University, Evanston, IL*

TP 750 **Charge State Dependent Fragmentation in Top-Down Analysis by RP-LC-MS/MS Using a Standard Protein Mix**; Benjamin Cutak[1]; Ken Chanthamontri[1]; Gordon Nicol[1]; Kevin Ray[1]; *[1]MilliporeSigma, Saint Louis, MO*

TP 751 **Revealing Tissue Specific Proteoforms by UVPD-MS**; Jolene K Diedrich[1, 2]; Daniel B. McClatchy[1]; John R. Yates III[1]; *[1]Scripps Research Institute, La Jolla, CA; [2]SALK Institute, La Jolla, CA*

TP 752 **Development of a Sensitive 2D RPLC-CZE Top-Down Approach for Sub-Microgram Sample Analysis**; Lushuang Huang[1]; Zhe Wang[1]; Si Wu[1]; *[1]University of Oklahoma, Norman, OK*

TP 753 **Combination of Native and Middle-Down Mass Spectrometry for In-Depth Characterization of a Site-Specific Antibody-Drug Conjugate**; Oscar Hernandez Alba[1]; Stéphane Erb[1]; Romain Huguet[2]; Jonathan Josephs[2]; Penelope Drake[3]; David Rabuka[3]; Alain Beck[4]; Stephane Houel[5]; Sarah Cianferani[1]; *[1]Institut Pluridisciplinaire Hubert Curien LSMBO, Strasbourg, France; [2]Thermo Fisher Scientific, San Jose, CA; [3]Catalent Biologics West, Emeryville, CA; [4]Centre d'immunologie Pierre Fabre, Saint-Julien-en-Genevois, France; [5]ThermoFisher, San Jose, CA*

TP 754 **Evaluation of a TIMS-UHRQ-TOF Bottom-Up Proteomics Platform for Proteoform Profiling and Top-Down Approaches**; Jim Kapron[1]; Kristina Marx[2]; Schmit Pierre-Olivier[3]; Gary Kruppa[1]; *[1]Bruker Daltonics Inc., Billerica, MA; [2]Bruker Daltonik GmbH, Bremen, Germany; [3]Bruker Daltonique S.A., Wissembourg, France*

TP 755 **Expanding Proteoform Identifications, Quantifying Proteoform Abundance Changes, and Visualizing Proteoform Families in Top-Down Proteomic Analyses**; Leah V. Schaffer[1]; Michael R. Shortreed[1]; Anthony J. Cesnik[1]; Jarred W. Rensvold[2]; Adam Jochem[2]; Brian L. Frey[1]; Stefan K. Solntsev[1]; Mark Scalf[1]; David J. Pagliarini[1, 2]; Lloyd M. Smith[1]; *[1]University of Wisconsin–Madison, Madison, WI; [2]Morgridge Institute for Research, Madison, WI*

TP 756 **Rapid and Automated SDS Depletion from Intact Proteins for Top Down Proteome Analysis**; Alan A. Doucette[1]; Nicole Unterlander[1]; Subin R Cheri Kunnumal Rajendran[1]; Philip Jakubec[1]; Khaldun Al Azzam[1]; *[1]Dalhousie University, Halifax, NS, Canada*

TP 757 **Altering the Charge-Pairing Environment within Tagged Protein Complexes for Improved Top-Down Sequencing**; Michael Keating[1]; Daniel A. Polasky[1]; Philip C. Andrews[1, 2]; Brandon T Ruotolo[1]; *[1]University of Michigan, Ann Arbor, MI; [2]University of Michigan Medical Center, Ann Arbor, MI*

TP 758 **Top-down SEQUENcing of Immunoglobulin Using Electron Capture Dissociation – Time of Flight Mass Spectrometer Combined with Online Disulfide Bond Reduction**; Takashi Baba[1]; J.C. Yves Leblanc[1]; Pavel Ryumin[1]; Bill Loyd[1]; *[1]SCIEX, Concord, ON, Canada*

TP 759 **Top-Down Mass Spectrometry Using Targeted MS2 Acquisition and BioPharma 3.0 software**; Robert O'meally[1]; Simion Kreimer[1]; Robert N. Cole[1]; *[1]Johns Hopkins School of Medicine, Baltimore, MD*

TP 760 **Optimization of RP-LC-MS Top-Down Protein Analysis on an Orbitrap Fusion Lumos Tribrid MS with the Advanced Peak Determination Algorithm**; Vlad Zabrouskov[1]; Luca Fornelli[2]; Kristina Srzentic[2]; Joshua A Silveira[1]; Christian Thoeing[3]; Graeme C McAlister[1]; Derek J Bailey[1]; Helene Cardasis[1]; Shannon Eliuk[1]; Romain Huguet[1]; Michael W. Senko[1]; Neil Kelleher[2]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Northwestern University, Evanston, IL; [3]Thermo Fisher Scientific, Bremen, Germany*

TP 761 **Improvements to ProSightPD Nodes in the Thermo Scientific™ Proteome Discoverer™ Software Framework**; David Horn[1]; Tara L. Schroeder[1]; Ioanna Ntai[1]; Joseph B. Greer[2]; Ryan Fellers[2]; Richard D. LeDuc[2]; Neil Kelleher[2]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Northwestern University, Evanston, IL*

TP 762 **Design of Novel Interface for Automated Mass Spectrometric Analysis Using Multiple Ionization Methods for Protein and PTM's Analyses**; Santosh Karki[1, 2]; Anil K. Meher[2, 3]; Milan Pophristic[2, 4]; Paul M. Stemmer[3]; Sarah Trimpin[2, 3, 5]; *[1]Wayne State University, Detroit, MI; [2]MSTM, LLC, Newark, DE; [3]Wayne State University, Detroit, MI; [4]University of the Sciences, Philadelphia, PA, 19104; [5]Wayne State University School of Medicine, Detroit, Michigan*

SMALL MOLECULES: QUANTITATIVE ANALYSIS
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TP 763 **Determination of Fipronil and Its Metabolites in Eggs by Ultra High Performance Liquid Chromatography-Tandem Mass Spectrometry**; Xin Zheng[1]; Feng JI[1]; Hui Gao[1]; Yueqi LI[1]; Taohong Huang[2]; *[1]Shimadzu Co.,LTD. Beijing, China; [2]Shimadzu Co.LTD, Shanghai, China*

TP 764 **Tackling Sample Matrix Effects in Trace Analysis of Reactive Genotoxic Impurities by Mass Spectrometry**; David Q Liu[1]; Naijun Wu[1]; *[1]Celgene, Summit, NJ*

TP 765 **Microtracer Absolute Bioavailability Studies: Comparison of Bioanalytical Data of Plasma Samples Using Accelerator Mass Spectrometry and Conventional LC-MS/MS**; Stefan Blech[1]; Martina Wein[2]; Heinz-Dieter Held[2]; Ralf Kiesling[2]; Sascha Keller[2]; Ralf Lotz[2]; Esther van Duijn[3]; *[1]Boehringer-Ingelheim Pharma GmbH & Co.KG, Biberach, Germany; [2]Boehringer-Ingelheim Pharma GmbH & CO KG, Biberach, Germany; [3]TNO, AJ Zeist, Netherlands*

TP 766 **An Ultrasensitive 2D-UHPLC-MS/MS Method for the Quantitation of Formoterol in Human Plasma**; Jingduan Chi[1]; Fumin Li[1]; Rand Jenkins[1, 2]; *[1]PPD, Middleton, WI; [2]PPD, Richmond, VA*

TP 767 **Highly Selective Bioanalytical Quantitation Method for Analysis of R and S Amlodipine Enantiomers in Human Plasma Using LC-MS/MS**; Rahul Baghla[1]; Ian Moore[1]; Sahana Mollah[1]; Matthew Brusius[2]; Marc Jacob[2]; *[1]SCIEX, Redwood City, CA; [2]Phenomenex, Torrance, CA*

TP 768 **Development and Validation of a Simple and Rugged LC-MS/MS Method to Measure Phytonadione E-isomer in Human Plasma**; Nick Peng[1]; Ben Gaboury[1]; Ardeshir Khadang[1]; *[1]Axis Clinicals, Dilworth, MN*

TP 769 **Validation of Non-Derivatization LC/MS/MS Method for Determination of Amino Acids in Infant and Adult Nutritional Formulas Following AOAC Requirements**; Zhe Sun[1]; Wantung Liw[1]; Nur Sadrina Binte Mohamed Shah[2]; Yu Jie Lee[3]; Jie Xing[1]; Zhaoqi Zhan[1]; *[1]Application Development and Support Centre, Shimadzu, Singapore, Singapore; [2]School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore, Singapore; [3]School of Chemical and Life Sciences, Singapore Polytechnic, Singapore, Singapore*

TP 770 **Screening of a Multiclass Drug Panel with Liquid Chromatography Coupled to High Resolution Mass Spectrometry (HRAM)**; Lawrence J Andrade[1]; Ana Celia Grenier[1]; *[1]Dominion Diagnostics, North Kingstown, RI*

TP 771 **Simultaneous Quantification of Six Major Grape Polyphenols in Mouse Liver Tissue by a New LC-MS/MS Method**; Qing Cai[1]; Divyank Soni[1]; EunJung Park[2]; Kenneth Morris[1]; John Pezzuto[2]; *[1]Long Island University - Lachman Institute, Brooklyn, NY; [2]Long Island University - Arnold & Marie Schwartz College of Pharmacy and Health Sciences, Brooklyn, NY*

TP 772 **High-Throughput Vitamin K Profiling in Human Plasma by LDTD-MS/MS**; Takeshi Ashida[1]; Tsuyoshi Nakanishi[1]; Mikael Levi[1]; Hiroyuki Yasuda[1]; Ichiro Hirano[1]; *[1]Shimadzu Corporation, MS Business Unit, Kyoto, Japan*

TP 773 **In-Vitro Cellular Uptake Study of Single Drug and Combination Therapy Treating Neuroblastoma**; Areum Hong[1]; Gyeongseo Min[1]; Hugh I. Kim[1]; *[1]Korea University, Seoul, South Korea*

TP 774 **Highly Sensitive Quantitative Analysis of Mometasone Furoate from Plasma Using LC-MS/MS**; Ashutosh Shelar[1]; Rashi Kochhar[1]; Shailendra Rane[1]; Shailesh Damale[1]; Deepti Bhandarkar[1]; Anant Lohar[1]; Purushottam Sutar[1]; Navin Devadiga[1]; Bhaumik H Trivedi[1]; Jitendra

Kelkar[1]; Pratap Rasam[1]; Ajit Datar[1]; *[1]Shimadzu Analytical (India) PVT LTD, Mumbai, India*

TP 775 **Analytical Determination of Drugs in Serum Using the Ultivo Triple Quad LC/MS**; Jarod N Grossman[1]; Yanan Yang[1]; *[1]Agilent Technologies, Santa Clara, CA*

TP 776 **New Simple and Fast SPE Protocols for Phospholipid Removal in Basic Analyte LC-MS/MS Bioanalytical Quantitation**; Thomas Swann[1]; Bonnie A. Alden[1]; Kenneth Berthelette[1]; Jon Finch[1]; Donna Osterman[1]; Thomas H. Walter[1]; *[1]Waters Corporation, Milford, MA*

TP 777 **Linear Dynamic Range Improvement in MS/MS Mode on X500® QTOF System**; Feng Zhong[1]; Suya Liu[1]; Wen Jin[1]; Doug Simmons[1]; Nic G Bloomfield[1]; *[1]SCIEX, Concord, ON, Canada*

TP 778 **A Sensitive LC-MS/MS Method for Detection and Quantification of Trace β-lactam Cross-Contamination**; Chen Qiu[1]; Hongbin Zhu[1, 2]; Connie Ruzicka[1]; David Keire[1]; Hongping Ye[1]; *[1]US FDA, St. Louis, MO; [2]ThermoFisher Scientific Inc., Rockford, IL*

TP 779 **Quantification and Confirmation of Impurities in Trazadone API for Quality Control by LC/MS/MS in Accordance to Pharmacopoeia Guidelines**; Vikrant Goel[1]; Samir Vyas[2]; *[1]Agilent Technologies, Gurgaon, India; [2]Agilent Technologies, Gurgaon, India*

TP 780 **Acoustic-Open Port-Mass Spectrometry (AOMS): A New Platform for Ultrafast, Direct Human PK Analysis without Sample Preparation**; Wenyi Hua[1]; Chang Liu[2]; Jianhua Liu[1]; Thomas Covey[2]; Hui Zhang[1]; *[1]Pfizer Inc., Groton, CT; [2]SCIEX, Concord, ON, Canada*

TP 781 **Improved Sensitivity for LC-MS Quantitation of Pharmaceutical Compounds in Human Plasma with MicroLC Using a New Microflow Source Design**; Ian Moore[1]; Carmai Seto[1]; Tom Biesenthal[1]; *[1]SCIEX, Concord, ON, Canada*

TP 782 **Simultaneous Quantitation/Profiling of Cell Culture Medium Components Using LCMS/MS**; Dilipkumar Reddy Kandula; *SCIEX, Gurugram, India*

TP 783 **A Novel Strategy to Overcome Isotopic Interferences in Applying LC-MS/MS Assay for Microdosing Absolute Bioavailability Study**; Long Yuan[1]; Christine Huang[1]; Peggy Liu-Kreyche[1]; Alban Allentoff[1]; R Fancher[1]; Naiyu Zheng[1]; Iyer Ramaswamy[1]; Li Zhu[1]; Pillutla Renuka[1]; Qin Ji[1]; *[1]Bristol-Myers Squibb, Princeton, NJ*

TP 784 **Simultaneous Determination of 10 Carbonyls in Electronic Cigarette Aerosols Using LC-MS/MS**; Yongquan Lai[1]; Yue Zhou[1]; Larry M. Mallis[1]; Philip J. Kuehl[1]; Jacob McDonald[1]; Steve Belinsky[1]; *[1]Lovelace Biomedical, Albuquerque, NM*

TP 785 **Determination of Polyglyceryl-3-Caprylate in Brazilian Personal Care Products by LC-MS**; Natália Figueiredo[1]; Simone Chiapetta[1]; *[1]INT, Rio De Janeiro, Brazil*

TP 786 **Analysis of Non-UV-Absorbing Impurities in an API by 2-Column Separation and Combined UV/MS Detection**; Laura Hayter[1]; Philip Anderson[1]; *[1]Avista Pharma Solutions, Longmont, CO*

TP 787 **Normalization of US Newborn Screening Labs MS/MS Analyte Results and Cutoffs Using the CDC NSQAP Reference Materials**; C. Austin Pickens[1]; Mary Seeterlin[2]; Victor R De Jesus[1]; Christopher Hayes[1]; Mark Morrissey[3]; Adrienne Manning[4]; Sonal Bhakta[5]; Patrice Held[6]; Konstantinos Petritis[1]; *[1]Centers for Disease Control and Prevention, Division of Laboratory Sciences, Atlanta, GA; [2]Michigan Department of Health & Human Services, Lansing, MI; [3]Wadsworth Center/New York State Department Of Health, Albany, NY; [4]Connecticut Department of Public Health, Rocky Hill, CT; [5]Arizona Department of Health Services, Phoenix, AZ; [6]Wisconsin State Laboratory of Hygiene, Madison, WI*

TP 788 **Failures of Hemolysis Testing, Assessment and Remediation Case Studies**; Michael Van Parys[1]; James Farnham[1]; Stephanie Cape[1]; Aaron Ledvina[1]; David Good[1]; Theodore Brus[1]; *[1]Covance Laboratories, Madison, WI*

TP 789 **A Fast and Simple Analysis of Underivatized Amino Acids in Pet Food Using Ultivo LC/TQ**; Jennifer Cottine Hitchcock[1]; Yanan Yang[2]; Gaëlle Bridon[3]; Hélène Lachance[4]; Mathieu D'Amours[4]; *[1]Agilent Technologies, Inc., Santa Clara, CA; [2]Agilent Technologies, Inc, Santa Clara, CA; [3]Agilent Technologies, Inc, Saint-Laurent, QC, Canada; [4]Shur-Gain/Nutreco, St-Hyacinthe, QC, Canada*

TP 790 **The Importance of Column Selection for Polar Compounds with LC/MS/MS Methods**; Rachel Sun[1]; Adrian Bott[1]; Hasantha Jayaratna[1]; Robert Clegg[1]; Juan Sanchez[1]; *[1]BASi, West Lafayette, IN*

TP 791 **A Rapid and Sensitive LC-MS/MS Method for Quantitative Analysis of Cardiolipin (18:2)4 in Human Leukocytes and Mouse Muscles**; Gang Xu[1]; Xiao Liu[2]; Yachun Shu[3]; Yan Xu[1]; *[1]Cleveland State University, Cleveland, OH; [2]Nanjing University of Chinese Medicine, Nanjing, China; [3]The First Affiliated Hospital of Nanjing University of Chinese Medicine, Nanjing, China*

TP 792 **Hydrolysis Kinetic Study by Mass Spectrometry for AEBSF Protease Inhibitor, Used in Cell Culture Process of HIV-1 Broadly Neutralizing Antibody**; Jesse Huang[1]; Cindy X Cai[1]; Vera B Ivleva[1]; Q Paula Lei[1]; *[1]NIH/NIAID/VPPL, Gaithersburg, MD*

TP 793 **Separation and Quantitation of Seven Cannabinoids Using Supercritical Fluid Chromatography-Tandem Mass Spectrometry (SFC-MS/MS)**; Guannan Li[1]; Jennifer Cottine Hitchcock[1]; Tony Brand[1]; *[1]Agilent Technologies, Inc., Santa Clara, CA*

TP 794 **Diagnostic Fragmentation Filtering for the Discovery of New Natural Products in Microbial Fermentations and Foods**; Justin J Renaud[1]; Mark W Sumarah[1]; *[1]Agriculture and Agri-Food Canada, London, ON, Canada*

TP 795 **Matrix Effect Challenges and Internal Standard Association in Mass Spectrometry**; Jean-Francois Bienvenu[1]; Gilles Provencher[1]; Patrick Bélanger[1]; René Bérubé[1]; Pierre Dumas[1]; Sébastien Gagné[1]; Éric Gaudreau[1]; Normand Fleury[1]; *[1]INSPQ, Quebec, QC, Canada*

TOXICOLOGY
796-819

TP 796 **Estimation of Median Lethal Doses Associated with Intravenous Exposure to the Stereoisomers of VX in Guinea Pigs *via* GC-MS/MS**; Jeffrey Michael McGuire[1]; Linnzi Wright[1]; Robert Kristovich[1]; Michael Busch[2]; *[1]US Army ECBC, Aberdeen Proving Ground, MD; [2]Excet, Inc., Springfield, VA*

TP 797 **A Validated and Practical UPLC-MS/MS Method for Methylenedianiline Determination in Human Urine**; Maggy Lepine[1, 2]; Lekha Sleno[2]; Jacques Lesage[2]; Sebastien Gagne[1]; *[1]IRSST, Montreal, QC, Canada; [2]UQAM, Montreal, QC, Canada*

TP 798 **Characterizing Flame Retardant-Induced Neurotoxicity in a Human Embryonic Stem Cell hESC Differentiation Model Using Proteomics and Transcriptomics**; Christie Hunter[1]; Hao Chen[2]; Katherine Williams[2]; Christopher Yan[2]; Joshua Robinson[2]; *[1]SCIEX, Redwood City, CA; [2]University of California San Francisco, San Francisco, CA*

TP 799 **Optimizing LS-MS/MS for the Detection of 44 drugs Including THC and Opioids in Oral Fluids**; Lisa Wanders[1]; Jill Yeakel[2]; Samuel Ellis[1]; *[1]Thomson Instrument Co, Oceanside, CA; [2]Lehigh Valley Toxicology, Bethlehem, PA*

TP 800 **Evaluating Contact Transfer and Skin Absorption of Carfentanil in a Pig Ear Model Utilizing LC-MS/MS Analysis**; Christopher Byers[1]; Richard Lawrence[1]; Ronald Evans[1]; *[1]US Army ECBC, Aberdeen Proving Ground, MD*

TP 801 **Determination of Agent BZ (3-quinuclidinyl benzilate) in Rat Plasma and Brain Homogenate by LC-MS/MS**; David Herman[1]; Nela Vanova[1]; Alzbeta Dlabkova[1]; Lenka

Cechova[1]; Jana Hatlapatkova[1]; Jana Zdarova-Karasova[1]; *[1]University of Defence in Brno, Faculty of Military Health Sciences, Department of Toxicology and Military Pharmacy, Hradec Kralove, Czech Republic*

TP 802 **Detection of Fentanyl and Related Synthetic Opioids in Biological Matrices**; Robert Lockwood[1]; Katie Pryor[2]; Michael Parks[2]; Christopher Gilles[2]; *[1]Conneticut Division of Scientific Services, Meriden, CT/ US; [2]Shimadzu Scientific Instruments Inc., Columbia, MD*

TP 803 **Clam- SPE On Line- UHPLC-MS/MS : Fully Automatic, Simultaneous and Quickly Quantification of Drugs of Abuse in Blood and Saliva**; Etienne Maout[1]; Doriane Toinon[2]; Mickael Nicolas[3]; Thierry Besnard[3]; *[1]Shimadzu, Noisiel, France; [2]Shimadzu France, Marne la Vallée, France; [3]laboratoire LTB, Narbonne, France*

TP 804 **Proteomic Characterization of Heavy Metal Exposure in Bladder Cells: PML as an Indicator**; Yi-Ting Chen[1]; Wei-Ting Ou Yang[1]; Chien-Lun Chen[2]; *[1]Chang Gung University, Taoyuan, Taiwan; [2]Chang Gung Memorial Hospital, Taoyuan, Taiwan*

TP 805 **Library Identification of Over 200 drugs of Abuse in Blood, Plasma and Urine Using MRM Spectrum Mode by LC-MS/MS**; Tiphaine Robin[1]; Alan Barnes[2]; Neil Loftus[2]; Sylvain Dulaurent[1]; Pierre Marquet[1]; Souleiman El Balkhi[1]; Franck Saint-Marcoux[1]; *[1]CHU Limoges, Limoges, France; [2]Shimadzu Corporation, Manchester, UK*

TP 806 **Simultaneous Determination of Synthetic Cathinones in Hair by Liquid Chromatography Tandem Mass Spectrometry**; Hsiu Chuan Chen; *Chung Shan Medical University, Taichung, Taiwan*

TP 807 **Analysis of β-N-Methylamino-L-Alanine in Environmental Samples Using a Novel Integrated Strategy**; Joshua Beri[1]; Kaylie I. Kirkwood[1]; Marco Valera[2]; Astrid Schnetzer[2]; David C Muddiman[1, 3]; Michael S. Bereman[1, 3, 4]; *[1]Department of Chemistry, North Carolina State University, Raleigh, NC; [2]Department of Marine, Earth, and Atmospheric Sciences, North Carolina State University, Raleigh, NC; [3]Center for Human Health and the Environment, North Carolina State University, Raleigh, NC; [4]Department of Biological Sciences, North Carolina State University, Raleigh, NC*

TP 808 **MALDI-MS Imaging Reveals Asymmetric Spatial Distribution of Lipid Metabolites from Bisphenol S-Induced Nephrotoxicity**; Chao Zhao[1]; Peisi Xie[1]; Hailin Wang[2]; Zongwei Cai[1]; *[1]Hong Kong Baptist University, Hong Kong, China; [2]Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences, Beijing, China*

TP 809 **Picogram Detection of the Marijuana Metabolite THC-COOH in Hair Samples Using an Efficient and Sensitive LC-MS/MS Analysis Workflow**; Xiang He[1]; Oscar G. Cabrices[1]; Alexandre Wang[1]; Casey Burrows[2]; Adrian Taylor[2]; *[1]SCIEX, Redwood City,, CA; [2]SCIEX, Redwood City, California*

TP 810 **Differentiate "Brown Mixture" Ingestion and Heroin Use by Monitoring Antimony in Urine**; Yan Zin Chang; *University, Taichung, Taiwan*

TP 811 **Single-Injection Screening of 664 Forensic Toxicology Compounds Using an Innovative Benchtop High Resolution Mass Spectrometer**; Oscar G. Cabrices[1]; Alexandre Wang[1]; Xiang He[1]; Holly McCall[1]; Adrian Taylor[2]; *[1]SCIEX, Redwood City,, CA; [2]SCIEX, Concord, ON, Canada*

TP 812 **Detection and Characterization of Polycyclic Aromatic Hydrocarbon DNA Adducts by Targeted and Untargeted Ultra-Performance Liquid Chromatography-High Resolution Multi-Stage Mass Spectrometry**; Jingshu Guo[1]; Sesha Krishnamachari[1]; Lihua Yao[1]; Robert J. Turesky[1]; *[1]University of Minnesota, Minneapolis, MN*

TP 813 **Validation of Generic Sample Extraction Workflow for Analysis of 62 Drugs in Urine by LDTD-MS/MS (Screening) and LC-MS/MS (Confirmation)**; Michael Barna[1]; Serge Auger[2]; Jonathan Rochon[3]; Jean Lacoursière[2]; Pierre Picard[2]; *[1]PSO Laboratory, Lansing, MI; [2]Phytronix Technologies, Quebec, QC, Canada; [3]Universite Laval, Quebec, QC, Canada*

TP 814 **Low Level Analysis of Extractable and Leachable Phthalates and Nitrosamine from Consumer Packaging Materials; from One Injection**; Ron Honnold[1]; Matthew Curtis[1]; David Weil[1]; *[1]Agilent Technologies, Inc., Santa Clara, CA*

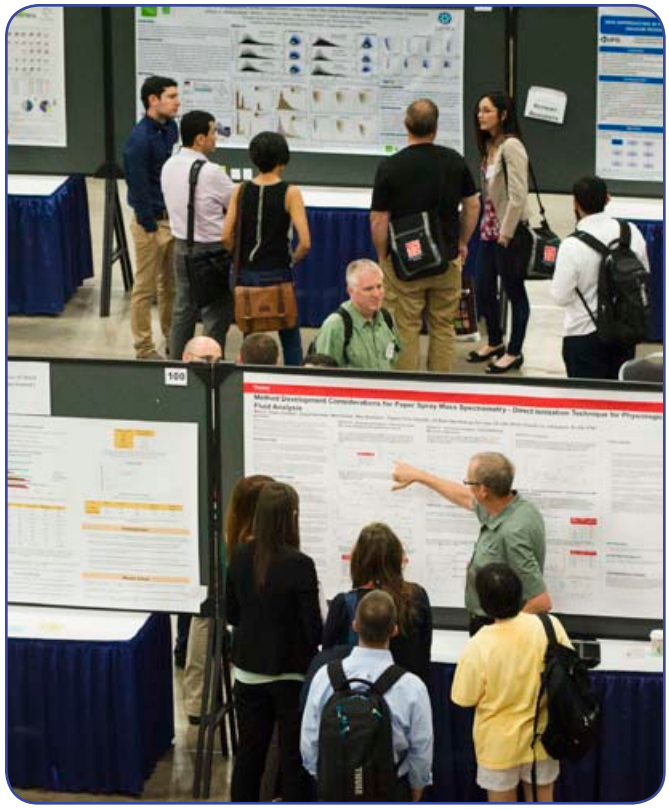
TP 815 **Increased Throughput with Alternate Column Regeneration Using Analytical LC/MS/MS Method for 126 Drugs and Metabolites in Urine in Clinical Research**; Andre Szczesniewski; *Agilent Technologies, Wood Dale, IL*

TP 816 **A New Approach to the Analysis of Unresolved Chromatographic Peaks in GC/MS**; Yongdong Wang[1]; Stacey Simonoff[1]; *[1]Cerno Bioscience, Norwalk, CT*

TP 817 **Challenges in Urine Testing: Overcoming Differences in Cleavage of Opioid Glucuronides Observed in Authentic Specimens Versus Standards in Synthetic Urine**; Gladis R Reyes Pimentel[1]; Zahra M Kashi[1]; Andrea E DeBarber[1, 2]; *[1]Kashi Clinical Laboratories, Portland, OR; [2]Oregon Health & Science University, Portland, OR*

TP 818 **A Quantitative Proteomic Study Identifies TRC8 and GP78 as New Targets of Arsenite to Inhibit HMGCR Ubiquitination**; Ji Jiang[1]; Yinsheng Wang[1]; *[1]University of California, Riverside, Riverside, CA*

TP 819 **Two Step Solid Phase Extraction Method of the Analysis of Carisoprodol and Meprobamate in Human Urine by LC/MS**; Peter Simms; *Lux Laboratories, Las Vegas, NV*



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 II
001-034

WP 001 **Automated Presentation of Solid Phase Microextraction Fibers to Facilitate High-Throughput DART-MS Analysis**; Brittany Laramee[1]; Frederick Li[2]; Taylor Feraco[2]; Joseph Tice[2]; Brian Musselman[2]; *[1]IonSense, Inc, Saugus, MA; [2]IonSense,Inc., Saugus, MA*

WP 002 **Open Air Ionization Mass Spectrometry for Online-Preconcentration, Separation, and Detection of Small Organics**; Yen-Chun Chen[1]; Arun Krishnamurthy[2]; Szu-Hua Chen[2]; Yu-Chie Chen[2]; *[1]National Chiao Tung University, Hsinchu, Taiwan; [2]National Chiao Tung University, Hsinchu, Taiwan*

WP 003 **Real-Time Monitoring of Alarm Pheromone Release of Western Honey Bee (Apis Mellifera) and Eastern Bumble Bee (Bombus Impatiens)**; Skylar M. Brodowski[1]; Yue Li[2]; *[1]Washington-Lee High School, Arlington, VA; [2]The University of Maryland, College Park, MD*

WP 004 **Enhanced Coupling of Acoustic Levitation Ambient Mass Spectrometry Miniaturized Direct Ionization and Reaction Monitoring**; Elizabeth A. Crawford[1]; Demian Dietrich[1]; Cemal Esen[2]; Dietrich A. Volmer[1]; *[1]Universität des Saarlandes, Saarbrücken, Germany; [2]Ruhr-Universität Bochum, Germany*

WP 005 **Investigation of a New Polymer Material for PaperSpray in Clinical Research**; Cornelia Leonie Boeser[1]; Maria Dulay[2]; Harikrishnan Sukumar[1]; Mari Prieto Conaway[1]; Richard N. Zare[2]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Stanford University, Palo Alto, CA*

WP 006 **Troubleshooting a Hair Cream Product Failure Using ASAP-Ion Mobility-Mass Spectrometry**; Sarah Dowd[1]; Eleanor Riches[2]; Jonathan Fox[2]; *[1]Waters Corp., Beverly, MA; [2]Waters Corporation, Wilmslow, UK*

WP 007 **Using Direct MS and Microextraction for Detection of Fentanyl and Analogs from Saliva**; Candace Price[1]; Craig Aurand[1]; Emily Barrey[1]; *[1]Millipore Sigma, Bellefonte, PA*

WP 008 **Fast Identification of Active Ingredients in Tablets Using Microwave Plasma Torch Mass Spectrometry**; Xinchen Wang[1]; Xiaoping Zhang[1]; Huanwen Chen[1]; *[1]East China University of Technology, Jiangxi Key Laboratory for Mass Spectrometry and Instrumentation, Nanchang, China*

WP 009 **Rapid Automated Single Cell Recognition and Analysis Using Laser Microdissection-Liquid Vortex Capture/ Electrospray Ionization-Mass Spectrometry**; Vilmos Kertesz[1]; John F. Cahill[1]; Gary J. Van Berkel[1]; *[1]Oak Ridge National Laboratory, Oak Ridge, TN*

WP 010 **Coated Blade Spray-Mass Spectrometry Parameter Optimization: Rapid Screening and Quantitation of Fentanyl and Related Analogs**; Daniel Rickert[1]; German Augusto Gómez-Ríos[1]; Varoon Singh[1]; Janusz Pawliszyn[1]; *[1]University of Waterloo, Waterloo, ON, Canada*

WP 011 **Apta Spray Mass Spectrometry**; David Romero Perez[1]; Barry Smith[1]; Behnam Bastani[1]; Iain Young[1]; Abraham Kwame Badu-Tawiah[2]; Tirayut Vilaivan[3]; Thanit Praneenararat[3]; Nuttapon Jirakittiwut[3]; Jutamat Prabphal[3]; Simon Maher[1]; *[1]University of Liverpool, UK; [2]Ohio State University, Columbus, OH; [3]Chulalongkorn University, Bangkok, Thailand*

WP 012 **Characterization of Breast Cancer Molecular Subtype in Fine-Needle Aspiration Biopsies Using Ambient Ionization Mass Spectrometry**; Qiuyu Li[1]; Kyana A. Garza[2]; John Q. Lin[2]; Stacey Carter[3]; Chandandeep Nagi[3]; LIVIA S. Eberlin[2]; *[1]University of Texas at Austin, Austin, TX; [2]University of Texas at Austin, Department of Chemistry, Austin, TX; [3]Baylor College of Medicine, Houston, TX*

WP 013 **Methodology for Profiling of Stained Bovine Enamel and Human Teeth Using Mass Spectrometry and Molecular Networking**; Kenneth L. Jones[1]; Alexey V. Melnik[2]; Ricardo Da Silva[2]; Alexander Aksenov[2]; Cajetan Dogo-Isonagie[3]; Paloma Pimenta[3]; Pieter C. Dorrestein[2, 4]; *[1]Biochemistry, Cell Biology, University of California, La Jolla, CA; [2]Collaborative Mass Spectrometry Innovation Center, Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA; [3]Colgate Palmolive Company, Piscataway, NJ; [4]Department of Pediatrics, University of California, San Diego, California*

WP 014 **High Throughput Compound Screening Using IR-MALDESI Mass Spectrometry**; Jon D. Williams[1]; Måns Ekelöf[2]; Nathaniel L. Elsen[1]; David C Muddiman[2]; *[1]AbbVie, North Chicago, IL; [2]North Carolina State University, Raleigh, NC*

WP 015 **Optimization of Carrier Gas Flow Dynamics to Improve Sensitivity and Molecular Coverage in Remote Laser Ablation Electrospray Ionization Mass Spectrometry**; Jarod Fincher[1]; Andrew Korte[1]; Nicholas J. Morris[2, 3]; Akos Vertes[1]; *[1]George Washington University, Washington, DC; [2]Air Force Research Laboratory, Materials and*

Manufacturing Directorate, AFRL/RXAS, WPAFB, WPAFB, Ohio; [3]UES, Inc., Beavercreek, Ohio

WP 016 **Development of a SPME Tool for the Determination of a Small Molecule-Drug Conjugate Directed against Carbonic Anhydrase in Cancer Chemotherapy**; Sahar Ghiasikhou[1]; Jorge Scheuermann[1]; Samuele Cazzamalli[1]; Dario Neri[1]; Renato Zenobi[1]; *[1]ETH, Zurich, Switzerland*

WP 017 **Accelerated Forced Degradation of Pharmaceuticals in Levitated Microdroplet Reactors**; Yangjie Li[1]; Yong Liu[2]; Hong Gao[3]; Roy Helmy[2]; W. Peter Wuelfing[2]; R. Graham Cooks[1]; *[1]Purdue University, West Lafayette, IN; [2]Merck Research Laboratories, West Point, PA; [3]Merck Research Laboratories, Rahway, NJ*

WP 018 **Developing Direct Analysis in Real Time Mass Spectral Libraries for the General Unknown Screening of Drugs**; Frederick Li[1]; Joseph Tice[1]; Mishka Repaska[2]; Chris Snyder[2]; Paul Kennedy[2]; Stephen Shrader[3]; Brian Musselman[1]; *[1]IonSense,Inc., Saugus, MA; [2]Cayman Chemical, Ann Arbor, MI; [3]Shrader Software Solutions, Grosse Pointe Park, MI*

WP 019 **In Source Preconcentration Ambient Ionization for the Analysis of PPT Level Environmental Contaminants**; Taoqing Wang[1]; Zhi Liu[1]; Xing Xu[1]; Alexander J. Tognazzi[1]; Anyin Li[1]; *[1]Department of Chemistry, University of New Hampshire, Durham, NH*

WP 020 **Assessing PaperSpray Ionization Technique for the Quantitation of Abiraterone in Human Plasma for Clinical Research**; Atul Bhatnagar[1]; Matthew J. McKay[2]; Maria Prieto Conaway[3]; Alex Chen[4]; Megan Crumbaker[5]; Howard Gurney[6]; Mark P Molloy[1, 2]; *[1]Department of Molecular Sciences, Macquarie University, Sydney, Australia; [2]Australian Proteome Analysis Facility, Macquarie University, Sydney, Australia; [3]Thermo Fisher Scientific, San Jose, CA; [4]Thermo Fisher Scientific, Melbourne, Australia; [5]Crown Princess Mary Cancer Centre, Westmead Hospital, Sydney, Australia; [6]Department of Clinical Medicine, Macquarie University, Sydney, Australia*

WP 021 **Micro Area Analysis of Bulk Alloys by Electrochemical Micro Probe Coupled Mass spectrometry**; Jiaquan Xu[1]; Lixue Zhu[2]; Huanwen Chen[2, 3]; *[1]East China University of Technology, Nanchang, China; [2]State Key Laboratory of Inorganic Synthesis and Preparative Chemistry, College of Chemistry, Jilin University, Changchun, China; [3]East China University of Technology, Jiangxi Key Laboratory for Mass Spectrometry and Instrumentation, NanChang, China*

WP 022 **Application of SPCP-Spray: A Rapid Disposable Separation Ambient Ionization Device with High Sensitivity and Selectivity**; Zong-Yi Wu[1]; PaiChi Syue[1]; Che-I Laio[1]; Kuo-Ching Jan[1]; Kuo-Lung Ku[1]; *[1]National Chiayi University, Chiayi City, Taiwan*

WP 023 **Rapidly Quantification of 3-Hydroxybenzo[a]pyrene in Human Urine by Using Magnetic Solid-Phase Extraction Coupled with Internal Extractive Electrospray Ionization Mass Spectrometry**; Xiaoping Zhang[1]; Jianchuan Liu[1]; Yi Li[2]; Jiaquan Xu[2]; Huanwen Chen[2]; *[1]East China University of Technology, Jiangxi Key Laboratory for Mass Spectrometry and Instrumentation, Nanchang, China; [2]East China University of Technology, Jiangxi Key Laboratory for Mass Spectrometry and Instrumentation, NanChang, China*

WP 024 **Stability of Labile Organic Compounds in Small-Volume Dried Blood Spheroids Studied by Hydrophobic Paper Spray Mass Spectrometry**; Deidre Damon[1]; Abraham K Badu-Tawiah[1]; *[1]The Ohio State University, Columbus, OH*

WP 025 **An Innovative Analysis Method for Fragrance of Sake Using an Introducing Device for Volatile Compounds Combined with DART-MS**; Chikako Takei[1]; Yukiko Ohtake[1]; Kenichi Yoshizawa[1]; Haruka Nishimoto[2]; Takahiro Akashi[2]; *[1]BioChromato, Inc., Fujisawa, Japan; [2]Hakutsuru Sake Brewing Co., Ltd., Kobe-shi, Japan*

WP 026 **Ruggedness Characterization of an Open-Air Paper Spray Ionization Source Operated Under Field Conditions on a Portable MS System**; Ashley Stelmack[1]; Shahnaz Mukta[1]; William L. Fatigante[1]; Christopher C. Mulligan[1]; *[1]Illinois State Univeristy, Normal, IL*

WP 027 **PaperSpray Methods for Agrochemical Analysis: Swab and Homogenate Testing for Screening and Targeted Quantitation**; Steven Lawrence Reeber[1]; John Glazier[1]; Mari Prieto Conaway[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

WP 028 **Paper Spray High – Resolution Accurate Mass Spectrometry for Quantitation of Voriconazole in Equine Tears and Plasma**; Michaela Lerch[1]; Rachel A. Allbaugh[2]; Lionel Sebbag[2]; Jonathan P. Mochel[1, 3]; David J. Borts[1]; *[1]Department of Veterinary Diagnostic & Production Animal Medicine, Iowa State University College of Veterinary Medicine, Ames, IA; [2]Department of Veterinary Clinical Sciences, Iowa State University College of Veterinary Medicine, Ames, IA; [3]Department of Biomedical Sciences, Iowa State University College of Veterinary Medicine, Ames, IA*

WP 029 **Study the Dehydrogenation Coupling Reaction of Pyrrole Compounds by On-line Electrospray Ionization Mass Spectrome**; Yi-Jin Li[1]; Wei Liu[1]; Huanwen Chen[1, 2]; *[1]East China University of Technology, Jiangxi Key Laboratory for Mass Spectrometry and Instrumentation, Nanchang, China; [2]State Key Laboratory of Inorganic Synthesis and Preparative Chemistry, College of Chemistry, Jilin University, Changchun, China*

WP 030 **Direct Analysis for Amino Acid of Intra-and Extracellular Fluids by Surface Desorption Atmospheric Pressure Chemical Ionization Mass Spectrometry**; Wei Liu[1]; Shuanglong wang[1]; Yi-Jin Li[1]; Huanwen Chen[1]; *[1]East China University of Technology, Jiangxi Key Laboratory for Mass Spectrometry and Instrumentation, Nanchang, China*

WP 031 **Direct Identificationand Quantification of Perfluorinated Compounds in Textiles by Dielectric Barrier Discharge Ionization Mass Spectrometry**; Chun Wang[1, 2]; Qiang Ma[1]; *[1]Chinese Academy of Inspection and Quarantine, Beijing, China; [2]Nanjing Agricultural University, Nanjing, China*

WP 032 **Microdroplet Electrocyclization and Radical Dimerization of 4-Ethynyl-N,N-Dimethylaniline**; Mei Zhang[1]; Robert Schrader[2]; R. Graham Cooks[2]; *[1]State Key Laboratory for Infectious Disease Prevention and Control, Beijing, China; [2]Purdue University, West Lafayette, IN*

WP 033 **Preparative Synthesis of Carboxylic Acids in Microdroplets from Aerobic Oxidation of Aldehydes**; Xin Yan[1]; Yin-Hung Lai[1]; Richard N. Zare[1]; *[1]Stanford University, Palo Alto, CA*

WP 034 **Paperspray Metabolomics of Urine for Diagnostic Potential in Prostate Cancer**; Timothy Garrett[1]; Joseph H. Kennedy[2]; Ranjan Perera[3]; *[1]Univ of Florida, Gainesville, FL; [2]Prosolia, Inc., Indianapolis, IN; [3]Sanford Burnham Prebys Medical Discovery Institute, San Diego, CA*

ANTIBODIES & ANTIBODY DRUG CONJUGATES II
035-067

WP 035 **Comparing Glycosylation, ADCC Activity and Structural Profiles of Rituximab and its Biosimilar**; Jukyung Kang[1]; Sang Yeop Kim[1]; Daniel Vallejo[2]; Tyler Hageman[3]; Alexander Benet[1]; K. Ilker Sen[4]; Sergei Saveliev[5]; David D. Weis[3, 6]; Brandon T. Ruotolo[2]; Anna Schwendeman[1, 7]; *[1]Department of Pharmaceutical Sciences, University of Michigan, Ann Arbor, MI; [2]Department of Chemistry, University of Michigan, Ann Arbor, MI; [3]Department of Chemistry, University of Kansas, Lawrence, KS; [4]Protein Metrics Inc., San Carlos, CA; [5]Promega Corporation, Madison, WI; [6]Department of Pharmaceutical Chemistry, University of Kansas, Lawrence, KS; [7]Biointerfaces Institute, University of Michigan, Ann Arbor, MI*

WP 036 **Large Scale Study of the W-ion Isoleucine and Leucine Determination (WILD) Method in Antibody De Novo Protein Sequencing**; Zac McDonald[1]; Qixin Liu[1]; Bin Ma[2]; Paul Taylor[3]; Jonathan R. Krieger[3]; *[1]Rapid Novor Inc., Kitchener, ON, Canada; [2]University of Waterloo, Waterloo, ON, Canada; [3]SPARC Biocentre, SickKids Hospital, Toronto, ON, Canada*

WP 037 **Antibody Isolation with Mimotope-Containing Porous Membranes Prior to Mass Spectrometry Analysis**; Weijing Liu[1]; Hui-Yin Tan[1]; Austin Landry Bennett[2]; Wenjing Ning[2]; Merlin Bruening[1]; *[1]University of Notre Dame, Notre Dame, IN; [2]Michigan State University, East Lansing, MI*

WP 038 **Multi-Attribute Monitoring (MAM) of Oxidized NIST mAb Using BioPharmaView™ Workflow**; Harini Kaluarachchi[1]; Annu Uppal[2]; Kerstin Pohl[3]; Sibylle Heidelberger[4]; *[1]SCIEX, Concord, ON, Canada; [2]Sciex India Pvt Ltd, Haryana, India; [3]SCIEX, Darmstadt, Germany; [4]SCIEX, Warrington, UK*

WP 039 **Increased Resolving Power and Detection Sensitivity of Two-Dimensional Liquid Chromatography for Bottom-Up Analysis of Therapeutic Proteins**; Hayley R. Lhotka[1]; David C. Harmes[1]; Benjamin Madigan[1]; Gregory O. Staples[2]; Dwight R. Stoll[1]; *[1]Gustavus Adolphus College, Saint Peter, MN; [2]Agilent Technologies, Inc., Santa Clara, CA*

WP 040 **Application of Immunoaffinity LC-MS/MS to Understand Antibody-Drug Conjugate Stability and Biotransformations**; Suk-Joon Hyung[1]; Surinder Kaur[1]; Ola Saad[1]; *[1]Genentech, San Francisco, CA*

WP 041 **Native Analysis of Monoclonal Antibodies by Microchip Capillary Electrophoresis-ESI-MS**; J. Scott Mellors[1]; Erin Redman[1]; *[1]908 Devices, Inc., Carrboro, NC*

WP 042 **Data Independent Acquisition Modes for Identification, Quantification and Monitoring of Low-Abundance Host Cell Proteins During Monoclonal Antibody Bioprocessing**; Catalin Doneanu[1]; Alex Xenopoulos[2]; Romas Skudas[2]; Ying Qing Yu[1]; Asish Chakraborty[1]; Weibin Chen[1]; *[1]Waters Corporation, Milford, MA; [2]EMD Millipore, Bedford, MA*

WP 043 **Deciphering Trisulfide Modification in a Monoclonal Antibody Using a Comprehensive Mass Spectrometry Approach**; Te-Wei Chu[1]; Gregory O. Staples[1]; Jordy J. Hsiao[1]; Hongfeng Yin[1]; *[1]Agilent Technologies, Santa Clara, CA*

WP 044 **Sensitive Quantitation of the ADC Trastuzumab Emtansine Free Cytotoxic Drug DM1 in Plasma Using MicroLC-MS**; Remco Van Soest[1]; Khatereh Motamedchaboki[2]; Ian Moore[3]; *[1]SCIEX, Redwood City, CA; [2]Sciex, Redwood City, CA; [3]SCIEX, Concord, ON, Canada*

WP 045 **Quantitation of Free Protein Thiols by Differential Cysteine Alkylation with Stable Isotopes**; Ioannis A. Papayannopoulos[1]; Shannon Renn-Bingham[1]; Jarrod M. Womble[1]; *[1]Celldex Therapeutics, Fall River, MA*

WP 046 **Monitoring Host Cell Proteins during Monoclonal Antibody Purification by Mass Spectrometry**; Chunxiang Yao[1]; Renpeng Liu[1]; Xuan Chen[1]; Xinrong Liu[1]; Virginia Liu-Compton[1]; Lintao Wang[1]; Alex Lazar[1]; *[1]ImmunoGen, Waltham, MA*

WP 047 **Detailed Characterization of Free Thiols in a Stressed Monoclonal Antibody**; Yutian Gan; *Genentech, Inc., San Francisco, CA*

WP 048 **Developing Recurrent Tandem Mass Spectral Libraries for Released Glycans from the NISTmAb Reference Material**; M. Lorna A De Leoz[1]; Yuri A. Mirokhin[1]; Stephen E. Stein[1]; *[1]National Institute of Standards & Technology, NIST, Gaithersburg, MD*

WP 049 **Infliximab Analysis Using High Resolution Mass Spectrometry**; Annu Uppal[1]; Yihan Li[2]; Sibylle Heidelberger[3]; *[1]Sciex India Pvt Ltd, Haryana, India; [2]SCIEX, Redwood City, California; [3]SCIEX, Warrington, UK*

WP 050 **A Unified Workflow for Automatic Mapping of Disulfide Bonds in Protein Therapeutics Based on High Resolution LC-QTOF**; Xianming Liu[1]; Kefei Wang[1]; Clark Chan[2]; Yi Liu[2]; Paul Shan[2]; *[1]Bruker Daltonics, Shanghai, China; [2]Bioinformatics Solutions Inc, Waterloo, ON, Canada*

WP 051 **Quantification of Intact Antibody Drug Conjugate (ADC) from Plasma Using Automated Affinity Purification Followed by UHPLC- UHR- qTOF MS Analysis**; Hetal Sarvaiya[1]; Rolf Kern[1]; Johannes Hampl[1]; *[1]Abbvie Stemcentrx LLC, South San Francisco, CA*

WP 052 **Application of PASEF MS/MS Scans to Monoclonal Antibody Peptide Mapping**; Anjali Alving[1]; Guillaume Tremintin[2]; Stuart Pengelley[3]; Detlev Suckau[4]; *[1]Bruker Daltonics Inc., Billerica, MA; [2]Bruker Daltonics, San Jose, CA; [3]Bruker Daltonics, Billerica, MA; [4]Bruker Daltonik GmbH, Bremen, Germany*

WP 053 **Extensive Characterization of Antibody Variable Regions Enabled by Parallel Ion Parking**; Josh D. Hinkle[1]; Robert D'Ippolito[1]; Elizabeth M. Duselis[1]; Jeffrey Shabanowitz[1]; Dina L. Bai[1]; Donald F. Hunt[1]; *[1]University of Virginia, Charlottesville, VA*

WP 054 **Complete Sequence Coverage of a Monoclonal Antibody Using a Nonspecific Protease**; Robert D'Ippolito[1]; Josh D. Hinkle[1]; Jeffrey Shabanowitz[1]; Dina L. Bai[1]; Donald F. Hunt[1]; *[1]University of Virginia, Charlottesville, VA*

WP 055 **Rapid Enzymatic Digest of Antibodies and Proteins Using CapturemTM Technology**; Christian Hoppmann[1]; Mandy Li[1]; Michael Vierra[1]; Boris Levitan[1]; Tim Larson[1]; Gia Jokhadze[1]; Andrew Farmer[1]; *[1]Takara Bio, Mountain View, CA*

WP 056 **Characterizing and Quantitating Therapeutic Antibody Multimer Degradation Using Affinity Capture Mass**; Neha Srikumar[1]; Wenjing Li[1]; Robert Tchelepi[1]; Chen Gu[1]; Diego Ellerman[1]; Greg A. Lazar[1]; Yichin Liu[1]; John C. Tran[1]; *[1]Genentech Inc., San Francisco, CA*

WP 057 **A New LC-MS Approach for Enhancing Subunit-Level Profiling of mAbs and ADCs**; Jennifer M. Nguyen[1]; Jacquelynn Smith[2]; Olga V. Friese[2]; Jason C. Rouse[3]; Daniel P. Walsh[1]; Ximo Zhang[1]; Nilini S. Ranbaduge[1]; Matthew A. Lauber[1]; *[1]Waters Corporation, Milford, MA; [2]Pfizer, St. Louis, MO; [3]Pfizer Inc., Andover, MA*

WP 058 **Analytical Scale Native SEC - MS for Robust Biotherapeutic Characterization**; Henry Shion[1]; Dale A. Cooper-Shepherd[2]; Laetitia Denbigh[2]; Maria Basanta-Sanchez[3]; Barbara Sullivan[4]; Ying Qing yu[1]; Weibin Chen[1]; *[1]Waters Corporation, Milford, MA; [2]Waters Corporation, Wilmslow, UK; [3]Waters Corporation, Pleasanton, CA; [4]Waters Corporation, Beverly, MA*

WP 059 **High Pressure-Accelerated Digestion of Unreduced IgG by Lys-C and Trypsin**; Vera S. Gross[1]; Nicole Cutri[1]; Gary Smejkal[1]; Alexander V. Lazarev[1]; *[1]Pressure Bioscience Inc., South Easton, MA*

WP 060 **Bi-Specific mAb Drug Monitoring *in vivo*: Concentration Determination by Intact and Subunit Masses in Monkey, with Ligand Binding Assay Comparison**; Kristen Pannullo[1]; John F Kellie[2]; *[1]GlaxoSmithKline, King Of Prussia, PA; [2]GlaxoSmithKline, King of Prussia, PA*

WP 061 **In Depth Analytical Comparison of Infliximab and Biosimilars**; Maria-Christina S. Malinao[1]; Morgan Kramer[1]; Chad Eichman[1]; Brian Rivera[1]; Sean Orlowicz[1]; *[1]Phenomenex, Torrance, CA*

WP 062 **Applying *de novo* Top-Down and Middle-Down MS/MS Strategies Towards the Discovery of Novel Polyclonal Antibodies from Ebola/Zika Convalescent Sera.**; Adrian Guthals[1]; Jared Shaw[2]; Crystal Moyer[1]; Pavlo Gilchuk[3]; Neha Malhan[2]; Stefano Bonissone[4]; Natalie Castellana[4]; Dafna Abelson[1]; Michael Pauly[1]; Cinque S. Soto[3]; Erica O. Saphire[5]; Zachary Bornholdt[1]; James E. Crowe, Jr[3, 6, 7, 8]; Kevin Whaley[1]; Larry Zeitlin[1]; *[1]Mapp Biopharmaceutical, San Diego, CA; [2]Pacific Northwest National Laboratory, Richland, WA; [3]Vanderbilt Vaccine Center, Nashville, TN; [4]Digital Proteomics, La Jolla, CA; [5]Scripps Research Institute, La Jolla, CA; [6]Department of Pathology, Microbiology, and Immunology, Vanderbilt University*

Medical Center, Nashville, TN; [7]Chemical and Physical Biology Program, Vanderbilt University, Nashville, TN; [8]Department of Pediatrics, Vanderbilt University Medical Center, Nashville, TN

WP 063 **Characterization of Ion Activation Methods for Middle-Down *de novo* Sequencing of Monoclonal Antibodies**; Adrian L. Guthals[1]; Neha Malhan[2]; Jared B. Shaw[2]; *[1]Mapp Biopharmaceutical, San Diego, CA; [2]Pacific Northwest National Laboratory, Richland, WA*

WP 064 **Characterization and Quantification of Antibody Microheterogeneity for Clone Selection**; Yan Jiang[1]; Fateme Tousi[1]; Anders Lund[1]; Stephen D'Eri[1]; Sharmila Sivendran[1]; Chantal Turner[1]; *[1]Sanofi, Framingham, MA*

WP 065 **Comprehensive Characterization of Therapeutic Protein Charge Variants**; Weitao Jia[1]; Jennifer Zhang[1]; *[1]Genentech Inc., San Francisco, CA*

WP 066 **IgG Isotype and Fc Variant Evaluation Using Automated MS Data Analysis**; Holly Yip; *Genentech, San Francisco, CA*

WP 067 **Improved Peptide Mapping of Therapeutic Antibodies Using Proteases with Orthogonal Cleavage Specificity**; Chris Hosfield[1]; Michael Rosenblatt[1]; Marjeta Urh[1]; *[1]Promega Corporation, Madison, WI*

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WP 068 **Challenges and Strategies to Determine Drug Receptor Occupancy as the Pharmacodynamic (PD) Biomarker by Immunocapture (IC)-LC-MS/MS for Clinical Drug Development**; Naiyu Zheng[1]; Ian M. Catlett[1]; Kristin Taylor[1]; Huidong Gu[1]; Mark Pattoli[1]; Robert J. Neely[1]; Wenying Li[1]; Alban Allentoff[1]; Xiling Yuan[1]; Eugene Ciccimaro[1]; Ming Yao[1]; Bethanne Warrack[1]; James R. Burke[1]; Yan J. Zhang[1]; Jianing Zeng[1]; *[1]Bristol-Myers Squibb Company, Princeton, NJ*

WP 069 **Quantitative Measurement of Squalene in Human Plasma by UPLC-APCI-MS/MS**; Liang Feng[1]; Guangchun Zhou[1]; Morgan Byrd[1]; Yong-Xi Li[1]; *[1]Medpace Inc., Cincinnati, OH*

WP 070 **Single Shot DIA Profiling of >1500 Plasma Proteomes of the Weight Loss and Maintenance Study DiOGenes**; Roland Bruderer[1]; Jan Muntel[1]; Sebastian Müller[1]; Oliver M. Bernhardt[1]; Tejas Gandhi[1]; Polina Mironova[2]; Ondine Walter[2]; Jérôme Carayol[2]; Arne Astrup[3]; Wim H.M. Saris[4]; Jörg Hager[2]; Armand Valsesia[2]; Loïc Dayon[2]; Lukas Reiter[1]; *[1]Biognosys AG, Schlieren, Switzerland; [2]Nestlé Institute of Health Sciences, Lausanne, Switzerland; [3]University of Copenhagen, Denmark; [4]Maastricht University Medical Centre, Maastricht, Netherlands*

WP 071 **Development of a Multiplexed Peptide Immunoaffinity LC-MS/MS Assay for the Quantification of Podocyte Injury Biomarkers in Glomerular Disease**; Carlos A. Morales Betanzos[1]; Hendrik Neubert[1]; Mireia Fernandez Ocana[1]; *[1]Pfizer, Andover, MA*

WP 072 **Quantitative Data Independent Acquisition Analysis of Pompe Disease Biomarkers: A Foundation for Improved Targeted Method**; Monica Lane[1]; Kelly George[1]; Mahmud Hossain[1]; Tejas Gandhi[2]; Lukas Reiter[2]; Brendan MacLean[3]; Josh Eckels[4]; Rena Baek[1]; Alison McVie-Wylie[1]; Petra Oliva[1]; Kate Zhang[1]; *[1]Sanofi, Framingham, MA; [2]Biognosys AG, Schlieren, Switzerland; [3]University of Washington, Seattle, WA; [4]LabKey, San Diego, CA*

WP 073 **Immunoaffinity-Micro Flow LC-MS/MS for the Quantitation of Immune Checkpoint Proteins PD1 and PD-L1 in Human Tumor Tissues**; Yongxin Zhu[1]; Petia Shipkova[1]; Jacob Zalaznick[1]; Zheng Yang[1]; Nataly Manjarrez Orduno[1]; Steven Nadler[1]; Adrienne Tymiak[1]; Timothy V. Olah[1]; *[1]Bristol Myers Squibb, Princeton, NJ*

WP 074 **Site-Specific Identification of Isomeric Glycopeptides Derived from Serum Alpha-1-Acid Glycoprotein (AGP) in Hepatocellular Carcinoma**; David M. Lubman[1]; Jianhui Zhu[1]; Jing Liang[1]; Yifan Huang[2]; Jie Zhang[1]; Mingrui An[1]; Yehia Mechref[2]; *[1]University of Michigan Medical Center, Ann Arbor, MI; [2]Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX*

WP 075 **Assessment of Catecholamines as Potential Biomarkers of Target Engagement in Non-Human Primate Cerebral Spinal Fluid Utilizing UPLC-MS/MS**; Kimberly A Navetta[1]; Tom Lanz[2]; Mireia Fernandez Ocana[3]; *[1]Pfizer Inc., Andover, MA; [2]Pfizer, Cambridge; [3]Pfizer, Andover, MA*

WP 076 **Bioactive Lipids Serve as Biomarkers of Host Immune Response during Severe Influenza Infection in Pediatric Patients**; Kent L Wong[1]; Adrienne G. Randolph[2]; Xiaoying Yang[3]; Allen Nguyen[1]; Carrie M Rosenberger[4]; William Rodney Mathews[1]; Jacqueline M. McBride[1]; Veronica G. Anania[1]; *[1]Department of OMNI Biomarker Development, Genentech Inc., San Francisco, CA; [2]Boston Children's Hospital and Harvard Medical School, Boston, MA; [3]Department of Clinical Biostatistics, Genentech, Inc., San Francisco, CA; [4]Department of Biomarker Discovery OMNI, Genentech, Inc, San Francisco, CA*

WP 077 **Improving the Sensitivity and Accuracy of Quantitative Protein Biomarker (Biomeasure) Mass Spectrometry Through the Use of SRM Transition Summing**; Jay S. Johnson[1]; Joe Palandra[1]; Katherine Wright[1]; Jason M. Walsh[1]; Hendrik Neubert[1]; *[1]Pfizer Inc., Andover, MA*

WP 078 **Use of High Resolution Mass Spectrometry for Spatial and Temporal Mapping of Proteins in Mouse GI tissues for Biomarker Discovery**; Faizan Zubair[1]; Melinda Manuel[1]; Kevin DeMent[1]; Anne Kanta[1]; Yunqing Shi[1]; Erica Pierce[1]; *[1]Takeda San Diego Inc, San Diego, CA*

WP 079 **Brain Quantitative Proteomic Analysis in Apolipoprotein-A2 Knockout Mice**; Sausan Azzam[1]; Neda Saleh[2]; Mark R. Chance[1]; Kingman P. Strohl[1]; *[1]Case Western Reserve University School of Medicine, Cleveland, OH; [2]University of Mount Union, Alliance, OH*

WP 080 **A Very Sensitive LC-MS/MS Method for Simultaneous Quantification of DNA Methylation and Hydroxymethylation Levels in Biological Samples**; Dongwei Zhu[1]; Fang Wang[1]; Yanyan Cui[2]; Jakal Amin[3]; Wei Liu[1]; Yue Chen[1]; Bin Wu[1]; Guowen Liu[1]; *[1]Agios Pharmaceuticals, Cambridge, MA; [2]Wave Life Sciences, Cambridge, MA; [3]Charles River Laboratories, Inc., Worcester, MA*

WP 081 **Novel Top-Down Proteomics Tools for the Quantitative Analysis of Serum Autoantibody Repertoires in Patient Samples**; Zhe Wang[1]; Xiaowen Liu[2]; Kenneth Smith[3]; Si Wu[1]; *[1]University of Oklahoma, Norman, OK; [2]Indiana University, Purdue University, Indianapolis, IN; [3]Oklahoma Medical Research Foundation, Oklahoma City, OK*

WP 082 **Development of an LC-MS Assay for PTEN, a Clinically Relevant Biomarker for Breast Cancer Therapy Resistance**; Sahar Ibrahim[1, 2]; Andre LeBlanc[1]; Rene Zahedi[1, 3]; Gerald Batist[4, 5]; Christoph H. Borchers[1, 3, 6, 7]; *[1]Jewish General Hospital Proteomics Centre, McGill University, Montreal, QC, Canada; [2]Department of Experimental Medicine, McGill University, Montreal, QC, Canada; [3]Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC, Canada; [4]Department of Medicine, McGill University, Montreal, QC, Canada; [5]Department of Oncology, McGill University, Montreal, QC, Canada; [6]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [7]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada*

WP 083 **Development and Characterization of an Immuno-MRM Assay Panel Targeting RAS Phospho-Signaling Dynamics**; Jeff Whiteaker[1]; Regine M. Schoenherr[1]; Melissa Hoffman[2]; Eric Kuhn[3]; William Bocik[4]; Lei Zhao[1]; Dongqing Huang[1]; Jacob Kennedy[1]; Kiah Bowers[2];

Alexandra Cocco[3]; Simona Colantonio[4]; Richard G. Saul[4]; Kanika Sharma[4]; Matthew Holderfield[4]; Steven A. Carr[3]; Gordon R. Whiteley[4]; John Koomen[2]; Amanda G. Paulovich[1]; *[1]Fred Hutchinson Cancer Research Center, Seattle, WA; [2]Moffitt Cancer Center, Tampa, FL; [3]Broad Institute, Cambridge; [4]Frederick National Laboratory for Cancer Research, Frederick, ML*

WP 084 **Quantitative Analysis of Human Tear Fluid by MALDI-TOF Mass Spectrometry**; Ryan Walsh; *Shimadzu Scientific Instruments Corp., Columbia, MD*

WP 085 **Characterizing Equine Specific Biomarkers Using nanoLC-MS/MS Methods to Monitor Growth Factors as Indicators of Prohibited Substance Abuse**; Sophie Bromilow[1]; Ben Moeller[1]; David Horohov[2]; Eric Huang[3]; Claudia Martins[3]; Scott Stanley[1]; *[1]Kenneth L. Maddy Equine Analytical Chemistry Laboratory, Davis, CA; [2]Gluck Equine Research Center, Lexington, KY; [3]Thermo Fisher Scientific, San Jose, CA*

WP 086 **An Analytical Pipeline for Discovery and Verification of Glycoproteins from Plasma-Derived Extracellular Vesicles as Breast Cancer Biomarkers**; Hillary Andaluz Aguilar[1]; I-Hsuan Chen[1]; J. Sebastian Paez[1]; Xiaofeng Wu[1]; Li Pan[1]; Michael K Wendt[1]; Anton B Iliuk[1]; Ying Zhang[2]; W. Andy Tao[1]; *[1]Purdue University, West Lafayette; [2]Fudan University, Shanghai, China*

WP 087 **A Novel Method for High-Throughput Analysis of Arginine, Ornithine, Citrulline and Urea in *in vitro* Human Hepatocyte**; Cheng Chen[1]; Xiaotong Li[1]; Hongmei Wang[1]; Xinxin Wen[1]; Zhiyu Li[1]; Yi Tao[1]; Xin Zhang[2]; *[1]Department of DMPK/Non-GLP Bioanalytical Service, WuXi AppTec Co., Shanghai, China; [2]Department of DMPK, WuXi AppTec Co., Shanghai, China*

WP 088 **Quantification of 19 Aldehydes in Human Serum by Headspace Solid-Phase Microextraction/Gas Chromatography/High-Resolution Mass Spectrometry**; Lalith K Silva; *Centers for Disease Control, Atlanta, GA*

WP 089 **Deep Un-Depleted Human Serum Proteome Profiling and Targeted Parallel Reaction Monitoring Mass Spectrometry toward Biomarker Discovery for Alzheimer's Disease**; Kaushik Kumar Dey[1]; Mingming Niu[1]; Hong Wang[2]; Bing Bai[1]; Yuxin Li[2]; Xusheng Wang[2]; Ji-Hoon Cho[2]; Ashutosh Mishra[2]; Haiyan Tan[2]; Ping-Chung Chen[1]; Anthony A High[2]; Thomas G Beach[3]; Junmin Peng[4]; *[1]Department of Structural Biology, St Jude Children's Research Hospital, Memphis, TN; [2]St. Jude Proteomics Facility, St. Jude Children's Research Hospital, Memphis, TN; [3]Banner Sun Health Research Institute, Sun City, AZ; [4]Department of Structural Biology and Developmental Neurobiology, St. Jude Proteomics Facility, St. Jude Children's Research Hospital, Memphis, TN*

WP 090 **A Stable-Isotope Labeled Protein and Peptide Mixture for Global Normalization in Targeted and Data-Independent Quantitative Bottom-Up Proteomics**; Irene Van Den Broek[1, 2]; Kelly Njine Mouapi[2]; Mitra Mastali[2]; Ronald Holewinski[2]; Vidya Venkatraman[2]; Qin Fu[2]; A.Lenore Ackerman[3]; Jayoung Kim[3]; Michael Freeman[3]; Jennifer T. Anger[3]; Kevin Millis[4]; Andrew Percy[4]; Jennifer E. Van Eyk[2]; *[1]Cedars-Sinai Precision Biomarker Laboratories, Cedars-Sinai Medical Center, Los Angeles, CA; [2]Advanced Clinical Biosystems Research Institute, Heart Institute, Cedars Sinai Medical Center, Los Angeles, CA; [3]Division of Urology, Department of Surgery, Cedars-Sinai Medical Center, Los Angeles, CA; [4]Cambridge Isotope Laboratories, Tewksbury, MA*

WP 091 **Brain Proteome Alterations in Living Patients after Traumatic Brain Injury Revealed by Shotgun Mass Spectrometry-Based Quantitative Proteomics**; Ganna Shevchenko[1]; Sami Abu Hamdeh[1]; Jia Mi[1]; Niklas Marklund[1]; Jonas Bergquist[1]; *[1]Uppsala University, Uppsala, Sweden*

WP 092 **Proteomic Profiling of Plasma samples from Pulmonary Hypertension Patients Using Label-Free Quantitation and Isobaric Tagging on Depleted and Non-Depleted Samples**; Ling Li[1]; Bo Hu[1]; Belinda Willard[1]; *[1]Cleveland Clinic, Cleveland, OH*

WP 093 **Supramolecular Assemblies for Enhanced Mass Spectrometric Detection of Breast Cancer Biomarkers in Breast Milk**; Bo Zhao[1]; Mahalia A. C. Serrano[1]; Kathleen F. Arcaro[1]; S. Thayumanavan[1]; Richard W. Vachet[1]; *[1]University of Massachusetts, Amherst, MA*

WP 094 **NOD Mice Display Unique Salivary Peptidome/Proteome Signatures at the Onset of Sjögren's Disease-like Hyposalivation (Salivary Gland Dysfunction)**; Fabian Schulte[1]; Shanshan Liu[1]; Jing Zhou[1]; Qing Yu[1]; Markus Hardt[1]; *[1]The Forsyth Institute, Cambridge, MA*

WP 095 **Multiplex Mass Spectrometry based Assay to Monitor the Effect of Glucocorticoid on Human Exosomal Proteome**; Alison M. Samsel[1]; Mansi V. Goswami[1]; Tchilabalo Alayi[1]; Marissa Barbieri[1]; Runia Roy[1]; Swati Mummidivarpu[1]; Nicole Rouhanna[2]; Eric P. Hoffman[1]; Yetrib Hathout[1]; *[1]School of Pharmacy and Pharmaceutical Sciences, Binghamton, NY; [2]Decker School of Nursing, Binghamton University, Binghamton, NY*

WP 096 **Origins of Elevated Plasma 8-ISO-Prostaglandin F2α Levels in Human Smokers**; Fred Bjorn Lih[1]; Thomas J. van 't Erve[1]; Maria B. Kadiiska[1]; Ronald P. Mason[1]; Leesa J. Deterding[1]; *[1]NIEHS/NIH/DHHS, Rtp, NC*

WP 097 **Designing a Survivor: Derivatization as Mode of Selectively Reducing Fragmentation**; Clementina Mesaros[1]; Lisa Bottalico[1]; Eugene Ciccimaro[2]; Nathaniel W. Snyder[3]; Ian A. Alexander Blair[1]; *[1]University of Pennsylvania School of Medicine, Philadelphia, PA; [2]Agilent Technologies, Inc., Wilmington, DE; [3]Drexel University, Philadelphia, PA*

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WP 098 **Analysis of Fentanyl and Its Analogues in Human Urine by LC-MS/MS**; Rob Freeman[1]; Shun-Hsin Liang[1]; Justin Steimling[1]; Landon Wiest[1]; dan li[1]; Ravali Alagandula[1]; Frances Carroll[1]; Ty Kahler[1]; Susan Steinike[1]; Paul Connolly[1]; *[1]Restek Corporation, Bellefonte, PA*

WP 099 **Automated Chemically-Driven Robotic Surgery Using Rapid Evaporative Ionisation Mass Spectrometry (REIMS)**; Eftychios Manoli[1]; Zsolt Bodai[1]; Petra Paizs[1]; JULIA BALOG[2]; Steven D. Pringle[2]; Ara Darzi[1]; Zoltan Takats[1]; Philip Pratt[1]; *[1]Imperial College London, London, UK; [2]Waters Research Center, Budapest, Hungary*

WP 100 **High-Performing Novel SPE Polymers Show Efficient Recoveries and Reduced Sample Preparation Times**; Xuejun Zang[1]; Slobodan Milasinovic[1]; David House[1]; Asha Oroskar[1]; *[1]Orochem Technologies Inc, Naperville, IL*

WP 101 **Small but Powerful: Antiepileptic Drugs in Human Serum Analyzed with a Miniature Triple Quadrupole Mass Spectrometer in Research**; Jennifer Cottine Hitchcock[1]; Lauren Frick[2]; Vaughn Miller[2]; *[1]Agilent Technologies, Inc, Santa Clara, CA; [2]Agilent Technologies, Inc, Lexington, MA*

WP 102 **Development and Integration of a Stable Isotope Label IDO1 PD Assay into Phase 1 Clinical Trials**; John Meissen[1]; Matt Blatnik[2]; *[1]Pfizer, Groton, CT; [2]Pfizer, Groton*

WP 103 **Development and Qualification of a Clinical Biomarker Assay for Very Long Chain Fatty Acids(VLCFA) in CSF for CNS Drug Development**; Kan Zhu; *Vertex, Boston, MA*

WP 104 **An Overview of Proteomic Analyses in Noise Induced Hearing Loss**; Nopporn Jongkamonwiwat[1]; Miguel Ramirez[1]; Jeffrey N. Savas[1]; *[1]Department of Neurology, Feinberg School of Medicine, Northwestern University, Chicago, IL*

WP 105 **Quantitation of Oxytocin in Serum, Saliva and Urine by Orbitrap LCMS after SPE**; Adrian Franke; *Univ of Hawaii Cancer Ctr, Honolulu, HI*

WP 106 **Urinary Cortisol Quantitation Using Ultra High Pressure Liquid Chromatography/Compact Mass Spectrometry**; Changtong Hao[1]; Daniel Eikel[1]; Simon Prosser[1]; Jack D Henion[1]; *[1]Advion Inc., Ithaca, NY*

WP 107 **Comparative Analysis of the Urine Peptidome in Case of Hypertensive Pathologies During Pregnancy by High Resolution Mass Spectrometry**; Alexey Kononikhin[1, 2]; Anna Bugrova[2, 3]; Victoria Sergeeva[1, 3]; Maria Indeykina[1, 3]; Natalia Starodubtseva[2]; Natalia V. Zakharova[3]; Evgeny Kukaev[1, 4]; Igor Popov[1, 2]; Vladimir Frankevich[2]; Eugene (Evgeny) Nikolaev[1, 4, 5]; *[1]Moscow Institute of Physics and Technology, Moscow, Russia; [2]Research Center for Obstetrics, Gynecology and Perinatology of the Ministry of Healthcare of the Russian Federation, Moscow, Russian Federation; [3]Emanuel Institute of Biochemical Physics, Moscow, Russia; [4]Institute for Energy Problems of Chemical Physics of RAS, Moscow, Russia; [5]Skolkovo Institute of Science and Technology, Moscow Region, Russian Federation*

WP 108 **The Reduced Activity of PP-1a Under Redox Stress Condition is a Consequence of GSH-Mediated Transient Disulfide Formation**; Simranjit Singh[1]; Simon Lämmle[2]; Hassan Dihazi[3]; Kaomei Guan[2]; Ali El-Armouche[2]; Florian Martin Richter[4, 5]; *[1]Institute of Pharmacology and Toxicology, Universitätsmedizin Goettingen (UMG), Goettingen, Germany; [2]Institute of Pharmacology and Toxicology, Technische Universität Dresden, Dresden, Germany; [3]Clinic for Nephrology and Rheumatology, UMG, Göttingen, Germany; [4]Medical Department, Goethe-University, Frankfurt Am Main, Germany; [5]Max Planck Institute for Immunbiology and Epigenetics, Freiburg im Breisgau, Germany*

WP 109 **Embryo-Maternal Molecular Networking During the Early Stage Embryogenesis**; Laszlo Mark[1, 2, 3]; Janos Schmidt[1, 2, 3]; *[1]Institute of Biochemistry and Medical Chemistry, University of Pecs, Hungary; [2]Imaging Center for Life and Material Sciences, University of Pecs,, Pecs, Hungary; [3]MTA-PTE Human Reproduction Scientific Research Group, Pecs, Hungary*

WP 110 **Breaking the Paradigm – The Value of Sub ng/mL Quantitation Limits for Monitoring Buprenorphine Compliance**; Judy Stone[1]; Heather Hochrein[1]; Robert L. Fitzgerald[2]; *[1]University of California San Diego Health Center for Advanced Laboratory Medicine, San Diego, CA; [2]University of California San Diego, Department of Pathology, San Diego, CA*

WP 111 **25-hydroxy Vitamin D Assay with Novel Integration of Liquid Chromatography Tandem Mass Spectrometry and Automated Sample Preparation**; Hikaru Shibata[1]; Akira Sasaki[1]; Brian Feild[2]; Tairo Ogura[2]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]Shimadzu Scientific Instruments, Inc, Columbia, MD*

WP 112 **Analysis of Immunosuppressive Drugs from Whole Blood by LC-MS/MS**; Paul Connolly[1]; Shun-Hsin Liang[1]; Sharon Lupo[1]; Justin Steimling[1]; Ty Kahler[1]; Susan Steinike[1]; *[1]Restek Corporation, Bellefonte, PA*

WP 113 **Development of a UPLC-MS/MS Assay for Monitoring of Pharmacotherpy in Patients with APRT Deficiency Utilizing Design of Experiments**; Unnur Arna Thorsteinsdottir[1, 2]; Hrafnhildur L Runolfsdottir[1]; Finnur F. Eiríksson[1, 2]; Thorsteinn Hjortur Bjarnason[1, 2]; Vidar O. Edvardsson[3]; Runolfur Palsson[1, 3]; Margret Thorsteinsdottir[1, 2]; *[1]University of Iceland, Reykjavik, Iceland; [2]ArcticMass, Reykjavik, Iceland; [3]Landspitali - The National University Hospital of Iceland, Reykjavik, Iceland*

WP 114 **Fast and Quantitative Determination of 11 Antibiotics in Urine by Liquid Chromatography-Triple Quadrupole Mass Spectrometry**; Che-Hui Ku[1]; Tai-Chia Chiu[1]; Cho-Chun Hu[1]; *[1]National Taitung University, Taitung, Taiwan*

WP 115 **Rapid Detection of Anesthetics in Blood Based on Paper Spray - Mass Spectrometry**; Ying Liu[1, 2]; Xiao-Hui Zhang[3]; Ying-Lin Zhou[3]; Hefang Wang[2]; Xin-Xiang Zhang[1]; *[1]Peking University, Beijing, China; [2]Nankai University, Tianjin, China; [3]Peking University, Beijing, China*

WP 116 **A Tailored MALDI Probe for Screening γ-Glutamyltranspeptidase Activity**; Xinhua Guo; *Jilin University, Changchun, China*

WP 117 **Determination of Total Fatty Acids from DBS Samples – An Optimized Substrate for Sample Collection, Storage and Analysis**; Ricardo Neto[1, 2]; Wei Boon Hon[1, 3]; Andrew Gooley[1, 3]; Ruben Dario Arrua[1, 2]; Emily Hilder[1, 2]; *[1]ARC Training Centre for Portable Analytical Separation Technologies, Ringwood, Australia; [2]Future Industries Institute, University of South Australia Adelaide, Mawson Lakes Campus, Australia; [3]Trajan Scientific and Medical, 7 Argent Place, Ringwood, Australia*

WP 118 **Cross Validation of Immunosuppressant Quantification in Whole Blood by LDTD-MS/MS and LC-MS/MS Using Triple Ion Source**; Francis Brière[1]; Pier-Luc Plante[1]; Serge Auger[2]; Jean Lacoursière[2]; Pierre Picard[2]; *[1]Universite Laval, Quebec, QC, Canada; [2]Phytronix Technologies, Quebec, QC, Canada*

WP 119 **Blood Plasma Proteome/Peptidome Comparative Study for Potential Biomarkers Search of Alzheimer's Disease**; Maria Indeykina[1, 2, 3]; Alexey Kononikhin[1, 2, 3]; Anna Bugrova[2]; Yana B. Fedorova[4]; Natalia V. Zakharova[1, 2]; Alexander Brhozovskiy[5]; Igor Popov[1, 3]; Svetlana I. Gavrilova[4]; Eugene (Evgeny) Nikolaev[1, 3, 5]; *[1]Moscow Institute of Physics and Technology, Moscow, Russia; [2]Emanuel Institute of Biochemical Physics, Moscow, Russia; [3]Institute for Energy Problems of Chemical Physics of RAS, Moscow, Russia; [4]Mental Health Research Center, Moscow, Russia; [5]Skolkovo institute of science and technology, Moscow Region, Russian Federation*

WP 120 **Improved Chiral MS Analysis with Superficially Porous Chiral Columns**; William Long[1]; Anne Mack[2]; Mia Summers[3]; *[1]Agilent Technologies, Wilmington, DE; [2]Agilent Technologies, Inc, Wilmington, DE; [3]Agilent Technologies, Inc., Wilmington, DE*

WP 121 **Early Diagnosis and Evaluation of Therapeutics for Anthrax Using a Validated MALDI-TOF MS Anthrax Lethal Factor Method**; John R. Barr[1]; Anne E. Boyer[1]; Maribel Gallegos-Candela[1]; *[1]CDC, Atlanta, GA*

WP 122 **Metrology for Clinical: The use of MS in Traceable Measurement for Higher Order Reference Materials**; Chris Hopley[1]; Emily Whyte[1]; Dima Almekdad[1]; Sabine Biesenbruch[1]; *[1]LGC, Teddington, UK*

WP 123 **A Streamlined Approach for Developing a Simple and Sensitive LC-MS/MS Method for Free Testosterone Measurement**; Yu Zhou[1]; Sihe Wang[1, 2]; *[1]Cleveland Clinic, Cleveland, OH; [2]Cleveland State University, Cleveland, OH*

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WP 196 **Exploiting API, UHRMS and UHPSFC-MS to Unlock Complexity to Detect and Understand Fuel Additives**; G. John Langley[1]; Edward Wilmot[1]; Julie Herniman[1]; Jim Barker[2]; *[1]University of Southampton, Southampton, UK; [2]Innospec Inc., Ellesmere Port, UK*

WP 197 **Characterization of Asphaltenes Precipitated at Different Solvent Power Conditions Using Magnetic Resonance Mass Spectrometry (MRMS)**; Matthias Witt[1]; Markus Godejohann[2]; Sven Oltmanns[3]; Estrella Rogel[4]; *[1]Bruker Daltonik GmbH, Bremen, Germany; [2]Bruker BioSpin GmbH, Rheinstetten, Germany; [3]Bruker Optik GmbH, Bremen, Germany; [4]Chevron Energy Technology Company, Richmond, CA*

WP 198 **In Situ Analysis of Neat Supercritical Fluids and Binary Mixtures of Fuel-Related Compounds Under Pyrolysis Conditions**; Andrew Deblase[1, 2]; William K Lewis[2]; Christopher E Bunker[2]; *[1]Spectral Energies, LLC, Beavercreek, OH; [2]Air Force Research Lab, Dayton, OH*

WP 199 **Petroleomic Characterization of Pyrolysis Oils from Scrap Tire–Biomass Blends by Fourier Transform Ion Cyclotron Resonance Mass Spectrometry**; Timo Kekäläinen[1]; MD Fahim Hossain[1]; Ilja Miettinen[1]; Janne Jänis[1]; *[1]University of Eastern Finland, Joensuu, Finland*

WP 200 **Advanced Structural Analysis of Heavy Oil Fractions by High-Resolution Tandem Mass Spectrometry and Ion Mobility Spectrometry**; Johann Le Maitre[1, 2, 3]; Marie Hubert-Roux[1, 3]; Benoit Paupy[2, 3]; Sabrina Marceau[2, 3]; Carlos Afonso[1, 3]; Pierre Giusti[2, 3]; *[1]University of Rouen, Mont Saint Aignan, France; [2]TOTAL Refining and Chemicals, Gonfreville l'Orcher, France; [3]TOTAL RC - CNRS Joint Laboratory C2MC: Complex Matrices Molecular Characterization, Pau, France*

WP 201 **High-Throughput Analysis Method for Hydrocarbons C20-C50 Using LDTD-HRMS System**; Houssem Loukil[1]; Pascal Belisle[1]; Serge Auger[1]; Jonathan Rochon[2]; Jean Lacoursière[1]; Pierre Picard[1]; *[1]Phytronix Technologies, Quebec, QC, Canada; [2]Université Laval, Québec, QC, Canada*

WP 202 **The Study of Ionization of Hydrocarbon Standards and Saturated Fractions Favored by Doping Agents (Benzyl and Alkyl Halides)**; Lindamara M Souza[1]; Fernanda E Pinto[1]; Mariana T Nascimento[2]; Christopher J. Thompson[3]; Valdemar Lacerda Jr.[4, 5]; Boniek G Vaz[6]; Wanderson Romão[7]; *[1]Petroleomic and Forensic Chemistry Laboratory, Department of Chemistry, Federal University of Espírito Santo, 29075-910 Vitória, ES, Brazil, Vitória, Brazil; [2]Federal Institute of Espirito Santo, Vila Velha, Brazil; [3]Bruker Daltonics, San Jose, CA; [4]Petroleomic and Forensic Chemistry Laboratory, Department of Chemistry, Federal University of Espírito Santo, 29075-910 Vitória, ES, Brazil, Vitória, Espirito Santo, Brazil, Vitória, Brazil; [5]Federal University of Espirito Santo, Vitória - ES, Brazil; [6]Chemistry Institute, Federal University of Goiás, 74001-970 Goiânia, GO, Brazil, Goiânia, Brazil; [7]Federal Institute of Education, Science and Technology of Espírito Santo, 29106-010 Vila Velha, ES, Brazil and Petroleomic and Forensic Chemistry Laboratory, Department of Chemistry, Federal University of Espírito Santo, 29075-910 Vitória, ES, Brazil, Vitória, Brazil*

WP 203 **A Comparison of PAH Levels in Used Engine Oils by GC-TOFMS and GCxGC TOF-MS**; Tom Enzweiler[1]; Christina Kelly[1]; Joseph E Binkley[1]; Lorne Fell[1]; *[1]LECO Corporation, Saint Joseph, MI*

WP 204 **Novel Approach to Molecular and Structural Analysis of Humic Substances Using FT-ICR MS and Synthetic Carboxylated Polystyrene for Internal Calibration**; Alexander Zherebker[1, 2]; Yuri Kostyukevich[1, 2, 3]; Alexey Kononikhin[2, 3, 4]; Oleg Kharybin[1]; Irina V Perminova[5]; Eugene (Evgeny) Nikolaev[1, 2, 3, 4]; *[1]Skolkovo institute of science and technology, Moscow, Russia; [2]Institute for Energy Problems of Chemical Physics of RAS, Moscow, Russia; [3]Emanuel Institute of Biochemical Physics, Moscow, Russia; [4]Moscow Institute of Physics and Technology, Moscow, Russia; [5]Lomonosov Moscow State University, Department of Chemistry, Moscow, Russia*

WP 205 **Evaluation of Degradation Degree of Lubricating Oil by Thermal Desorption and Pyrolysis Combined with DART-MS (TDP/DART-MS)**; Chikako Takei[1]; Derek Gonzales[1]; Kenichi Yoshizawa[1]; *[1]BioChromato, Inc., Fujisawa, Japan*

WP 206 **Elucidation of Engine Oil Deposits by Mass Spectrometry Methods**; Savannah R Snyder[1]; Chrys Wesdemiotis[1]; *[1]The University of Akron, Akron, OH*

WP 207 **Optimizing GCxGC Parameters for Petroleum Analysis Using a Free Web-Based Tool**; Christina Kelly[1]; David E Alonso[1]; Lorne M. Fell[1]; Joseph E Binkley[1]; *[1]LECO Corporation, Saint Joseph, MI*

WP 208 **Analysis of Trace Levels Nitrogen Containing Species Present in Crude Oil Hydro Processing Products by High Resolution Mass Spectrometry**; Matthew Hurt[1]; Bi-Zeng Zhan[1]; *[1]Chevron Energy Technology Company, Richmond, CA*

WP 209 **Molecular-Beam Mass Spectrometry Study of the Impact of Hydrogen Addition to Natural Gas Mixtures in Partial Oxidation Reactions**; Dennis Kaczmarek[1]; Tina Kasper[1]; Burak Atakan[1]; *[1]University of Duisburg-Essen, Duisburg, Germany*

WP 210 **Lean Partial Oxidation of Methane in the Presence of Nitrogen Monoxide as a Model for Exhaust Gas Recirculation**; Martin Hoener[1]; Dennis Kaczmarek[1]; Tina Kasper[1]; *[1]University Duisburg-Essen, Duisburg, Germany*

WP 211 **Comprehensive Mass Spectrometric Evolved Gas Analysis (EGA) in the Context of Petroleomics**; Christopher Paul Rüger[1, 2]; Anika Neumann[1, 2]; Christoph Grimmer[1, 2]; Uwe Käfer[1, 3]; Martin Sklorz[1, 2]; Thomas Gröger[1, 3]; Thorsten Streibel[1, 2]; Ralf Zimmermann[1, 2, 3]; *[1]Joint Mass Spectrometry Centre (University of Rostock and Helmholtz Zentrum Munich), Rostock, Germany; [2]University of Rostock, Institute of Chemistry, Division of Analytical and Technical Chemistry, Rostock, Germany; [3]Helmholtz-Zentrum München (CMA), Munich, Germany*

WP 212 **Mass Profiling Study to Understand the Molecular Cause of Jet Fuel Thermal Oxidative Instability**; Krege Matthew Christison[1, 2]; David O Sparkman[2]; *[1]Chevron, Richmond, CA; [2]University of the Pacific, Stockton, CA*

WP 213 **VIZMASS© Software Package for Workflow Automatization in Complex Mixture Analysis**; Kat Maksimova[1]; Vlad Lobodin[2]; *[1]MAXIKAT, INC., Tallahassee, FL; [2]Maxicat, Inc., Tallahassee, FL*

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WP 215 **The Impacts of Wipe Sampling Variables on Method Performance for Hazardous Pesticide Environmental Samples**; Stuart Willison[1]; Daniel Stout[2]; James Starr[2]; Amy Mysz[3]; Dennis Tabor[2]; Barbara Wyrzykowska-Ceradini[4]; Eric Morris[4]; Josh Nardin[4]; Emily Snyder[1]; *[1]EPA/NHSRC, Cincinnati, OH; [2]EPA, Research Triangle Park, NC; [3]EPA, Chicago, IL; [4]Jacobs Technology, Inc., Research Triangle Park, NC*

WP 216 **Analysis of Ibuprofen and its Main Metabolites in Roots, Shoots and Seeds of Cowpea (Vigna Unguiculata L.Walp) Using LC-QTOF-MS**; Damia Barcelo[1]; Yolanda Pico[2]; Rodrigo Alvarez-Ruiz[2]; Leonard Wijaya[3]; Ahmed Alfarhan[3]; Mohammed Alyemeni[3]; *[1]ICRA, Girona, Spain; [2]Environmental and Food Safety Research Group (SAMA-UV), Desertification Research Centre CIDE (CSIC-UV-GV), Faculty of Pharmacy, University of Valencia, Valencia, Spain; [3]Department of Botany and Microbiology, College of Science, King Saud University, P.O. Box 2455, Riyadh 11451, Saudi Arabia, Riyadh, Saudi Arabia*

WP 217 **Novel Ionisation Technique Offers Increased Spectral Clarity in the UPLC-MS/MS Analysis of a Range Crop Protection Chemicals & Their Metabolites**; Michael Jones[1]; Peter Hancock[2]; *[1]Waters Corporation, Wilmslow, UK; [2]Waters Corporation, Wilmslow, UK*

WP 218 **Multi-Residue Analytical Method for Determination of Emerging Contaminants in Various Aqueous Environmental Matrices by Solid-Phase Extraction and Liquid Chromatography/Mass Spectrometry**; Renee N.G Huang[1]; Jim Scott[1]; Katherine Hyland[2]; Steve Tersigni[1]; *[1]Santa Clara Valley Water District, San Jose, CA; [2]SCIEX, Redwood City, California*

WP 219 **Detection and Evaluation of Antibiotics in Seven Wastewater Treatment Plants in Southwest Illinois**; Qianqian Zhang[1]; Clayton Donald[1]; Jillian Rhomberg[1]; Kevin R Tucker[1]; *[1]Southern Illinois University Edwardsville, Edwardsville, IL*

WP 220 **Magnetic Molecularly Imprinted Polymers for Dispersive Micro Solid-Phase Extraction Coupled to LC-MS/MS for Analyzing of Estrogens in Environmental Aqueous Samples**; Cheng-Chieh Huang[1]; Chien-Yun Hsueh[1]; Maw-Rong Lee[2]; *[1]National Chung Hsing University, Taichung, Taiwan; [2]National Chung-Hsing University, Taichung, Taiwan*

WP 221 **The Analysis of Natural and Synthetic Estrogens at Low PPQ Levels in Surface Water and Final Effluent Water by LC-ESI-MS/MS**; Benjamin Wuyts[1]; Euan Ross[1]; Angela Boag[2]; Simon Hird[1]; Kenneth Rosnack[3]; Samantha Mora[4]; *[1]Waters Corporation, Wilmslow, UK; [2]Scottish Water, Edinburgh, UK; [3]Waters Corporation, Milford, MA; [4]Waters Corporation, Beverly, MA*

WP 222 **Rapid Determination of Polar Pesticides and Plant Growth Regulators in Fruits/Vegetables Byliquid Chromatography/Tandem Mass Spectrometry**; Narong Chamkasem; *FDA, Atlanta, GA*

WP 223 **Determination of Multi-Residue Antibiotics in Surface Water by SPE and UHPLC-MS/MS**; Yiwen Li[1]; Zhiwei Gan[1]; Ruoying Liao[1]; Xiang Li[2]; Xiangdong Zhou[2]; Chengyuan Cai[2]; Yongming Xie[2]; Feng Qin[3]; Jingcun Wu[3]; *[1]Department of Environmental Science and Engineering, School of Architecture and Environment, Sichuan University, Chengdu, China; [2]Perkinelmer Management (Shanghai) Co., Ltd., Shanghai, China; [3]PerkinElmer Inc., Woodbridge, ON, Canada*

WP 224 **Combined Approach for the Screening and Identification of Microbial Secondary Metabolites for Applications in Biocontrol**; Mickael Chevalier[1]; Emma Ricart[2]; Frédérique Lisacek[2]; Maude Pupin[3, 4]; Sandra Matthijs[5]; Philippe Jacques[6]; Christophe Flahaut[7]; Valérie Leclère[1]; *[1]Charles Viollette Institute, University of Lille, Vileneuve d'Ascq, France; [2]Proteome informatics Group, Geneva, Switzerland; [3]Univ Lille, CNRS, Centrale Lille, UMR 9189 – CRIStAL- Centre de Recherche en Informatique Signal et Automatique de Lille, Lille, France; [4]Inria-Lille Nord Europe, Bonsai team, Lille, France; [5]Institut de Recherches Microbiologiques-Wiame, Campus du CERIA, Brussels, Belgium; [6]TERRA Research Centre, Microbial Processes and Interactions (MiPI), Gembloux Agro-Bio Tech, University of Liege, Gembloux, Belgium; [7]Charles Viollette institute, Lille & Lens, France*

WP 225 **Automatic, Simultaneous and Rapid Analysis of Pesticides in Surface and Underground Water by Online SPE and UHPLC-MS/MS**; Sascha Giegold[1, 2]; Doriane Toinon[3]; Sara Sambissa[3]; *[1]Shimadzu Europa GmbH, Duisburg, Germany; [2]shimadzu Deutschland GMBH, 47269 Duisburg, Germany; [3]Shimadzu France, Marne la Vallée, France*

WP 226 **Study on the Degradation Mechanism of Atrazine in Sewage by UHPLC-MS/MS**; Jun Li[1]; Jianfei Yan[1]; Bo Lai[1]; Xiang Li[2]; Xiangdong Zhou[2]; Chengyuan Cai[2]; Yongming Xie[2]; Feng Qin[3]; Jingcun Wu[3]; *[1]Department of Environmental Science and Engineering, School of Architecture and Environment, Sichuan University, Chengdu, China; [2]Perkinelmer Management (Shanghai) Co., Ltd., Shanghai, China; [3]PerkinElmer Inc., Woodbridge, ON, Canada*

WP 227 **Determination of Psychotropic Drugs (Benzodiazepines) in Environmental Sample Of River Water and Sediments by MALDI-TOF-MS**; Chalder Nunes[1]; Emy Komatsu[2]; Hélène Perreault[2]; Sueli Pércio Quináia[1]; *[1]Universidade Estadual do Centro-Oeste - Unicentro, Guarapuava, Brazil; [2]University of Manitoba, Winnipeg, MB, Canada*

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WP 229 **The Coffee Effects on Bioavailability of Acrylamide in Mice**; Da-Jung You[1, 2]; Soo Hyun Lee[3]; Miyeon Lee[1]; Yuri Cho[4, 5]; Hyun-Jin Park[6]; Hyun-Mee Park[7]; *[1]Korea Institute of Science and Technology, Korea, Seoul, South Korea; [2]Korea University, Korea, Seoul, South Korea; [3]Kongju National University, Kongju, South Korea; [4]Korea Institute of Science and Technology, Seoul, South Korea; [5]Kyunghee Univercity, Seoul, South Korea; [6]Korea University, Seoul, South Korea; [7]Korea Institute of Science and Technology, Seoul, South Korea*

WP 230 **Exploring the Capabilities of a Newly Built Automation Platform For Food Safety**; Anil Kumar Meher[1]; Santosh Karki[1, 2]; Milan Pophristic[2]; Wenzhe Jiao[1]; Charles N McEwen[2, 3]; *[1]Wayne State University, Detroit; [2]MSTM, LLC, Newark, DE; [3]University of the Sciences, Philadelphia, Pennsylvania*

WP 231 **Residual Fipronil and Threemetabolites Determination in Chicken Egg by Gas Chromatography Tandem Mass Spectrometry**; Li Xianjiang[1]; Zhen Guo[1]; Xiuqin Li[1]; Hongmei Li[1]; *[1]National Metrology of China, Beijing, China*

WP 232 **From Signal to Analytical Reporting for Allergen Detection by Mass Spectrometry**; Philip Johnson; *University of Nebraska, Lincoln, Lincoln, NE*

WP 233 **Comparison of Various Data-Acquisition Modes in High Resolution Mass Spectrometry (HRMS) for Contaminants Screening in Aquacultured Products**; I-Lin Wu[1]; Sherri B Turnipseed[1]; Joseph M Storey[1]; Wendy C Andersen[1]; *[1]US Food and Drug Administration, Denver, CO*

WP 234 **Broad Screening of Illicit Ingredients in Cosmetics Using UPLC-Hybrid Quadrupole-Orbitrap Mass Spectrometry with Customized Accurate-Mass Database and Mass Spectral Library**; Xianshuang Meng[1]; Qiang Ma[1]; *[1]Chinese Academy of Inspection and Quarantine, Beijing, China*

WP 235 **A Simple Analysis of 4-Methylimidizole Using Automated Solid Phase Extraction and High Performance Liquid Chromatography with MS/UV Detection**; William Jones[1]; Alicia Cannon[1]; Michael Ebitson[1]; Paul Monroy[2]; *[1]Horizon Technology, Salem, NH; [2]Babcock Laboratories, Riverside, California*

WP 236 **Validation of N-terminal Labeling Strategy for Analysis of Partially Hydrolyzed Gluten Proteins**; Wanying Cao[1]; Joe L. Baumert[1]; Melanie Downs[1]; *[1]Food Allergy Research and Resource Program, Department of Food Science and Technology, University of Nebraska-Lincoln, Lincoln, NE*

WP 237 **Comparing LC-MS/MS and GC-MS for the Characterization of Terpenes in Plant Extracts**; Kevin J. Mchale[1]; Suresh Seethapathy[1]; Rory Doyle[1]; *[1]Thermo Fisher, Somerset, NJ*

WP 238 **Determination of Furfuryl Alcohol Levels in Caramel Food Colorings and Food Products**; Brad Mangrum[1]; Lowri DeJager[1]; *[1]FDA-CFSAN, College Park, MD*

WP 239 **Validation of A Low-Cost and Highly-Sensitive Method for Determination of Eighteen Mycotoxins in Food Matrixes Using SPE and LC/MS/MS**; Yin Ling Chew[1]; Rui Bing Shannon Peck[2]; Zhaoqi Zhan[1]; Jie Xing[1]; *[1]Shimadzu Asia Pacific, Singapore, Singapore; [2]National University of Singapore, Singapore, Singapore*

WP 240 **Determination of Glyphosate and Aminomethylphosphonic Acid in Tea byLC-MS/MS**; Haijuan An[1]; Jian Kang[2]; Shizhong Chen[3]; *[1]Shimadzu-GL Sciences (Shanghai) Laboratory Supplies Co.,LTD. Beijing Branch, Beijing, China; [2]Shimadzu-GL Sciences (Shanghai) Laboratory Supplies Co.,LTD. Beijing Branch, Beijing, China; [3]School of Pharmaceutical Sciences, Peking University, Beijing, China*

WP 241 **Determination of Methyl-3-Quinoxaline-2-Carboxylic Acid in Pork by LC-MS/MS**; Fulan Zhu[1]; Haijuan An[2]; Hong Wang[3]; *[1]Shimadzu-GL Sciences (Shanghai) Laboratory Supplies Co.,LTD., Shanghai, China; [2]2. Shimadzu-GL Sciences (Shanghai) Laboratory Supplies Co.,LTD, Beijing Branch, Beijing, China; [3]3. School of Pharmaceutical Sciences, Peking University, Beijing, China*

WP 242 **Evaluating the Effects of the Addition of Adulterants in Milkusing Direct-Infusion High-Resolution Mass Spectrometry**; Tatiane Melina Guerreiro[1]; Diogo Noin de Oliveira[1]; Carlos Fernando Odir Rodrigues Melo[1]; Estela de Oliveira Lima[1]; Marta Ribeiro da Silva[1]; Rodrigo Ramos Catharino[1]; *[1]Innovare Biomarkers Laboratory, Campinas, Brazil*

WP 243 **Evaluation of a Mass Spectrometry-Based Method for Detecting Enzymatically Active Botulinum Neurotoxins in Foods**; Whitney L. Stutts[1]; Gowri Manickam[1]; Timothy R. Croley[1]; Shashi K. Sharma[1]; *[1]U.S. Food and Drug Administration, Center for Food Safety and Applied Nutrition, College Park, MD*

WP 244 **Radiolysis Products Of Tris(Nonylphenyl) Phosphite Gamma-Irradiated at Low Doses**; Mary Dawn Celiz[1]; Kim M. Morehouse[1]; Lowri S. de Jager[1]; Timothy H. Begley[1]; *[1]US FDA, College Park, MD*

WP 245 **A Simple, Sensitive and Specific Assay to Simultaneously Quantify Methylcobalamin, Cyanocobalamin and Cobamamide in Protein/Non-Protein Dietary Supplements Using LC/MS/MS**; Aihua Liu[1]; Daniel Taylor[1]; Uri Hong[1]; Edgar Grigorian[1]; Spencer Carter[1]; *[1]Dyad Labs, Salt Lake City, UT*

WP 246 **Development of LC-MS/MS Method for Determination Of Hydrophilic Phycotoxins**; Renat Selimov[1]; Pavel Metalnikov[1]; Elizaveta Goncharova[1]; Irina Goncharova[1]; Ilya Batov[1]; Alexander Komarov[1]; *[1]VGNKI, Moscow, Russian Federation*

WP 247 **Rapid Semi-Quantification of Zilpaterol from Biological Matrices Using ASAP and DESI-like MS from a Commercial Heated Electrospray Ionization Probe**; Shubhashis Chakrabarty[1]; Weilin L. Shelver[1]; David J. Smith[1]; *[1]USDA, Fargo, ND*

WP 248 **Development and Validation of Analytical Method of Boric Acid in Caviars by ICP-AES and ICP-MS**; Jaewook Shin[1]; Jung Bok Kim[1]; *[1]Korea Advanced Food Research Institute, Uiwang-si, Gyeonggi-do, South Korea*

WP 249 **Determination of Pyrrolizidine Alkaloids in plant Material Using On-Line SPE Coupled to UHPLC-MS/MS**; Sven Vedder[1]; Anja Grüning[1]; Julia Sander[1]; *[1]Shimadzu Europa GmbH, Duisburg, Germany*

WP 250 **Quantitative Analysis of Lysozyme in a Wine Matrix by LC-MS/MS with multiple Instrument Platforms**; Beth Anne McClure[1]; Tony Ribeiro[1]; Shyamali Jayasena[2]; Michael Krawitzky[2]; Melanie Downs[2]; *[1]E & J Gallo Winery, Modesto, CA; [2]Food Allergy Research and Resource Program, Department of Food Science and Technology, University of Nebraska-Lincoln, Lincoln, NE*

WP 251 **Determination of fipronil and its Metabolite Fipronil Sulfone in Eggs by LC-MS/MS Using a Modified QuEChERS Method**; Renata Jandova[1]; Eimear McCall[1]; Euan Ross[1]; Simon Hird[1]; Kenneth Rosnack[2]; *[1]Waters Corporation, Wilmslow, UK; [2]Waters Corporation, Milford, MA*

WP 252 **A Sensitive, Specific and High-Throughput LC/MS/MS Assay to Quantify Glyphosate and Its Metabolite in Protein, Non-protein, and Botanical Dietary Supplements**; Aihua Liu[1]; Daniel Taylor[1]; Edgar Grigorian[1]; Spencer Carter[1]; *[1]Dyad Labs, Salt Lake City, UT*

WP 253 **Simultaneous Determination of γ-Hydroxybutyrate and its Precursor Substances γ-Butyrolactone and 1,4-Butanediol in Beverages Using UHPLC-MS/MS**; Shaoming Jin[1]; Xiao Ning[1]; Qilei Guo[2]; Tao Bo[2]; *[1]China National Institutes for Food and Drug Control, Beijing, China; [2]Agilent Technologies Inc., Beijing, China*

WP 254 **Determination of 298 Pesticides in Fish and Shellfish by Modified QuEChERS Extraction Gas Chromatography with Tandem Mass Spectrometry Detection (GC-MS/MS)**; Andrew D Sullivan; *Canadian Food Inspection Agency, Calgary, AB, Canada*

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WP 256 **Questioning the Status Quo: Decrease of Ethyl Glucuronide Concentrations in Hair After Prolonged Exposure to Water**; Marc Joel Luginbühl[1]; Susanne Nussbaumer[1]; Wolfgang Weinmann[1]; *[1]Institute of Forensic Medicine Bern, Bern, Switzerland*

WP 257 **Here Comes the Boom: Derivatization to Enhance Detection and Quantification of Emerging Threat Compounds Using Mass Spectrometry**; Connor J Graca[1]; Luke Metzler[1]; Michael Van Stipdionk[1]; Stephanie Wetzel[1]; *[1]Duquesne University, Pittsburgh, PA*

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WP 259 **Toward Universal Extraction and Detection of Multitudinous Exogenous Peptides in Equine Plasma and Urine for Doping Control**; Fuyu Guan[1]; Mary A Robinson[2]; *[1]University of Pennsylvania, West Chester, PA; [2]University of Pennsylvania, Kennett Square, PA*

WP 260 **Rapid Screeing of Drugs in Blood by the Coupling of ATLAS-USIS and Method Package for Rapid Toxcoloy Screening**; Lun Song; *Shimadzu (China) Co., Ltd,, Shanghai, China*

WP 261 **MRM Spectrum Mode and Library Searching for Enhanced Reporting Confidence in Forensic Toxicology analysis**; Eishi Imoto[1]; Takeshi Ashida[1]; Kazuya Ukai[1]; *[1]Shimadzu corp., Kyoto, Japan*

WP 262 **Use of High-Resolution Mass Spectrometry for Targeted/Non-Targeted Screening in Equine Doping Control Analysis**; Youwen You[1]; Rachel M. Proctor[2]; Kevin Guo[3]; Fuyu Guan[2]; xiaoqing Li[2]; Mary A Robinson[2]; *[1]University of Pennsylvani, West Chester, PA; [2]University of Pennsylvania, Kennett Square, PA; [3]Thermo Fisher Scientific, San Jose, CA*

WP 263 **Quantification of Apple Juice in Commercial Grape Juice by ESI-FT-ICR MS: A Forensic Approach**; Bruno G Oliveira[1]; Flávia Tosato[1]; Fernada E Pinto[1]; Lindamara S Souza[1]; Mariana T Nascimento[2]; Paulo R Filgueiras[1]; José A Ventura[3]; Denise C Endringer[2, 4]; Wanderson Romão[1, 2]; *[1]Federal University of Espirito Santo, Vitória - ES, Brazil; [2]Federal Institute of Espirito Santo, Vila Velha, Brazil; [3]Capixaba Institute for Research, Technical Assistance and Rural Extension, Vitória - ES, Brazil; [4]University Vila Velha, Vila Velha, Brazil*

WP 264 **Anticipating the Admissibility of Forensic Evidence Screened On-Site via Ambient Sampling, Portable Mass Spectrometry**; Chase M. Deberry[1]; Sara E. Bell[1]; Angelica Traub[1]; Donald Bernardi[2]; Christopher C. Mulligan[1]; *[1]Department of Chemistry, Illinois State University, Normal, IL; [2]Department of Politics and Government, Illinois State University, Normal, IL*

WP 265 **Spray Solvent Dependence Observed During the Analysis of Synthetic Cannabinoids via Paper Spray Ionization-Mass Spectrometry**; Sara E. Bell[1]; Shahnaz Mukta[1]; Chase M. Deberry[1]; Christopher C. Mulligan[1]; *[1]Department of Chemistry, Illinois State University, Normal, IL*

WP 266 **Solid-phase Extraction with Paper Spray Mass Spectrometry for Improving Detection Limits of Chemical Warfare Agent Hydrolysis Products in Water Samples**; William R. A. Wichert[1]; Trevor G. Glaros[2]; Nicholas E. Manicke[1]; *[1]IUPUI, Indianapolis, IN; [2]BioSciences Division, BioDefense Branch, US Army Edgewood Chemical Biological Center, Aberdeen Proving Ground, Maryland*

WP 267 **Human Hair Proteomics – Using Genetically Variant Peptides to Infer Individuals SNPs in Forensic Contexts**; Brett S Phinney[1]; Michelle S Salemi[1]; Zachary C Goecker[2]; Robert H Rice[2]; Glendon J Parker[2]; *[1]UC Davis Genome Center, Davis, California; [2]UC Davis, Davis, CA*

WP 268 **Improvement of an LC/Q-TOF Method for the Trace Analysis of Peroxide-Based Explosives**; Nan Hu[1]; Tao Bo[1]; *[1]Agilent Technologies (China) Co.,Ltd, Beijing, China*

WP 269 **Fully-Automated LC-MS/MS System as a Beneficial Alternative to Conventional Immunoassay Screening**; Zhi Wei Edwin Ting[1]; Shao Hua Chia[1]; Yi Ju Yao[2]; Hooi Yan Moy[2]; Daisuke Kawakami[3]; Zhaoqi Zhan[1]; *[1]Application Development and Support Centre, Shimadzu (Asia Pacific) Pte Ltd, 79 Science Park Drive #02-01/08, Singapore 118264, Singapore, Singapore; [2]Analytical Toxicology Division, Health Science Authority, 11 Outram Road, Singapore, Singapore; [3]Clinical & Biotechnology Business Unit, Shimadzu Corporation, 1 Nishinokyo Kuwabara-cho, Nakagyo-ku, Kyoto, Japan*

WP 270 **Automated Micro Solid Phase Extraction (µSPE) for Quick and Easy in the Detection of Aqueous Nitro Aromatic Explosives**; Matthew Diplock[1]; Andrew Minett[2]; Philip Doble[1]; *[1]School of Mathematical and Physical Sciences, University of Technology Sydney, Sydney, Australia; [2]Eprep Pty Ltd, Mulgrave, Australia*

WP 271 **The Internal Standard Metabolites for Applying Previous Analysis of Bloodstain to the Field**; Hyo-Jin Kim[1]; You-Rim Lee[1]; Jiyeong Lee[2]; Ae Eun Seok[1]; Arum Park[1]; Sora Mun[1]; Yoo-Jin Lee[1]; Hee-Gyoo Kang[1, 2]; *[1]Laboratory of Signal Transduction and Disease Biomarker Discovery, Department of Senior Healthcare, BK21 Plus Program, Graduate School, Eulji University, Daejeon-si, South Korea; [2]Department of Biomedical Laboratory Science, College of Health Sciences, Eulji University, Seongnam-si, Gyeonggi-do, South Korea*

WP 272 **Cannabis Leaf Analysis by MALDI-FT-ICR MSI**; Lindamara M. Souza[1]; Nayara A. dos Santos[1]; Fernanda E Pinto[1]; Lilian V. Tose[1]; Mariana T Nascimento[2]; Christopher J. Thompson[3]; Sidnei Moura[4]; Ronaldo Mohana-Borges[5]; Wanderson Romão[6]; *[1]Federal University of Espirito Santo, Vitória, Brazil; [2]Federal Institute of Espirito Santo, Vila Velha, Brazil; [3]Bruker Daltonics Inc., Billerica, MA; [4]University of Caxias do Sul, Caxias Do Sul, Brazil; [5]Federal University of Rio de Janeiro, Rio de Janeiro, Brazil; [6]IFES/UFES, Vitoria, Brazil*

WP 273 **Optimization of Design Drugs Analysis by LDI(+), MALDI(+) and MALDI(+)-Imaging Coupled to FT-ICR MS**; Fernanda E Pinto[1]; Lilian V. Tose[1]; Nayara A. dos Santos[2]; Valdemar Lacerda Jr[1]; Ronaldo Mohana-Borges[3]; Sidnei Moura[4]; Lindamara S Souza[1]; Mariana T Nascimento[5]; Christopher Thompson[6]; Wanderson Romão[7]; *[1]Federal University of Espirito Santo, Vitória - ES, Brazil; [2]Federal University of Espirito Santo, Vitória, Brazil; [3]Federal University of Rio de Janeiro, Rio de Janeiro, Brazil; [4]University of Caxias do Sul, Caxias Do Sul, Brazil; [5]Federal Institute of Espirito Santo, Vila Velha, Brazil; [6]Bruker Daltonics Inc., Billerica, MA; [7]IFES/UFES, Vitoria, Brazil*

WP 274 **Cannabis-Related Bioanalysis (from Plant to Forensic) Using LC-CMS (Single Quad)**; Ben Nie[1]; Jack D Henion[1]; George A Maylin[2]; *[1]Advion Inc., Ithaca, NY; [2]New York Drug Testing & Research Program, Ithaca, NY*

WP 275 **Chemical Imaging of Latent Fingerprints Deposited on Porous Surfaces Developed by Ninhydrin and Iodine Fuming**; Emily C King[1]; Paige Hinners[1]; Young-Jin Lee[1]; *[1]Iowa State University, Ames, IA*

WP 276 **Analysis of Amino Acids in Human Hair to Assist in the Differentiation of Ancestral Origins by Gas Chromatography/Mass Spectrometry**; Sirena Lam[1]; Robert H. Powers[1]; Alyssa L. M. Marsico[1]; *[1]University of New Haven, West Haven, CT*

WP 277 **Lifestyle Profiling Using Metabolomics of Personal Objects**; Xavier A. Holmes[1]; Louis-Felix Nothias[1]; Kathleen Dorrestein[1]; Ricardo R. da Silva[1]; Chris Callewaert[2]; Rob Knight[2, 3]; Amina Bouslimani[1]; Pieter C. Dorrestein[1, 4]; *[1]Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California, San Diego, La Jolla, California; [2]Department of Pediatrics, University of California, San Diego, California; [3]Department of Computer Science and Engineering, University of California, San Diego, La Jolla, California; [4]Departments of Chemistry, Biochemistry and Pharmacology, University of California, San Diego, La Jolla, California*

WP 278 **Forensic Sampling Using Gas-pulse Displacement and Vacuum Capture**; Jamira A Stephenson[1]; Fabrizio Donnarumma[2]; Kermit K Murray[1]; *[1]Louisana State University, Baton Rouge, LA; [2]Louisiana State University, Baton Rouge, LA*

WP 279 **Comprehensive Screening and Identification of Multiclass of Drugs and Poisons in Body Fluid by LC-HRMS for Toxicological Analysis**; Dai-Yong Huang[1]; Wen-Yen Lee[2]; Jun-Gang Lu[3]; Shan-An Chan[4]; *[1]Agilent Technologies Ltd. Hong Kong, Hong Kong, Hong Kong; [2]Agilent Technologies, Inc, Taipei, Taiwan; [3]Agilent Technologies, Inc., Guangzhou, China; [4]Agilent Technologies, Inc, Taipei, Taiwan*

WP 280 **Analysis of Doping and Forensic Drugs in Urine Using High-Resolution GC/Q-TOF**; Sofia Nieto[1]; Nathan Eno[1]; Wim Van Gansbeke[2]; Peter Eenoo[2]; *[1]Agilent Technologies, Inc., Santa Clara, CA; [2]DoCoLab, Ghent University, Ghent, Belgium*

WP 281 **Quantitative Analysis of Trace Levels of Explosives, Gunshot Residues, Propellants, Suppressors and Stabilizers Using LC/MS/MS and GC/MS**; RORY M DOYLE[1]; Suresh Seethapathy[1]; Dominic Andrada[2]; *[1]Thermo Fisher Scientific, Somerset, NJ; [2]Thermo Fisher Scientific, San Jose, CA*

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WP 282 **Effect of Tag on Spectral Perturbation in Infrared Predissociation Spectroscopy of Biomolecules**; Taylor A. Harmon[1]; Caroline Liu[2]; Christian Bleiholder[3]; Nicolas C. Polfer[1]; *[1]University of Florida Department of Chemistry, Gainesville, FL; [2]Florida State University, Tallahassee, FL; [3]Deparament of Chemistry and Biochemistry, The Florida State University, Tallahassee, FL*

WP 283 **Multiplexed IR Tagging Spectroscopy Inside a Mass-Selective Cryogenic Linear Ion Trap**; Larry Tesler[1]; Nicolas C. Polfer[1]; *[1]University of Florida Department of Chemistry, Gainesville, FL*

WP 284 **Intramolecular CH-C interactions Can Switch Off H-Tunneling Reactivity of Hydroxycarbenes; A Gas-Phase Study by IR Ion Spectroscopy**; Mathias Schaefer[1]; Jos Oomens[2]; Giel Berden[2]; Jonathan Martens[2]; Anthony Meijer[3]; Albrecht Berkessel[1]; Katrin peckelsen[1]; Mathias Paul[1]; *[1]University Cologne, Department of Chemistry, Cologne, Germany; [2]Radboud University, Nijmegen, Netherlands; [3]University of Sheffield, Sheffield, UK*

WP 285 **Probing Peptide Solvation with IR Spectroscopy of Cold Ions**; Jonathan M. Voss[1]; Kaitlyn Fischer[1]; Etienne Garand[1]; *[1]University of Wisconsin-Madison, Madison, WI*

WP 286 **REMPI andMATIspectroscopy of Methyl and Halo Pyridines**; Niklas Helle[1]; Sascha Krüger[1]; Jurgen Grotemeyer[1]; *[1]Christian-Albrechts-Univ, Kiel, Germany*

WP 287 **Cryogenic Ion Spectroscopy for Identification of Monosaccharide Anomers**; Valeriu Scutelnic[1]; Thomas R. Rizzo[1]; *[1]EPFL, Lausanne, Switzerland*

WP 288 **The Largest Blue-Shift of O-H Vibration Frequency Observed in the Gas Phase**; Xianglei Kong; *Nankai University, Tianjin, China*

WP 289 **Exploring Conformational Folding and Proton Migration within DNA Dinucleotide Cation-Radicals in the Gas Phase with UV Action Spectroscopy**; Andy Dang[1]; Frantisek Turecek[1]; Joe Korn[1]; Huong T.H. Nguyen[1]; Yang Liu[1]; Camille Houferak[1]; *[1]University of Washington, Seattle, WA*

WP 290 **Gas-Phase Ubiquitin Conformation Probed by Förster Resonance Energy Transfer (FRET) between Multiple Residue Pairs**; Jocky Chun Kui Kung[1]; Matthew Kusinski[1]; Martin F. Czar[1]; Benjamin Schuler[2]; Rebecca A. Jockusch[1]; *[1]University of Toronto; [2]University of Zurich, Switzerland*

WP 291 **Influence of a Peptide Composition on its Conformational Dynamics: Time-Resolved Pump-Probe Action Spectroscopy**; Luke MacAleese[1]; Mathilde Bouakil[1]; Philippe Dugourd[1]; *[1]Institut Lumière Matière, UMR5306 CNRS & Univ. Lyon 1, Villeurbanne, France*

WP 292 **Identification of Lasso and Branched-Cyclic Topoisomers Using Trapped Ion Mobility Spectrometry – Mass Spectrometry and Ion Spectroscopy**; Kevin Jeanne Dit Fouque[1]; Julian D. Hegemann[2]; Severine Zirah[3]; Sylvie Rebuffat[3]; Philippe Maitre[4]; Francisco Fernandez-Lima[1]; *[1]Florida International University, Miami, FL; [2]University of Illinois at Urbana-Champaign, Urbana, IL; [3]Laboratory Molecules of Communication and Adaptation of Microorganisms, National Museum of Natural History, Sorbonne Univ, Paris, France; [4]Laboratoire de Chimie Physique, UMR 8000, Université Paris Sud, Orsay, France*

WP 293 **IR Photons as Structural Probe for Transient Intermediates in Glycosylation**; Anouk M. Rijs; *Radboud University, FELIX Laboratory, Nijmegen, Netherlands*

WP 294 **Gas-Phase Conformational Investigation of 2′-Ribose Methylation on Protonated Pyrimidine Nucleosides**; Chenchen He[1]; Lucas A Hamlow[1]; Yanlong Zhu[1]; Yuan-wei Nei[1]; Lin Fan[1]; Christopher P. McNary[2]; Philippe Maitre[3]; Vincent Steinmetz[3]; Baptiste Schindler[4]; Isabelle Compagnon[4, 5]; Peter B. Armentrout[2]; Mary T. Rodgers[1]; *[1]Wayne State University, Detroit , MI; [2]University of Utah, Salt Lake City, UT; [3]Université Paris-Sud, Orsay, France; [4]Université de Lyon, Université Claude Bernard Lyon 1, France; [5]Institut Universitaire de France IUF, 103 Boulevard St Michel, France*

WP 295 **Characterization of Gas-Phase Conformations of Protonated Arabinose Nucleosides**; Lucas A. Hamlow[1]; Chenchen He[2]; Zachary J. Devereaux[2]; Harrison Roy[2]; Nathan Cunningham[2]; Erik Soley[2]; Justin K. Lee[2]; Giel Berden[3]; Jos Oomens[3]; Mary T. Rodgers[2]; *[1]Wayne State University, Detroit, MI; [2]Wayne State University, Detroit , MI; [3]Radboud University, FELIX Laboratory, Nijmegen, Netherlands*

WP 296 **IRMPD Spectroscopy Investigation of the Addition of Molecular Oxygen to Anionic U(V) Carboxylate Complexes**; Irena Tatosian[1]; Amanda R Bubas[1]; John K Gibson[2]; Jonathan Martens[3]; Giel Berden[3]; Jos Oomens[3]; Michael J. Van Stipdonk[1]; *[1]Duquesne University, Pittsburgh, PA; [2]Lawrence Berkeley Laboratory, Berkeley, CA; [3]Radboud University, FELIX Laboratory, Nijmegen, Netherlands*

WP 297 **IRMPD Studies of Non-Proteinogenic Peptides: The Shifts of Amide Bands**; Jianhua Ren[1]; Patrick M. Batoon[1]; Jos Oomens[2]; Giel Berden[3]; *[1]University of the Pacific, Stockton, CA; [2]Radboud University, FELIX Laboratory, Nijmegen, Netherlands; [3]Radboud University, FELIX Laboratory, Nijmegen, Netherlands*

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WP 298 **Semi-quantitative LC/ESI/MS Analysis Using Predictive Models of ESI Ionization Efficiencies**; Jaanus Liigand[1]; Anneli Kruve[1, 2]; Karl Kaupmees[1]; Piia Liigand[1]; Mari Ojakivi[1]; *[1]University of Tartu, Institute of Chemistry, Tartu, Estonia; [2]Free University of Berlin, Institute of Chemistry and Biochemistry, Berlin, Germany*

WP 299 **Investigating LTP ionization Products of Terpene Species via FT-ICR-MS and Twin-Trap-MS**; Björn Raupers[1]; Tassilo Muskat[1]; Jurgen Grotemeyer[1]; *[1]Christian-Albrechts-Univ, Kiel, Germany*

WP 300 **Crown Ethers Modulate the Location of Charge Carriers in Electrospray Droplets: Implications for the Mechanism of Protein Charging and Supercharging**; Haidy Metwally[1]; Lars Konermann[1]; *[1]Western University, London, ON, Canada*

WP 301 **Ionization Mechanism of Matrix-Assisted Ionization (MAI)**; Chuping Lee[1]; Sarah Trimpin[1]; Jien Lian Chen[2]; Chi-Kung Ni[2]; *[1]Department of Chemistry, Wayne State University, Detroit, MI; [2]Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan*

WP 302 **Exploration of Solvent Effect on the Reaction between Triazine and H2S Using Paper Spray Mass Spectrometry**; Weiwei Han[1]; Yue Ji[1]; Xiaoting Wang[1]; Zhiping Zhang[1]; *[1]Xi'an Shiyou University, Xi'an, China*

WP 303 **Measuring Masses of Intact Bacterial Macroions**; Shao-Yu Liang[1]; Avinash A. Patil[1]; Chou-Hsun Han[1]; Szu-Wei Chou[1]; Wen Chang[2]; Po-Chi Soo[3]; Huan-Cheng Chang[2]; Wen-Ping Peng[1]; *[1]National Dong Hwa University, Shoufeng, Hualien, Taiwan; [2]Academia Sinica, Taipei, Taiwan; [3]Tzu Chi University, Hualien, Taiwan*

WP 304 **Investigation of Fragmentation Processes during Atmospheric Pressure Laser Ionization**; Stefan Hellhake[1]; Alexander Haack[1]; Walter Wißdorf[1]; Hendrik Kersten[1]; Nils Helge Schebb[1]; Thorsten Benter[1]; *[1]University of Wuppertal, Wuppertal, Germany*

WP 305 **Investigations into the Decay Time of Corona Discharge Ionization through Spectroscopic Probing of a Pulsed Ionization Event**; Cassidy Crandell[1]; David Walker[2]; Luke Garcia[2]; Eric Davis[2]; *[1]Azusa Pacific University, Azusa, CA; [2]Department of Biology and Chemistry, Azusa Pacific University, Azusa, CA*

WP 306 **Systematic Investigation on Difference in (+) APPI Efficiency of Ortho, Meta, and Para Isomers**; Arif Ahmed[1]; Nissa Nurfajrin Solihat[2]; Thamina Acter[2]; Sunghwan Kim[2]; *[1]Kyungpook National University, Daegu, South Korea; [2]Kyungpook National University, Daegu, South Korea*

WP 307 **Ion-Solvent Interactions in nanoESI-MS: Characterization of Charge Depletion and Charge Conservation (Supercharging) Processes**; Christine Polaczek[1]; Alexander Haack[1]; Marco Thinius[1]; Walter Wissdorf[1]; Hendrik Kersten[1]; Thorsten Benter[1]; *[1]University of Wuppertal, Wuppertal, Germany*

WP 308 **Electrospray Droplet Exposure to Polar Organic Vapors Provides Evidence for Different Mechanisms for Native Versus Denatured Protein Ionization**; Andre Venter[1]; Richard B. Cole[2]; *[1]Western Michigan University, Kalamazoo, MI; [2]Sorbonne Université - Paris 06, Paris, France*

WP 309 **Capture of Electrochemically-Generated Fleeting Carbazolium Radical Cations and Elucidation of Carbazole Dimerization Mechanism by Mass Spectrometry**; Chengyuan Liu[1, 2]; Brian E Hivick[2]; Yang Pan[1]; Hao Chen[2]; *[1]National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei, China; [2]Center for Intelligent Chemical Instrumentation, Department of Chemistry and Biochemistry, and Edison Biotechnology Institute, Ohio University, Athens, OH*

WP 310 **Supercharging through the Looking Glass: The Use of Silicon-Based Supercharging Reagents in Electrospray Ionization Mass Spectrometry**; Jacob M. Shaner[1]; Daniel N. Mortensen[1]; David V. Dearden[1]; *[1]Brigham Young University, Provo, UT*

WP 311 **Enhanced Protonation of Fatty Acids, Bile Acids, and Steroids Using Chromium(III) Nitrate during Electrospray Ionization Mass Spectrometry**; Matthew Mireles[1]; Carolyn J. Cassady[1]; *[1]University of Alabama, Tuscaloosa, AL*

WP 312 **How is the Equilibrium Constant of a Non-Covalently Bound Protein Assembly Affected by The Droplet Environment?**; Styliani Consta; *University of Western Ontario, London*

WP 313 **Spectroscopic and Total Ion Current Characterization of Electrospray/Coronaspray Ionization with Respect to Dissolved Analyte Species and Sheath Gas Composition**; Molly Gibney[1]; David Walker[1]; Nathan Michael Hoffman[2]; Brian H Clowers[2]; Eric Davis[1]; *[1]Department of Biology and Chemistry, Azusa Pacific University, Azusa, CA; [2]Department of Chemistry, Washington State University, Pullman, WA*

FUNDAMENTALS: METAL ION CATIONIZATION, METAL-LIGAND INTERACTIONS, CATALYSIS
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WP 314 **Using Chromium(III) Complexes and Salts to Enhance Peptide Protonation by Electrospray Ionization**; Xinyao Jing[1]; Kyle Edwards[1]; John B. Vincent[1]; Carolyn J. Cassady[1]; *[1]The University of Alabama, Tuscaloosa, AL*

WP 315 **A Mass Spectrometric Study of Tripeptides Cationized by Tripositively-charged Lanthanide Ions**; Yating Wang[1]; K. W. Michael Siu[1, 2]; Alan C. Hopkinson[1]; *[1]York University, Toronto; [2]University of WIndsor, Windsor, On*

WP 316 **Acenitobactin-FeIII Complexes – Pre, SN2, and Oxidized Forms: an Empirical and Theoretical Study**; Daryl Giblin[1]; Justin Shapiro[2]; Tabbetha Bohac[1]; Michael L. Gross[1]; Timothy Wencewicz[1]; *[1]Washington University, St. Louis, St. Louis, MO; [2]Emory University, Antlanta, Georgia*

WP 317 **Investigating Ligand Effect on the Oxidative Addition Reactivity of Low Valent Metal Complexes Using a Modified LTQ Mass Spectrometer**; Mariah Parker[1]; Scott Gronert[1]; *[1]Virginia Commonwealth University, Richmond, VA*

WP 318 **Mechanistic study of C-H Activation by Using a Cationic Iridium(III) Dichloride Phenanthroline Complex**; Rozalie Sharon Corea[1]; Scott Gronert[1]; *[1]Virginia Commonwealth University, Richmond, VA*

WP 319 **Synthesis and Reactivity of Zero-Valent Metal Complexes in the Gas Phase**; Michael Borrome[1]; Malissa Grose[1]; Scott Gronert[1]; *[1]Virginia Commonwealth University, Richmond, VA*

WP 320 **The Generation of Exotic Anions Such as [AlH4]-, [SrH3]-, [Pb(0)H]-, [SbH2]-, [Bi(I)H2]-, and Bi- in Gas Phase Manifests Period**; Zhaoyu Zheng; *Stevens Institute of Technology, Hoboken, NJ*

WP 321 **Gas Phase C-C Reactions of Functionalized Alkanes Catalyzed by Nickel Complexes**; Elettra L. Piacentino[1]; Edwin Rodrigues[1]; Thomas M. Gilbert[1]; Victor Ryzhov[1]; *[1]Northern Illinois University, Dekalb*

WP 322 **Biological Light Bulbs: Mass Spectrometry for the Study of Lanthanide Metal-Ligand Complexes Conjugated to Peptides and Proteins**; Jackie Mosely; *Durham University, Durham, UK*

WP 323 **Olefin Production from Carboxylic Acids via Decarbonylation of Pd(II) Ternary Complexes in the Gas Phase**; Kenneth Mundorf[1]; Elettra L. Piacentino[2]; Richard A. J. O'hair[3]; Victor Ryzhov[2]; *[1]Northern Illinois University, DEKALB; [2]Northern Illinois University, Dekalb; [3]University of Melbourne, Victoria, Australia*

WP 324 **Fragmentation of N-Terminally Derivatized Peptides Cationized with Cu2+**; Susan Kline[1]; Amanda Bubas[1]; Michael J. Van Stipdionk[1]; *[1]Duquesne University, Pittsburgh, PA*

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WP 325 **Whole Gut Lavage Fluid Fractionation Using COmbination HILIC/C-18 LC/MS/MS Demonstrates Robust Coverage of Glycopeptides and Potential for Biomarker Discovery Applications**; Crystal Daniels[1]; Lewis Pannell[1]; *[1]Mitchell Cancer institute, Mobile, AL*

WP 326 **Combined LC-MS/MS and Hybrid Search Facilitates the Structural Elucidation of N/O Glycopeptides in NIST Human Plasma Standard Reference Material 1950**; Connie Remoroza[1]; Meghan C. Burke[1]; Yuxue Liang[1]; Stephen E. Stein[1]; *[1]NIST, Gaithersburg, MD*

WP 327 **Comprehensive Domain-Specific [Fc vs. Fab] N-Glycosylation Analysis of Therapeutic Proteins**;

Charles Nwosu[1]; Shuangqi Sally Liu[2]; Lei Wang[2]; May Zhu[2]; Anne Kowal[2]; *[1]Takeda Pharmaceuticals International Co, Cambridge, MA; [2]Takeda Pharmaceuticals International Co., Cambridge, MA*

WP 328 **Cold Spray Ionization Mass Spectrometry Preserves Labile Protein Glycosylation**; Natalia Gasilova[1]; Daniel Ortiz[2]; Yury O. Tsybin[3]; Laure Menin[2]; *[1]EPFL SB ISIC-GE, Sion, Switzerland; [2]EPFL SB ISIC-GE, Lausanne, Switzerland; [3]Spectroswiss, Lausanne, Switzerland*

WP 329 **Mass Spectrometry-Based Characterization of Recombinant Human Immunodeficiency Virus Type 1 (HIV-1) Envelope Glycoprotein Vaccine**; Vaneet Kumar Sharma; *International AIDS Vaccine Initiative (IAVI), New York, NY*

WP 330 **Differentiation of α2,3 and α2,6 Sialic Acid-Linked Glycan Isomers Using Differential Mobility Spectrometry**; Catherine S Lane[1]; Kirsty McManus[2]; Philip Widdowson[2]; Sarah A Flowers[3]; Gerard Powell[2]; Ian Anderson[2]; J. Larry Campbell[4]; *[1]SCIEX, Warrington, UK; [2]Allergan Biologics Limited, Liverpool, UK; [3]Georgetown University, Washington Dc, DC; [4]SCIEX, Concord, ON, Canada*

WP 331 **Parallel Reaction Monitoring of Fucosylated Glycopeptides in Alpha-Fetoprotein Immunoprecipitated from Hepatocellular Carcinoma Serum**; Kwang Hoe Kim[1, 2]; Heeyoun Hwang[2]; Ju Yeon Lee[1]; Eun Sun Ji[1]; Hyun Joo An[2]; Soo-Youn Lee[3]; Jin Young Kim[1]; Jong Shin Yoo[1]; *[1]Korea Basic Science Institute, Cheongju, South Korea; [2]Chungnam national university, Daejeon, South Korea; [3]Sungkyunkwan University School of Medicine, Seoul, South Korea*

WP 332 **High Throughput Characterization of Site-specific Glycoforms by a Virtual Multistage Mass Spectrometry Method**; Hongqiang Qin[1]; Yao Chen[2]; Jiawei Mao[2]; Mingliang Ye[2]; *[1]Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China; [2]457 Zhongshan Road, Dalian, Dalian City, China*

WP 333 **Towards universal Glycoproteome Analysis Using pGlycoNovo: Intact N-glycopeptide Profiling Across Seven Model Species**; Mingqi Liu[1]; Wen-Feng Zeng[2]; Weiqian Cao[3]; huali shen[3]; si-min he[2]; pengyuan yang[3]; *[1]Fudan University, Shanghai, China; [2]Institute of Computing Technology, Chinese Academy of Sciences, Beijing, China; [3]Fudan Universiry, Shanghai, China*

WP 334 **Urinary Glycoproteomics Identify Novel Putative Host Defense Factors for UTI**; John Froehlich[1, 2]; Richard Lee[1, 2]; *[1]Children's Hospital Boston, Boston, MA; [2]Harvard Medical School, Boston, MA*

WP 335 **Comprehensive Evaluation of Sample Preparation Protocols and Multistep Enrichment for Extraction of N- and O- Glycopeptides from Breast Cancer Cells**; Fengfei Ma[1]; Kellen DeLaney[2]; Matthew Glover[1]; Fabao Liu[3]; Wei xu[3]; Lingjun Li[1]; *[1]School of Pharmacy, University of Wisconsin-Madison, Madison, WI; [2]Department of chemistry University of Wisconsin Madison, Madison, Wisconsin; [3]University of Wisconsin–Madison, Madison, WI*

WP 336 **GlikeN: A New Bioinformatic Tool to Evaluate Biosimilarity of Antibody Drugs Using Intact Glycoprotein Analysis with LC-MS/MS**; Heeyoun Hwang[1, 2]; Unyong Kim[3]; Youngsuk Seo[1, 2]; Myung Jin Oh[1, 2]; Hyun Joo An[1, 2]; *[1]Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, South Korea; [2]Asia-Pacific Glycomics Reference Site, Chungnam National University, Daejeon, South Korea; [3]Glycan Co. Ltd., Sungnam, South Korea*

WP 337 **Systematic Evaluation of Chemical Labeling-Based Quantitative Glycoproteomics**; Pan Fang[1]; Yanlong Ji[1, 2]; Kuan-Ting Pan[1]; Henning Urlaub[1, 3]; *[1]Max-Planck Inst for Biophysical Chemistry, Goettingen, Germany; [2]Johann Wolfgang Goethe University, Frankfurt am Main, Germany; [3]Department of Clinical Chemistry, University Medical Center Goettingen, Goettingen, Germany*

WP 338 **Site-specific Glycosylation of Flu Hemagglutinin H4**; Lisa M Parsons[1]; John F. Cipollo[1]; *[1]FDA, Silver Spring, MD*

WP 339 **Computationally Efficient Strategy to Generate Multiple Glycopeptide Decoys on Demand**; Josh Shipman[1]; Xiaomeng Su[1]; David Hua[1]; Heather Desaire[1]; *[1]University of Kansas, Lawrence, KS*

WP 340 **Analysis of Fragmented Porcine Immunoglobulin G (IgG) by MALDI-MS and UPLC-ESI-MS**; Helene Perreault[1]; Claudia Nelson[2]; *[1]University of manitoba, Winnipeg; [2]University of Manitoba, Winnipeg, MB, Canada*

WP 341 **Microwave-Assisted Pronase Digestion Allowing Efficient Release of O-Glycans for Sensitive LC-MS/MS Analysis**; Parvin Mirzaei[1]; Andrew cho[1]; Mona goli[1]; Yehia mechref[1]; *[1]Texas Tech University, Lubbock, TX*

WP 342 **A Novel O-Glycoprotease with Applications in O-glycan Analysis Using Mass Spectrometry**; Rolf Lood[1, 2]; Maria Nordgren[1]; Fredrik Leo[1]; Stephan Björk[1]; Malin Mejáre[1]; Fredrik Olsson[1]; *[1]Genovis AB, Lund, Sweden; [2]Department of Infectious Diseases, Lund University, Lund, Sweden*

WP 343 **Quantification and Identification of Glycan from Proteins with Multiple Glycosylation Sites with Automated LC-MS Data Processing**; Sven Bahrke[1]; Robert Wilmanowski[1]; *[1]Glycotope GmbH, Berlin, Germany*

WP 344 **Comprehensive Glycopeptide Profiling in Blood Plasma for Clinical Applications**; Hans JCT Wessels[1]; Anouk Suppers[1]; Maurice van Dael[1]; Koen Rademaker[1]; Esther Willems[1]; Nurulamin Abu Bakar[1]; Monique van Scherpenzeel[1]; Dirk J Lefeber[1]; Alain J Van Gool[1]; *[1]Radboudumc, Nijmegen, Netherlands*

WP 345 **A Rapid, Streamlined Workflow for Glycan Sample Preparation and Analysis by LC-MS**; Judy Boland[1]; Nicolas Caffarelli[1]; Amber Henry[1]; Gordon Nicol[1]; Jeffrey Turner[1]; Kevin Ray[1]; *[1]MilliporeSigma, St. Louis, MO*

WP 346 **Glycoproteomics Analysis of Plasma Membrane Proteins in Mammalian Glioma by MALDI-TOF/TOF MS and nLC-ESI-QTOF-MS**; Milan Teraiya[1, 2]; Emy Komatsu[1]; Jenna Noordenbos[2]; Helene Perreault[1]; Vincent Chen[2]; *[1]University of Manitoba, Winnipeg, MB, Canada; [2]Brandon University, Brandon, MB, Canada*

WP 347 **Energy-Resolved Collision-Induced Dissociation of Protonated O-Linked Glycopeptides**; Maia I Kelly[1]; Eric D Dodds[1]; *[1]University of Nebraska - Lincoln, Lincoln, NE*

WP 348 **Deciphering the Role of Protein N-Glycosylation on Collagen-Protein Interactions**; Christian Toonstra[1]; Yingwei Hu[1]; Hui Zhang[1]; *[1]Johns Hopkins School of Medicine, Baltimore, MD*

WP 349 **Site-Specific Glycosylation Analysis of Influenza A/H1N1/09 Neuraminidaseexpressed in Human and Insect Cells**; Shisheng Sun; *Northwest University, Xi'an, China*

WP 350 **Deciphering Complex O-Glycosylation: Solid-Phase Chemoenzymatic Cleavage and Enrichment**; Shuang Yang[1]; Philip Onigman[2]; Jonathan Sjogren[2]; Wells W. Wu[3]; Rong-fong Shen[3]; John Cipollo[1]; *[1]LBP, CBER, FDA, Silver Spring, MD; [2]Genovis AB Inc., Boston, MA; [3]FBR, CBER, FDA, Silver Spring, MD*

H/D EXCHANGE: PROTEIN STRUCTURE/FUNCTION
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WP 351 **Uncovering a Dynamic Immunogen's Structure and Epitope Exposure Using HDX-MS**; Edgar A Hodge[1]; Mark Benhaim[1]; Brooke Nickerson[1]; Kelly Lee[1]; Neil King[1]; David Baker[1]; Laurent Perez[1]; Jessica Marcandalli[1]; *[1]University of Washington, Seattle, WA*

WP 352 **Tracking the Sequence of Conformational Changes in a Viral Membrane Fusion Protein by Pulse Labeling Hydrogen/Deuterium-Exchange Mass Spectrometry**;

Mark Benhaim[1]; Natalie K Garcia[1]; Miklos Guttman[1]; Kelly Lee[1]; *[1]University of Washington, Seattle, WA*

WP 353 **Thermally Activated Conformational Motions of Wild-Type and Mutant Enolase Studied Using Hydrogen/Deuterium Exchange Mass Spectrometry**; Anthony T. Iavarone[1]; Emily J. Thompson[1]; Judith P. Klinman[1]; *[1]UC Berkeley, Berkeley, CA*

WP 354 **Investigating Bone Remodeling Proteins by HDX-MS: Ligand Interactions of Monomeric and Dimeric OPG**; Yiming Xiao[1]; Ding Xu[2]; Lars Konermann[1]; *[1]University of Western Ontario, London, ON, Canada; [2]University at Buffalo, Buffalo, NY*

WP 355 **Studying the Aggregation Propensity of Glyco-Engineered Plant Produced Anti-Rabies Monoclonal Antibodies Using HDX-MS**; Sindisiwe G. Buthelezi[1, 2]; Lennart Martens[3]; Heini W. Dirr[2]; Tsepo Tsekoa[1]; Elien Vandermarliere[3]; Stoyan Stoychev[1]; *[1]Council for scientific and industrial research, Pretoria, South Africa; [2]University of the Witwatersrand, Johannesburg, South Africa; [3]Ghent University, Ghent, Belgium*

WP 356 **Epitope Identification and Conformational Characterization of IgG2 Disulphide Isoforms Interaction with Anti-Human IgG2 mAb by Hydrogen Deuterium Exchange Mass Spectrometry**; Devrishi Goswami[1]; Thomas Dillon[1]; Jun Zhang[1]; Michael Treuheit[1]; Ping Yeh[1]; *[1]Amgen, Thousand Oaks, CA*

WP 357 **Examining the Interaction between Cytochrome P450 Reductase and Heme Oxygenase 2 via Hydrogen Deuterium Exchange Mass Spectrometry**; Brent Kochert[1]; Angela S. Fleischhacker[2]; Stephen W. Ragsdale[2]; John R. Engen[1]; *[1]Northeastern University, Boston, MA; [2]University of Michigan, Ann Arbor, MI*

WP 358 **Investigating the Conformational and Dynamic Aspects of Beta-Lactamases Inhibitory Resistance by Integrated Mass Spectrometric Approaches**; Liwen Huang[1]; Pui-Kin So[1]; Yun-Chung Leung[1]; Zhongping Yao[1]; *[1]Department of Applied Biology and Chemical Technology, The Hong Kong Polytechnic University, China*

WP 359 **Structural Basis for Ligand and Inhibitor Binding in Cytochrome BD-Oxidases Revealed by HDX-MS**; Martin L. Eisinger[1]; Schara Safarian[1]; Kristina Desch[1]; Hideto Miyoshi[2]; Junshi Sakamoto[3]; Hartmut Michel[1]; Julian D Langer[1, 4]; *[1]Max Planck Institute of Biophysics, Frankfurt, Germany; [2]Kyoto University, Kyoto, Japan; [3]Kyushu Institute of Technology, Iizuka, Japan; [4]Max Planck Institute for Brain Research, Frankfurt, Germany*

WP 360 **Application of Differential Hydrogen/Deuterium Exchange Mass Spectrometry to Support a Proposed Mechanism of Vitamin D Receptor Antagonism**; Ryan Stites[1]; Keith R Stayrook[1]; James Patrick Steele[1]; Scott J Novick[2]; Bruce D Pascal[2]; Michael Chalmers[1]; Patrick R. Griffin[2]; Jeffrey A Dodge[1]; *[1]Eli Lilly and Company, Indianapolis; [2]The Scripps Research Institute, Jupiter, Florida*

WP 361 **Programming Water Transporter Aquaporin Z by Lipid Composition-altered Protein Dynamics**; Xin Shan Lim; *National University of Singapore, singapore, Singapore*

WP 362 **The Application of Hydrogen Deuterium Exchange Mass Spectrometry in Biopharmaceutical Comparability Study with Statistical Analysis**; Hanwei Zhao[1]; Yaping Sun[1]; Paul Salinas[1]; Scott Li[1]; Bernice Yeung[1]; Chris Barton[1]; *[1]Shire, Lexington, Massachusetts*

WP 363 **The Effects of Deamidation on the Conformation of γS-Crystallin Probed by HDX MS**; Charles Mundorff[1]; Calvin Vetter[2]; Thomas E. Wales[1]; John R Engen[1]; Kirsten J Lampi[2]; Larry L David[2]; *[1]Northeastern University, Boston, MA; [2]OHSU, Portland, OR*

WP 364 **Determining the Potential Deuterium Uptake Regions of Monoclonal Antibody Fragment Using Hydrogen Deuterium Exchange Mass Spectrometry**; Gencer Kaan Akyüz[1]; Baran Dingiloglu[1]; Duygu Yalcinkaya[1]; Gizem Dinler Doganay[1]; *[1]Istanbul Technical University, istanbul, Turkey*

WP 365 **Dynamics of Viron Capsid and its Implications for Antibody Interactions Captured by Amide Hydrogen/Deuterium Exchange Mass Spectrometry**; Ganesh S Anand[1]; Xin Xiang Lim[1]; *[1]NUS Singapore, Singapore, Singapore*

WP 366 **The Action of Molecular Machines Revealed by HX-MS**; Xiang Ye[1]; Leland Mayne[1]; S.Walter Englander[1]; *[1]University of Pennsylvania, Philadelphia, PA*

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WP 367 **Multimodal Lipidomic Imaging of Germinal Center Microenvironments in Spleen Utilizing MALDI FT-ICR IMS, IHC, and Autofluorescence Microscopy**; Marissa Jones[1, 2]; Nathan Heath Patterson[2, 3]; William J. Perry[1, 2]; Sung Hoon Cho[4]; Mark R. Boothby[4, 5, 6, 7, 8]; Jeffrey M. Spraggins[1, 2, 3]; Richard M. Caprioli[1, 2, 3, 5, 8]; *[1]Department of Chemistry, Vanderbilt University, Nashville, TN; [2]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [3]Department of Biochemistry, Vanderbilt University, Nashville, TN; [4]Department of Pathology, Microbiology and Immunology, School of Medicine, Vanderbilt University, and Vanderbilt University Medical Center, Nashville, TN; [5]Department of Medicine, Vanderbilt University, Nashville, TN; [6]Department of Cancer Biology, Vanderbilt University, Nashville, TN; [7]Vanderbilt-Ingram Cancer Center, Vanderbilt University, Nashville, TN; [8]Department of Pharmacology, Vanderbilt University, Nashville, TN*

WP 368 **Multifaceted Imaging Approach for Liposomal Drug Delivery in Tumor Spheroids**; Jessica K. Lukowski[1]; William T. Andrews[1]; Amanda B. Hummon[2]; *[1]University of Notre Dame, Notre Dame, IN; [2]Ohio State University, Columbus, OH*

WP 369 **A Promising Pathway in Immuno-Oncology: CD73-Adenosine Axis Highlighted by Quantitative Mass Spectrometry Imaging**; Lauranne Poncelet[1]; Rima Ait-Belkacem[1]; Bruno Gomes[2]; Jonathan Stauber[1]; *[1]Imabiotech, Loos, France; [2]Iteos, Gosselies, Belgium*

WP 370 **Impact of IDO Inhibitor on Tryptophan&Kynurenine Pathway Reflected in the Tumor Microenvironment and Highlighted Using Quantitative Mass Spectrometry Imaging**; Lauranne Poncelet[1]; Rima Ait-Belkacem[1]; Bruno Gomes[2]; Gregory Hamm[1]; Jonathan Stauber[1]; *[1]Imabiotech, Loos, France; [2]Iteos, Gosselies, Belgium*

WP 371 **Analysis of Fungicides on Plant Leaves with LAESI-Mass Spectrometry Imaging (MSI) and LC-MS**; Erin Gemperline[1]; Suresh Annangudi[1]; Todd Mathieson[1]; Mariela Fernandez[1]; John Atkinson[1]; Courtney Gallup[1]; Jinglin Liu[1]; *[1]Dow-DuPont, Indianapolis, IN*

WP 372 **Visualizing Metabolites in Plant-Pathogen and Plant-Herbivore Interactions with High-Resolution AP-MALDI MSI**; Dhaka Ram Bhandari[1]; Sven Gottwald[1]; Georg Petschenka[2]; Andreas Römpp[3]; Bernhard Spengler[1]; *[1]Institute of Inorganic and Analytical Chemistry, Justus Liebig University Giessen, Heinrich-Buff-Ring 17, Giessen, Germany; [2]Institute of Insect Biotechnology, Justus Liebig University Giessen, Heinrich-Buff-Ring-58, Giessen, Germany; [3]Chair of Bioanalytical Sciences and Food Analysis, University of Bayreuth, Universitätsstr.-30, Bayreuth, Germany*

WP 373 **DESI-MS of Accelerated Aged Energetic Material and Encapsulant Systems**; Christina L Crawford; *Sandia National Laboratories, Albuquerque, NM*

WP 374 **MALDI-Mass Spectrometric Imaging for the Investigation of Metabolites in Linum Usitatissimum L. Roots Inoculated with Fusarium Oxysporum**; Gleb Vladimirov[1, 2]; Nataliya Melnikova[3]; Alexey Dmitriev[3]; Nadezhda Bolsheva[3]; Roman Novakovskiy[3]; Alexander

Zherebker[1]; Artur Yablokov[2, 4]; Eugene (Evgeny) Nikolaev[1]; *[1]Skolkovo institute of science and technology, Moscow Region, Russian Federation; [2]Institute of Energy Problems of Chemical Physics, Russian Academy of Sciences, Moscow, Russia; [3]Engelhardt Institute of Molecular Biology, Russian Academy of Sciences, Moscow, Russia; [4]Moscow Infectious Clinical Hospital № 2, Moscow, Russia*

WP 375 **Integrated MALDI Imaging and LC/MS Workflow for Spatial Lipidome Analysis of Liver Tissues**; Bindesh Shrestha[1]; Hernando Olivos[1]; Qi Li[2]; Xinmin Yin[2]; Wenke Feng[2]; Xiang Zhang[2]; *[1]Waters Corp., Beverly, MA; [2]University of Louisville, Louisville, KY*

WP 376 **Monoamine Mapping by Mass Spectrometry Identified Brain Nuclei Regulating Anxiety in a Serotonin Deficiency Model**; Yuki Sugiura[1]; Eiji Sugiyama[1]; *[1]Keio University, Tokyo, Japan*

WP 377 **AP-SMALDI MSI of lipids in Schistosoma Mansoni Parasites**; Patrik Kadesch[1]; Thomas Quack[2]; Stefanie Gerbig[1]; Katharina Henrich[1]; Tobias Hollubarsch[1]; Christoph G. Grevelding[2]; Bernhard Spengler[1]; *[1]Institute of Inorganic and Analytical Chemistry, Justus Liebig University Giessen, Giessen, Germany; [2]Institute of Parasitology, Justus Liebig University, Giessen, Germany*

WP 378 **Multimodal Mass Spectrometry Imaging Pipelines for Large Oncology Studies Across Multiple Sites**; Rory T. Steven[1]; Andrew D. Campbell[2]; Yulia Panina[1, 3]; Alex Dexter[1]; James S. McKenzie[4]; Stephanie Ling[5]; Spencer A. Thomas[1]; Adam J. Taylor[1]; Paolo Inglese[4]; Arafath K Najumudeen[2]; Jean-Luc Vorng[1]; Gregory Hamm[5]; Rasmus Havelund[1]; Renata Filipe-Soares[4]; Efstathios Elia[1]; David Gay[2]; Teresa Murta[1]; Bin Yan[1]; Chelsea Nikula[1]; Ala Al-Afeef[1]; Tingting Fu[1]; Robin Philip[1]; Ian S Gilmore[1]; Mariia O. Yuneva[3]; Richard J.A. Goodwin[5]; Zoltan Takats[4]; Owen J. Sansom[2]; Josephine Bunch[1]; *[1]National Physical Laboratory, Teddington, UK; [2]Cancer Research UK Beatson Institute, Glasgow, UK; [3]The Francis Crick Institute, London, UK; [4]Imperial College, London, UK; [5]AstraZeneca, UK, Cambridge, UK*

WP 379 **High Resolution Single Cell Imaging of Phospholipids by a Combination of GCIB-ToF-SIMS with Fluorescence Microscopy**; L.J. Sparvero[1, 2]; Hua Tian[3]; Andrew A. Amoscato[1, 2]; Simon C. Watkins[4]; Nicholas Winograd[3]; Valerian E. Kagan[1, 2, 5]; Hülya Bayır[1, 2, 6]; *[1]Department of Environmental and Occupational Health, University of Pittsburgh, Pittsburgh, PA; [2]Center for Free Radical Research and Antioxidant Health, University of Pittsburgh, Pittsburgh, PA; [3]Department of Chemistry, Pennsylvania State University, State College, PA; [4]Departments of Cell Biology and Immunology, University of Pittsburgh, Pittsburgh, PA; [5]Departments of Chemistry, Pharmacology and Chemical Biology, University of Pittsburgh, Pittsburgh, PA; [6]Department of Critical Care Medicine and Safar Center for Resuscitation Research, University of Pittsburgh, Pittsburgh, PA*

WP 380 **Enhancing the MALDI MS Signal of 2-Arachidonoylglycerol in Tissues by Imaging MS Through Chemical Derivatization with Betaine Aldehyde**; Lisa Manier[1]; Michelle L. Reyzer[1, 2]; Michael D. Tuck[1]; Jennifer L. Harvey[1]; Philip J. Kingsley[2]; Gaurav Bedse[3]; Sachin Patel[3]; Richard M. Caprioli[1, 2, 4, 5]; *[1]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [2]Department of Biochemistry, Vanderbilt University, Nashville, TN; [3]Department of Psychiatry and Behavioral Sciences, Vanderbilt University Medical Center, Nashville, TN; [4]Department of Chemistry, Vanderbilt University, Nashville, TN; [5]Department of Pharmacology and Medicine, Vanderbilt University, Nashville, TN*

WP 381 **Imaging Mass Spectrometry Analysis of lipid Changes in the Human Ocular Lens with Aging**; Md Amir Hossen[1]; David M.G. Anderson[1]; Kevin L. Schey[1]; *[1]Department of Biochemistry, Vanderbilt University, Nashville, TN, Nashville, Tennessee*

WP 382 **A Matrix-Mediated Selective Ionization Strategy for Lipidomics Mapping of DB/DB Mouse Brain by MALDI-MS Imaging**; Jianing Wang[1]; Xianlin Han[1]; *[1]University of Texas Health Science Center, San Antonio, Texas*

WP 383 **Implementing Multimodal Mass Spectrometry Imaging to Explore the Molecular Interactions within Environmental Microbiomes**; Dusan Velickovic[1]; Rosalie K. Chu[1]; Alyssa A Carrell[2]; Ljiljana Pasa Tolic[1]; Roeland L Berendsen[3]; David J Weston[4]; Christopher R Anderton[1]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]Oak Ridge National Laboratory, Oak Ridge, TN; [3]Utrecht University, Utrecht, Netherlands; [4]Oak Ridge National Laboratory, Oakridge, TN*

WP 384 **Comparative MALDI-Based Imaging Mass Spectrometry of Potato Psyllids Infected with Candidatus Liberibacter Solanacearum to Uninfected Insects**; Jing Wang[1]; David R Gang[1]; *[1]Washington State University, Pullman, WA*

WP 385 **Lipid dynamics in Mosquito Ovaries Using Mass Spectrometry Imaging**; Anthony Castellanos[1]; Mario E Gomez-Hernandez[1]; Veronika Michalkova[2]; Marcela Nouzova[2]; Fernando Noriega[2]; Francisco A Fernandez-Lima[2]; *[1]Florida International University, Miami, FL; [2]Florida International University, Miami*

WP 386 **Analyses of Minor Chemical Components of Ostrich Eggshell by MALDI-Imaging Mass Spectrometry**; Akiko Kubo[1]; Taku Ito[1]; Suguru Kato[1]; Masaya Nakata[1]; Yoko Saikawa[1]; Makoto Suematsu[1]; *[1]Keio University, Tokyo, Japan*

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WP 387 **Low Temperature Catalytic Combustion Reactor for Gas Chromatography Isotope Ratio Mass Spectrometry**; Herbert Tobias[1]; Andrew Jones[2]; Charlie Spanjers[2]; J. Thomas Brenna[1]; *[1]University of Texas at Austin, Austin, TX; [2]Activated Research Company, Eden Prairie, MN*

WP 388 **Exploring the Size Limit and Range of Compounds Amenable for Electron Ionization LC-MS**; Svetlana Tsizin[1]; Tal Alon[1]; Alexander B. Fialkov[1]; Aviv Amirav[1]; *[1]Tel-Aviv University, Tel-Aviv, Israel*

WP 389 **Coxiella Burnetii Proteome Analyzed by µ-Pillar Arrayed Columns**; Goran Mitulovic[1]; Maksym Danchenko[2]; Gabriela Flores Ramírez[3]; *[1]Medical University of Vienna, KIMCL, Vienna, Austria; [2]Institute of Virology, Biomedical Research Center, Bratislava, Slovakia; [3]Department of Rickettsiology Institute of Virology Slovak Academic of Science, Bratislava, Slovakia*

WP 390 **Design and Performance of a Dual-Polarity Instrument for Soft-Landing of Mass-Selected Ions**; Pei Su[1]; Hang Hu[1]; Jonas Warneke[1]; Mikhail Belov[2]; Gordon A. Anderson[3]; Julia Laskin[1]; *[1]Department of Chemistry, Purdue University, West Lafayette, IN; [2]Spectroglyph, LLC, Kennewick, WA; [3]GAA Custom Engineering, LLC, Benton City, WA*

WP 391 **High Velocity Impact Fragmentation Pathways of Neutral Molecules in Flyby and Orbiter Mass Spectrometers**; Brandon Turner[1]; Logan Sweet[2]; Eric Sevy[1]; Daniel Austin[1]; *[1]Brigham Young University, Provo, UT; [2]Brigham Young University-Idaho, Rexburg, ID*

WP 392 **Dual Polarity Ion Confinement and Ion Mobility Separations in Traveling Wave-Based Structures for Lossless Ion Manipulations (SLIM)**; Isaac Kwame Attah[1]; IAN K. WEBB[1]; Yehia M. Ibrahim[1]; Christopher D. Chouinard[1]; Gabe Nagy[1]; Sandilya Garimella[1]; Richard D. Smith[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

WP 393 **Ion Mobility Electrophoresis: A Novel Separation and Biomolecule 3D Structure Analysis Technique**; Muyi He[1]; Xiaofeng Wang[2]; Pan Luo[3]; Jie Hong[1]; Rongkai Zhang[1]; Haimei Wu[1]; Ye Xiang[4]; Wei Xu[1]; *[1]Beijing Institute*

of Technology, Beijing, China; [2]Institute of High Energy Physics, Chinese Academy of Sciences, Beijing, China; [3]Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China; [4]Tsinghua University, Beijing, China

WP 394 **Droplet Capture Tip-enhanced Laser Ablation Sampling for Mass Spectrometry**; Fan Cao[1]; Fabrizio Donnarumma[1]; Kermit K Murray[1]; *[1]Louisiana State University, Baton Rouge, LA*

WP 395 **Dipole Tunnel as a Novel Ion Guide to Maximize the S/N in a Mass Spectrometer**; Xiaoqiang Zhang[1]; Keke Wang[1]; Qiao Jin[1]; Siyu Wu[1]; Lin Liu[1]; Xu Zhou[1]; Wenjian Sun[1]; *[1]Shimadzu Research Laboratory (Shanghai) Co., Ltd., Shanghai, China*

WP 396 **A Computational Fluid Dynamics Study of a Pulsed Hydrogen Atom Gun for Ion Activation-Dissociation on the Omnitrap Platform**; Athanasios Zacharos[1]; Dimitris Papanastasiou[1]; Ioannis Nikolos[2]; Roman Zubarev[3]; *[1]Fasmatech, Athens, Greece; [2]School of Production Engineering & Management, TUC, Chania, Greece; [3]Karolinska Institutet, Stockholm, Sweden*

WP 397 **Soft Ionization of Volatile Organic Compounds Using a Novel Dual Mode Electron Ionization Source**; Anna Kornilova[1]; Lisa Cousins[1]; Heather Gamble[1]; Chuck Jolliffe[1]; Marius Radu[1]; Dante Sanchez[1]; Mehrnaz Sarrafzadeh[1]; Harpreet Singh[1]; Victor Titov[1]; Dmitry Valyaev[1]; Reza Javahery[1]; *[1]PerkinElmer Inc., Woodbridge, ON, Canada*

WP 398 **GC-MS/MS with a Novel Plasma Source for Profiling and Identification of Hydrocarbons**; Mehrnaz Sarrafzadeh[1]; Reza Javahery[1]; Miles Snow[1]; Chuck Jolliffe[1]; *[1]PerkinElmer Inc., Woodbridge, ON, Canada*

WP 399 **Implementation of an Array of Traps and Ion Elevators in Structures of Lossless Ion Manipulations**; Aneesh Prabhakaran[1]; Sandilya Garimella[1]; Randolph V. Norheim[1]; Colby E. Schimelfenig[1]; Spencer A. Prost[1]; Cameron Giberson[1]; Yehia M. Ibrahim[1]; Richard D. Smith[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

WP 400 **Design and Performance of a Segmented Ion Trap with Inductive Detection used as a Charged Particle Mass Analyser**; Toby O Rose[1, 2]; Robert Appleby[1, 2]; Keith Richardson[3]; Peter Nixon[3]; Martin Green[3]; *[1]Cockcroft Institute, Daresbury, UK; [2]University of Manchester, Manchester, UK; [3]Waters Corporation, Wilmslow, UK*

WP 401 **Ion Source Multiplexing on a Single Mass Spectrometer**; Yury Kostyukevich[1]; Eugene (Evgeny) Nikolaev[2]; *[1]Russian Academy of Sciences, Moscow, Russian Federation; [2]Skolkovo institute of science and technology, Moscow Region, Russian Federation*

WP 402 **Development of a Novel LC Concept for Clinical Proteomics**; Nicolai Bache[1]; Philipp E Geyer[2]; Ole B Hoerning[1]; Lasse Falkenby[1]; Peter Treit[2]; Sophia Doll[2]; Igor Paron[2]; Florian Meier[2]; Ole Vorm[1]; Matthias Mann[2]; *[1]Evosep, Odense, Denmark; [2]Max-Planck Institute of Biochemistry, Martinsried, Germany*

WP 403 **Novel Integration of a Separation Column to an Ion Source for LC-MS**; Michael O Fogwill[1]; Wade P Leveille[1]; Jacob N Fairchild[1]; Joseph D Michienzi[1]; Theodore A Dourdeville[1]; Jeffrey Musacchio[1]; *[1]Waters Corporation, Milford, MA*

WP 404 **The Optimal Parameters of Flow Focusing Mechanism for Mass Spectrometry Tissue Imaging**; Vincen Wu[1]; Jocelyn Tillner[1]; Emrys Jones[2]; James McKenzie[1]; Dipa Gurung[3]; Anna Mroz[3]; Francesca Rosini[3]; Josephine Bunch[4]; Ian Gilmore[4]; Zoltan Takats[3]; *[1]Imperial College London, London, UK; [2]Waters, Wilmslow, UK; [3]Imperial College London, London, UK; [4]National Physical Laboratory, Teddington, UK*

WP 405 **Ion Transmission through dual Field Tapered Multipoles: Cyclone Ion Guide and Vortex Collision Cell**; Laura L. Pollum[1]; Haopeng Wang[1]; Kenneth R. Newton[1]; Shane E. Tichy[1]; *[1]Agilent Technologies, Inc., Santa Clara, CA*

WP 406 **Online Epitope Fishing nanoLC-MS/MS of Protein Biomarkers**; Maren Levernæs[1]; Ole Kristian Brandtzæg[2]; Elsa Lundanes[2]; Steven Ray Wilson[2]; Léon Reubsaet[1]; Trine Grønhaug Halvorsen[1]; *[1]Farmasoytisk Institute, Oslo, Norway; [2]Department of Chemistry, University of Oslo,, Oslo, Norway*

WP 407 **Fast Peptide Disulfide Bond Cleavage in Fused Silica Capillary by Using A UV Lamp**; Yixin Zhu[1]; Yu Gao[2]; John Yates[2]; Kai Tang[1]; *[1]Zhejiang Haochuang Biotech Co. Ltd., Hangzhou, China; [2]The Scripps Research Institute, La Jolla, CA*

WP 408 **Systematic Optimization and Validation of On-Line Supercritical Fluid Extraction/Supercritical Fluid Chromatography – Mass Spectrometry for Polyaromatic Hydrocarbons in Soil**; Alison P Wicker[1]; Kenichiro Tanaka[2]; Masayuki Nishimura[3]; Vivian Chen[3]; Tairo Ogura[3]; William Hedgepeth[3]; Kevin A. Schug[1]; *[1]University of Texas at Arlington, Arlington, TX; [2]Shimadzu Corporation, Kyoto, Japan; [3]Shimadzu Scientific Instruments Inc., Columbia*

WP 409 **Development and Validation of On-Line SFE-SFC-MS/MS Method for Screening of Aflatoxins B1, B2, G1 and G2 in Grain Matrices**; Jun Xiang Lee[1]; Udi Jumhawan[1]; Lin Min Lee[2]; Yun Wei Yat[2]; Sheot Harn Chan[2]; Tanaka Kenichiro[3]; Zhaoqi Zhan[1]; *[1]Shimadzu Asia Pacific, Singapore, Singapore; [2]Food Safety - Division, Health Sciences Authority, Singapore, Singapore; [3]Shimadzu corp., Kyoto, Japan*

WP 410 **Simulation Study of a U-shaped Mobility Analyzer for Multiple Operation Modes**; Keke Wang[1]; Kent Gillig[2]; Xiaoqiang Zhang[1]; Long Chen[3]; Wenjian Sun[1]; *[1]Shimadzu Research laboratory (Shanghai) Co. Ltd., Shanghai, China; [2]Academia Sinica, Taipei, Taiwan; [3]Nanjing University of Aeronautics and Astronautics, Nanjing, China*

WP 411 **Metabolomics Profile of the Stroke Induced Model using Blood-Brain Barrier of the Neurovascular Unit (NVU)**; Simona G Codreanu[1, 2]; Stacy D Sherrod[1, 2]; Jacquelyn A Brown[1, 3]; Diana M Neely[4, 5, 6]; Aaron B Bowman[4, 5, 6]; BethAnn McLaughlin[1, 3]; John P Wikswo[1, 3]; John A McLean[1, 2, 3]; *[1]Vanderbilt University, Nashville, TN; [2]Center for Innovative Technology, Vanderbilt University, Nashville, TN; [3]Vanderbilt Institute for Integrative Biosystems Research and Education, Nashville, TN; [4]Vanderbilt University Medical Center, Nashville, TN; [5]Vanderbilt Kennedy Center, Nashville, TN; [6]Vanderbilt Brain Institute, Nashville, TN*

WP 412 **Selective Extraction and Release of Peptides for Sensitive MS Analysis Using Self-Assembling Polymers**; Meizhe Wang[1]; Bo Zhao[1]; S. Thayumanavan[1]; Richard W. Vachet[1]; *[1]University of Massachusetts-Amherst, Amherst, MA*

WP 413 **Utility of QDa® Mass Detection for the Monitoring of Product Quality Attributes**; Monica Sadek[1]; Melissa Alvarez[1]; Nisana Andersen[1]; Christopher Yu[1]; *[1]Genentech Inc., South San Francisco, CA*

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WP 414 **The Difference in Modification Pattern of Hydrophobized Hyaluronan as Revealed by LC-IMS-MS**; Martina Hermannova[1]; Romana Šuláková[1]; Kristýna Šinovská[1]; Matěj Šimek[1]; Jaromír Kulhánek[1]; Petra Lišková[1]; Vladimír Velebný[1]; *[1]Contipro a.s., Dolni Dobrouc, Czech Republic*

WP 415 **Comparing Solution-Phase and Gas-Phase Protein Stability of a Homotetrameric Model System Using Ion Mobility and Differential Mobility Mass Spectrometry**; Lucienne Nouchikian[1]; Katherine A. Donovan[2]; Renwick C.J. Dobson[2]; Yves J.C. LeBlanc[3]; Derek J. Wilson[1]; *[1]York University, Toronto, ON, Canada; [2]Biomolecular Interaction Centre and School of Biological Sciences, Christchurch, New Zealand; [3]SCIEX, Concord, ON, Canada*

WP 416 **Using Drift Tube Ion Mobility for Enhancing Lipidome Coverage**; Russell L. Lewis[1]; Jeremy P. Koelmel[1]; Robin H. J. Kemperman[1]; John A. Bowden[2]; Timothy J. Garrett[1]; Richard A. Yost[1]; *[1]University of Florida, Gainesville, FL; [2]National Institute of Standards and Technology, Charleston, SC*

WP 417 **Online Electrochemistry/Trapped Ion Mobility/ Mass Spectrometry for the Simulation of Phase-I Metabolism of Metoprolol**; Simon Gereon Scheeren[1]; Jens Fangmeyer[1]; Robin Schmid[1]; Uwe Karst[1]; *[1]University of Münster, Münster, Germany*

WP 418 **On the Stability of Oligomeric Species Measured by Temperature-Controlled ESI-IMS-MS**; Daniel R. Fuller[1]; Tarick J. El-Baba[1]; Christopher R. Conant[1]; David E. Clemmer[1]; *[1]Indiana University, Bloomington, IN*

WP 419 **Towards High-Throughput Identification and Quantitation of Lipids Using LC-TIMS-MS/MS**; Cesar E. Ramirez[1]; Kendra J. Adams[1]; Anthony Castellanos[1]; Alyssa Garabedian[1]; Francisco Fernandez-Lima[1, 2]; *[1]Florida International University, Miami; [2]Biomolecular Sciences Institute, Florida International University, Miami, FLORIDA*

WP 420 **Structural Characterization of HMGA2 and HMGA2-DNA interactions Using LC-HDX-TIMS-MS/MS**; Alyssa Garabedian[1]; David Butcher[1]; Fenfei Leng[1]; Mario E Gomez-Hernandez[1]; Francisco Fernandez Lima[1]; *[1]Florida International University, Miami*

WP 421 **Performance of a timsTOF Pro Mass Spectrometer in Shotgun Proteomics Evaluated with a Tryptic HeLa Digest Mixture**; Guoting Qin[1]; Yanxin Chen[2]; Jong Min Choi[3]; Sung Yun Jung[3]; Chengzhi Cai[2]; *[1]College of Optometry, University of Houston, Houston, TX; [2]Department of Chemistry, University of Houston, Houston, TX; [3]Baylor College of Medicine, Houston, TX*

WP 422 **Impurities Identification of Synthetic B-type Natriuretic Peptide Using UPLC Coupled Ion Mobility Mass Spectrometry**; Peng Xiao; *National Institute of Metrology, Beijing, China*

WP 423 **Characterizing TDP-43307-319 Oligomeric Assembly to Elucidate Mechanistic and Structural Implications Involved in the Etiology of ALS**; Veronica Laos[1]; Thanh D. Do[1, 2]; Dezmond Bishop[1]; Yingying Jin[1]; Nicole Marsh[3]; Brady Quon[3]; Megan Korff[3]; Kristi Lazar Cantrell[3]; Steve K Buratto[1]; Michael T Bowers[1]; *[1]Department of Chemistry & Biochemistry, University of California, Santa Barbara, Santa Barbara, CA; [2]Department of Chemistry and the Beckman Institute, University of Illinois at Urbana-Champaign, Urbana, IL; [3]Department of Chemistry, Westmont College, Santa Barbara, CA*

WP 424 **IMTBX+Grppr: Software Suite for Peak Detection, Isotopic Clustering and Precursor-Fragment Matching in Ion Mobility Enabled Data**; Dmitry Avtonomov[1]; Daniel Polasky[1]; Sarah Haynes[1]; Brandon Ruotolo[1]; Alexey Nesvizhskii[1]; *[1]University of Michigan, Ann Arbor, MI*

WP 425 **Site specific structural and stability analysis of MHC-associated phosphopeptides**; Zhichao Zhang[1]; Goran W Tumbic[2]; Fuller R Daniel[2]; Christopher R Conant[2]; David E Clemmer[2]; *[1]Indiana University, Bloomington, IN; [2]Indiana University Bloomington, Bloomington, IN*

WP 426 **Influence of Mobile Phase Composition on Collision Cross-Section (CCS): Towards a Universal Ion-Mobility-Mass Spectrometry (IM-MS) Method for Extractables Identification**; Rodrigo Feliciano[1]; Vincent Hanot[1]; Peifeng Hu[2]; Christopher Jones[2]; *[1]Baxter R&D Europe, Braine L'Alleud, Belgium; [2]Baxter Healthcare Corporation, Round Lake, IL*

WP 427 **Peptide Catabolite Identification Using HDMSE data and Mass-MetaSite Processing**; Ismael Zamora[1]; Christopher J Kochansky[2]; Mark Cancilla[2]; Mark Wrona[3]; Russell Mortishire-Smith[4]; Jayne Kirk[4]; Gordon Murray[5]; Tatiana Radchenko[1]; *[1]Lead Molecular Design, S.L., Sant Cugat Del Valles, Spain; [2]Merck, West Point, PA; [3]Waters Corporation, Milford, MA; [4]Waters Corporation, Wilmslow, UK; [5]Waters Corp., Beverly, MA*

WP 428 **Combining Ion Mobility Spectrometry with Ambient Mass Spectrometry: Towards Spatial Profiling of Protein Conformations**; Rian L. Griffiths[1]; Emma K Sisley[1]; Anna L Simmonds[1]; Klaudia I. Kocurek[1]; James Hughes[1]; Jana Havlikova[1]; Iain B. Styles[1]; Helen J. Cooper[1]; *[1]University of Birmingham, Birmingham, UK*

WP 429 **Simultaneous Determination of Four PHOTOCYANINE Isomers Using Differential Ion Mobility Tandem Mass Spectrometry and its Application in Clinical Pharmacokinetic Study**; Xin Zheng[1]; Xinge Cui[1]; Huaidong Yu[2]; Ji Jiang[1]; *[1]Peking Union Medical College Hospital, Beijing, China; [2]Sciex, shanghai, China*

WP 430 **Investigating Structures of Compounds in Processed Oils by Ion Mobility Mass Spectrometry (IM-MS)**; Dongwan Lim[1]; Arif Ahmed[2]; Sunghwan Kim[2]; *[1]Kyungpook National University, Daegu, South Korea; [2]Kyungpook National University, Daegu, South Korea*

WP 431 **PASEF on a TIMS-QTOF for Reproducible, Sensitive and High-Throughput Shotgun Proteomics**; Scarlet Koch[1]; Markus Lubeck[1]; Heiner Koch[1]; Romano Hebeler[1]; Florian Meier[2]; Andreas-David Brunner[2]; Paul Shan[3]; Jürgen Cox[2]; Matthias Mann[2]; *[1]Bruker Daltonik GmbH, Bremen, Germany; [2]Max Planck Institute of Biochemistry, Martinsried, Germany; [3]Bioinformatics Solutions Inc., Waterloo, ON, Canada*

WP 432 **Separation of Isomeric Metabolites Using High Performance Ion Mobility in Various Drift Gases on an Orbitrap Mass Spectrometer**; Julia Kaszycki[1]; Aurelio La Rotta[1]; Benoit Colsch[2]; François Fenaille[2]; Claire Dauly[3]; Anas Kamleh[4]; Ching Wu[1]; *[1]Excellims Corporation, Acton, MA; [2]CEA Saclay, DRF, Institut Joliot, Service de Pharmacologie et d'Immunoanalyse- CEA-INRA UMR 0496, Laboratoire d'Etude du Métabolisme des Médicament, Gif-sur-Yvette, France; [3]Thermo Fisher Scientific, Paris, France; [4]Thermo Fisher Scientific, Hägersten, Sweden*

WP 433 **Separation and Structural Characterization of Middle-Down Proteoforms Using Linear Trapped IMS-FT-ICR MS/MS**; Jacob Porter[1]; Kevin Jeanne Dit Fouque[1]; Matthew A. Baird[2]; Alexandre A. Shvartsburg[2]; Philippe Maitre[3]; Mark E Ridgeway[4]; Melvin A Park[4]; Francisco Fernandez-Lima[1]; *[1]Florida International University, Miami, FL; [2]Wichita State University, Wichita, KS; [3]Laboratoire de Chimie Physique, UMR 8000, Université Paris Sud, Orsay, France; [4]Bruker Daltonics Inc., Billerica, MA*

WP 434 **Classifying Ligand Binding Behavior of the Integral Membrane Translocator Protein (TSPO) via Collision Induced Unfolding from Micelles and Nanodiscs**; Sarah M. Fantin[1]; Kristine F. Parson[1]; Shuai Niu[1]; Dan A. Polasky[1]; Jian Liu[2]; Shelagh M. Ferguson-Miller[2]; Brandon T. Ruotolo[1]; *[1]University of Michigan, Ann Arbor, MI; [2]Michigan State University, East Lansing, MI*

WP 435 **An Open Source Pipeline for Ion Mobility-Enabled Mass Spectrometry Proteomics**; Sarah Haynes[1]; Dmitry Avtonomov[1]; Alexey Nesvizhskii[1]; Brent Martin[1]; *[1]University of Michigan, Ann Arbor, MI*

WP 436 **Insight Into Distinct Conformations of Therapeutic Monoclonal Antibody Fragment: Evidence From Ion Mobility Mass Spectrometry ofVEGF-Induced Fab**; Baran Dingiloglu[1]; Gencer Kaan Akyüz[2]; Gizem Dinler Doganay[2]; *[1]Istanbul Technical University, Istanbul, Turkey; [2]Istanbul Technical University, istanbul, Turkey*

WP 437 **A Comprehensive Ion Mobility Characterization of Calibration Compounds Used in Mass Spectrometry**; Jody C May[1]; John A McLean[1]; *[1]Vanderbilt University, Nashville, TN*

WP 438 **Ion Mobility Spectrometry, Gas-Phase Hydrogen Deuterium Exchange for Distinguishing Disaccharides**

isomers; Sandra N Majuta[1]; Hossein Maleki[2]; Joseph Stein[2]; Stephen J Valentine[2]; *[1]West Virginia University.C. Eugene Bennett Department of Chemistry, Morgantown, WV; [2]West Virginia University, Morgantown, WV*

WP 439 **Ion Mobility Spectrometry-Mass Spectrometry Reveals the Effects of Phosphorylation on the Stability of Immunologically Stimulating Peptides**; Chris Conant[1]; Daniel R. Fuller[1]; Zhichao Zhang[1]; David E Clemmer[1]; *[1]Indiana University, Bloomington, IN*

WP 440 **Liquid Chromatography-Trapped Ion Mobility-Mass Spectrometry (HPLC-TIMS-MS) for the Analysis of Juvenile Hormone III from Insects**; Alan A McKenzie-Coe[1]; Cesar E. Ramirez[2]; Francisco Fernandez Lima[2]; Veronika Michalkova[2]; Marcela Nouzova[2]; Fernando Noriega[2]; *[1]Florida Int'l University, Miami, FL; [2]Florida International University, Miami*

WP 441 **The Use of Protein Modification and Ion Mobility-Mass Spectrometry to Probe Protein Structure**; Asia Aljabiry[1]; Neil Oldham[2]; *[1]University of Nottingham, nottingham, UK; [2]University of Nottingham, Nottingham, UK*

WP 442 **Increasing Annotation Rates in Untargeted Lipidomics Research Using Ion Mobility-Mass Spectrometry**; Ivana Blazenovic[1]; Tong Shen[1]; Sajjan Singh Mehta[1]; Tobias Kind[1]; Jian Ji[2]; Marco Piparo[3]; Oliver Fiehn[1]; *[1]UC Davis, Davis, CA; [2]Joint International Research Laboratory on Food Safety, Jiangnan University, Wuxi, China; [3]University of Messina, Messina, Italy*

WP 443 **Probing Peptide Conformational Stabilities by Collisional Activation Using Multidimensional Ion Mobility Spectrometry-Mass Spectrometry**; Goran Tumbic[1]; Zhichao Zhang[2]; Michael Przybylski[3]; David E Clemmer[2]; *[1]Indiana University, Bloomington, IN; [2]Indiana University Bloomington, Bloomington, IN; [3]Steinbeis Centre for Biopolymer Analysis and Biomedical Mass Spectrometry, Rüsselsheim am Main, Germany*

WP 444 **Separation and Analysis of Disaccharides by SCIEX SelexION® Differential Ion Mobility Spectrometry (DMS)**; Craig Butt[1]; Christopher Borton[2]; Katherine Hyland[3]; *[1]Sciex, Framingham, MA; [2]SCIEX, Redwood City, California; [3]SCIEX, Redwood City, CA*

WP 445 **LipidIMMS Analyzer: Integration of Multi-Dimensional Information to Support Ambiguous Lipid Identification for Ion Mobility-Mass Spectrometry based Lipidomics**; Zhiwei Zhou[1]; Zhengjiang Zhu[1]; *[1]Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai, China*

WP 446 **PASEF for Sensitive Shotgun Proteomics**; Romano Hebeler[1]; Matt Willetts[2]; Heiner Koch[1]; Markus Lubeck[1]; Scarlet Koch[1]; *[1]Bruker Daltonik GmbH, Bremen, Germany; [2]Bruker Daltonics, Billerica, MA*

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WP 447 **Separations of D-Amino Acid Containing Peptides of all Sizes Using High-Resolution FAIMS Followed by Electron Transfer Dissociation**; Matthew Baird[1]; Alexandre Shvartsburg[1]; *[1]Wichita State University, Wichita, KS*

WP 448 **Exploring the Trends and Structural Specificity of Isotopologic Shifts in High-Field Ion Mobility Spectra**; Pratima Pathak[1]; Matthew A. Baird[1]; Julia L. Kaszycki[1]; Gordon A. Anderson[2]; Alexandre A. Shvartsburg[1]; *[1]Wichita State University, Wichita, KS; [2]GAACE, Kennewick, WA*

WP 449 **Deep Proteomic Coverage Using Fast and Sensitive FAIMS Device Coupled to a Thermo Scientific™ Orbitrap Fusion™ Lumos™ Tribid™ Mass Spectrometer**; Satendra Prasad[1]; Michael W Belford[1]; Derek J Bailey[1]; Joshua A Silveira[1]; Romain Huguet[1]; Eloy R Wouters[1]; Jean-Jacques Dunyach[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

WP 450 **Characterization of a Field Asymmetric Ion Mobility Spectrometer with a Micro-Fabricated Ion Filter**; Katsuya Ujimoto[1]; Shinichi Kubota[1]; Kunihiro Tan[1]; Tomofumi Kiyomoto[1]; Junichi Konishi[1]; Kazutaka Niigata[1]; Saori Yoshida[1]; *[1]Ricoh Company, Ltd., Ikeda-city, Japan*

WP 451 **A Selective Method for the Quantitation of Allopurinol in Human Plasma Using Differential Ion Mobility Spectrometry**; Georges Koudssi[1]; Milton Furtado[1]; Jeff Plomley[1]; Anahita Keyhani[1]; *[1]Altasciences, Laval , QC, Canada*

WP 452 **Selective and Sensitive Quantitation of Fingolimod and Fingolimod Phosphate in Human Blood Using Differential Ion-Mobility Spectrometry**; Laurence Mayrand-Provencher[1]; Milton Furtado[1]; Anahita Keyhani[1]; *[1]Altasciences, Laval , QC, Canada*

WP 453 **Selective Quantitation of 1,3-Propanediol in Dog Plasma Using Differential Ion Mobility Spectrometry**; Ming-Luan Chen[1]; Milton Furtado[1]; Jeff Plomley[1]; Anahita Keyhani[1]; *[1]Altasciences, Laval , QC, Canada*

WP 454 **Characterization of Biologic Compounds with Differential Mobility and SWATH**; Brendon Seale[1, 2]; Lyle Burton[1]; J.c. Yves Leblanc[3]; *[1]SCIEX, Concord, ON, Canada; [2]York University, Toronto, ON, Canada; [3]SCIEX, Concord, ON, Canada*

WP 455 **Characterization Analysis of Glycopeptides through Arrival Time Correlation Using Concurrent RPLC Fraction Monitoring and FAIMS Filtering**; Daniel G. Delafield[1]; Matthew A. Baird[2]; Zhe Wang[1]; Alexandre A. Shvartsburg[2]; Si Wu[1]; *[1]University of Oklahoma, Norman, OK; [2]Wichita State University, Wichita, KS*

WP 456 **Improved Selectivity in Narcotics Detection by Tandem DMS through Combination of Chemical Modifiers and Ion-Molecule Reactions**; Marlen R. Menlyadiev[1]; Peter E. Fowler[2]; Hartwig Schmidt[1]; Stefan R. Lukow[1]; Gary A. Eiceman[2]; *[1]Rapiscan Systems, Andover, MA; [2]Department of Chemistry and Biochemistry, New Mexico State University, Las Cruces, NM*

WP 457 **Liquid extraction Surface Analysis Mass Spectrometry of Bacterial Colonies: Expanding Capabilities with High-Field Asymmetric Waveform Ion Mobility Spectrometry**; Klaudia I Kocurek[1]; Josephine Bunch[2, 3]; Robin C May[1]; Helen J Cooper[1]; *[1]University of Birmingham, Birmingham, UK; [2]National Physical Laboratory, Teddington, UK; [3]Imperial College London, London, UK*

WP 458 **High Field Asymmetric Waveform Ion Mobility Spectrometry (FAIMS) Expand the Comprehensiveness and Precision of Multiplex Proteomics**; Sibylle Pfammatter[1]; Eric Bonneil[1]; Pierre Thibault[1]; *[1]Universite de Montreal, Montréal*

WP 459 **Gas-Phase Uranyl Ion Prefiltration and Speciation Using Differential Mobility Spectrometry - Mass Spectrometry**; Ifeoluwa Ayodeji[1]; Theresa Evans-Nguyen[1]; Jake T Shelley[2]; *[1]University of South Florida, Tampa, FL; [2]Rensselaer Polytechnic Institute, Troy, NY*

WP 460 **Extending the Detection Boundary of Immunopeptidome Analyses Using High-Field Asymmetric Waveform Ion Mobility (FAIMS) and Isobaric Peptide Labelling**; Eric Bonneil[1]; Sibylle Pfammatter[2]; Joel Lanoix[2]; Marie-Pierre Hardy[2]; Claude Perreault[2]; Pierre Thibault[2]; *[1]Université de Montréal, Montréal, QC, Canada; [2]Université de Montréal, Montréal, Québec*

WP 461 **Exploring the Figures of Merit of Differential Mobility Spectrometry (DMS) Cells of Varied Geometries**; J. Larry Campbell[1]; Bradley B. Schneider[1]; *[1]SCIEX, Concord, ON, Canada*

WP 462 **Separation of Intact Protein Isoforms with Differential Mobility**; J.C. Yves Leblanc[1]; Sibylle Heidelberger[2]; Annu Uppal[3]; *[1]SCIEX, Concord, ON, Canada; [2]SCIEX, Concord, ON, Canada; [3]SCIEX, Gurugram, India*

WP 463 **Segmented Ion Fractionation Using High Field Asymmetric Waveform Ion Mobility Spectrometry Expand the Depth and Comprehensiveness of**

Proteomics Analyses; Sibylle Pfammatter[1, 2]; Eric Bonneil[1]; Pierre Thibault[2, 3]; *[1]Institute for Research in Immunology and Cancer, University of Montreal, Montreal, QC, Canada; [2]Department of chemistry, University of Montreal, Montreal, Québec; [3]Univ.of Montreal, Montreal, QC, Canada*

WP 464 **Influence of Cluster/De-Cluster Reactions on Ion Separation in Differential Mobility Spectrometry (DMS) in Dependence of the Analyte Structure**; Florian Stappert[1]; Christine Polaczek[1]; Walter Wissdorf[1]; Hendrik Kersten[1]; Thorsten Benter[1]; Bradley B. Schneider[2]; Tom Covey[2]; *[1]Bergische Universität Wuppertal, Wuppertal, Germany; [2]SCIEX, Concord, ON, Canada*

WP 465 **Strategies for Improving FAIMS-MS Separation of Drug Isomers**; Michael Wei[1]; Richard Yost[1]; Robin H. J. Kemperman[1]; *[1]University of Florida, Gainesville, FL*

WP 466 **Improving Constitutional Isomer Separation in FAIMS by Addition of Two Solvent Vapors**; Kevin Davis[1]; Richard A. Yost[2]; Michael Wei[2]; *[1]University of Florida, Gainesville, FL; [2]University of Florida, Department of Chemistry, Gainesville, FL*

WP 467 **Chemical Kinetic and Ion Transport Simulations: Temperature Dependence of Ion Mobility and its Impact on Cluster Equilibria**; Duygu Erdogdu[1]; Walter Wissdorf[1]; Florian Stappert[1]; Hendrik Kersten[1]; Thorsten Benter[1]; Bradley B. Schneider[2]; Tom Covey[2]; *[1]Bergische Universität Wuppertal, Wuppertal, Germany; [2]SCIEX, Concord, ON, Canada*

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WP 468 **Automated Online Solid Phase Derivatization for Rapid and Sensitive Determination of Endogenous Low-Molecular-Mass S-Nitrosothiols**; Xin Wang[1]; Carlos T. Garcia[1]; Guanyu Gong[1]; John S. Wishnok[1]; Steven R. Tannenbaum[1]; *[1]Massachusetts Institute of Technology, Cambridge, MA*

WP 469 **Simultaneous Analysis of Multiclass Veterinary Antibiotics in Animal Body Fluids by UHPLC-MS/MS**; Viet D Dang[1]; Edwin J. George[2]; DAVID J. BORTS[1]; *[1]Iowa State University, Ames, IA; [2]Thermo Fisher Scientific, San Jose, CA*

WP 470 **Comparison of Sample Preparation Options for the Extraction of a Panel of Endogenous Steroids from Serum Prior to UHPLC-MS/MS Analysis**; Katie-Jo Teehan[1]; Lee Williams[1]; Adam Senior[1]; Alan Edgington[1]; Rhys Jones[1]; Helen Lodder[1]; Geoff Davies[1]; Steve Jordan[1]; Claire Desbrow[1]; Paul Roberts[1]; Stephanie Marin[2]; Dan Menasco[2]; Candice Summitt[2]; Elena Gairloch[2]; *[1]Biotage GB Limited, Cardiff, UK; [2]Biotage LLC, Charlotte, NC*

WP 471 **Development of an Automated "Cells-To-Peptides" Sample Preparation Workflow for High-Throughput Quantitative Proteomic Applications**; Yan Chen[1]; Joel M. Guenther[1]; Leanne Jade G. Chan[2]; Jennifer W. Gin[1]; Paul D. Adams[1]; Christopher J. Petzold[1]; *[1]LBNL, Berkeley, CA; [2]Calico Life Sciences, South San Francisco, CA*

WP 472 **Systematic Evaluation of Extraction Recovery for Protein Precipitation to Address the Common Issue of Over 100% of Recovery**; Aimin Tan[1]; Xuan Susan Gui[1]; John C. Fanaras[1]; *[1]Nucro-Technics, Scarborough, ON, Canada*

WP 473 **A Fully Automated Tip-Based Solid Phase Extraction for Released Nanoparticle Quantitation Using LC-MS/MS**; Amy Rose Boisvert[1]; Joseph A Tweed[1]; Zhenhua Gu[2]; Rago Brian[2]; *[1]Pfizer Inc., Groton, CT; [2]Pfizer, Groton*

WP 474 **An Optimized Protocol for Global Proteome and Phosphoproteome Analysis that Yields Highly Reproducible and Deep Coverage within and Across Laboratories**; Philipp Mertins[1]; Lauren C Tang[1]; Karsten Krug[1]; David J Clark[2]; Marina A Gritsenko[3]; Lijun Chen[2]; Karl R Clauser[1]; Therese R Clauss[3]; Punit Shah[2]; Michael A. Gillette[1]; Vladislav A Petyuk[3]; Stefani N Thomas[2]; D. R. Mani[1]; Filip Mundt[1]; Ronald J. Moore[3]; Yingwei Hu[2]; Rui Zhao[3]; Michael Schnaubelt[2]; Hasmik Keshishian[1]; Matthew E. Monroe[3]; Zhen Zhang[2]; Namrata D Udeshi[1]; Deepak Mani[1]; Sherri R Davies[4]; R. Reid Townsend[4]; Daniel W Chan[2]; Richard D. Smith[3]; Hui Zhang[2]; Tao Liu[1]; Steven A Carr[1]; *[1]The Broad Institute of MIT and Harvard, Cambridge, MA; [2]Johns Hopkins School of Medicine, Baltimore, MD; [3]Pacific Northwest National Laboratory, Richland, WA; [4]Washington University School of Medicine, St Louis, MO*

WP 475 **Development of a Simple and Rapid Digestion Protocol for Proteomics Sample Preparation**; Zhiyun Cao[1]; Amber Henry[1]; Judy Boland[1]; Nicolas Caffarelli[1]; Jeffrey Turner[1]; Kevin Ray[1]; *[1]MilliporeSigma, St. Louis, MO*

WP 476 **Online Sol-Gel Capillary Microextraction-Mass Spectrometry (CME-MS): Microextraction of Illicit Drugs in CME-MS Applications**; Emre Seyyal[1]; Theresa Evans-Nguyen[1]; *[1]University of South Florida, Tampa, FL*

WP 477 **Subcellular Fractionation with Stable Isotope Labeling by Essential Nutrients**; Sophie Trefely[1, 2]; Jimmy Xu[1]; Mary Doan[1]; Helen Jiang[1]; Nathaniel W Snyder[1]; *[1]Drexel University, Philadelphia, PA; [2]University of Pennsylvania School of Medicine, Philadelphia, PA*

WP 478 **Electromagnetic Mixer for Low Response Paramagnetic Particles**; Chang Liu[1]; Thomas R Covey[1]; *[1]SCIEX, Concord, ON, Canada*

WP 479 **Case Studies Evaluating Automated Vs. Manual Digestion of mAbs**; Alexander Barnakov[1]; HARSHA GUNAWARDENA[1]; Jefferey Brelsford[1]; Darryl Davis[1]; Hirsh Nanda[1]; Subinay Ganguly[1]; *[1]Janssen Research & Development, Spring House, PA, 19002*

WP 480 **Optimizing In-Solution Urea-Based Digestion to Minimize Missed Cleavage Rate and Maximize Identifications**; Deepak Mani[1]; Lauren Tang[1]; Luke Wallace[1]; Tanya Svinkina[1]; Hasmik Keshishian[1]; Philipp Mertins[1]; Namrata D Udeshi[1]; Steven A Carr[1]; *[1]Broad Institute of MIT and Harvard, Cambridge, MA*

WP 481 **Practical Considerations of Matrix Effects Using Quantisal Oral Fluid Collection Devices & SPE**; Dan Menasco[1]; Candice Summit[2]; Jillian Neifeld[1]; Stephanie Marin[1]; Lee Williams[3]; Elena Gairloch[1]; *[1]Biotage, Charlotte, NC; [2]Biotage LLC, Charlotte, NC; [3]Biotage GB Limited, Cardiff, UK*

WP 482 **Comprehensive Evaluation of S-Trap Approach as an Alternative to Highly Efficient and Effective Shotgun Proteomics**; Yanbao Yu[1]; Milkessa Haile Mariam[2]; Harinder Singh[1]; Gobena Ameni[2]; Rembert Pieper[1]; *[1]J. Craig Venter Institute, Rockville, MD; [2]Aklilu Lemma Institute of Pathobiology, Addis Ababa University, Addis Ababa, Ethiopia*

WP 483 **Quantitative Determination of Multi-class Multi-residue Veterinary Drugs in Beef Using Captiva EMR-Lipid cleanup and LC/MS/MS**; Limian Zhao[1]; Derick Lucas[1]; *[1]Agilent Technologies, Wilmington, DE*

WP 484 **Phase Transfer Surfactants-based Sample Preparation toward Unbiased Proteomics**; Arisu Furukawa[1]; Takeshi Masuda[1]; Yuma Inamori[1]; Shingo Ito[1]; Sumio Ohtsuki[1]; *[1]Kumamoto univ., Kumamoto, Japan*

WP 485 **Surface Phase Cleanup (SPC): An Optimized Peptide Cleanup Method for Mass Spectrometry Using Carboxylate-Coated Magnetic Beads**; Michael Pereckas[1]; Matthew Waas[1]; Rachel A. Jones Lipinski[1]; Rebekah L. Gundry[1]; *[1]MCW, Milwaukee, WI*

WP 486 **The Pros and Cons of Two Commercial Hemoglobin-Depletion Kits for Red Blood Cell Cytosol Proteomics**; Yi Wang[1]; James Zimring[1, 2]; Xiaoyun Fu[1, 2]; *[1]Bloodworks Research Institute, Seattle, WA; [2]Department of Medicine, University of Washington, Seattle, WA*

WP 487 **A Surfactant-Aided Extraction/Precipitation/On-Pellet Digestion Strategy (SEPOD) Enables Rapid, Efficient**

and Reproducible Sample Preparation for Large-Scale Quantitative Proteomics; Shichen Shen[1]; Bo An[1]; Xue Wang[1]; Jun Li[1]; Jin Cao[2]; Andrew Ng[1]; Chengjian Tu[1]; Martin S Zand[3]; Jun Qu[1]; *[1]University at Buffalo, Buffalo, NY; [2]China Academy of Chinese Medical Sciences, Beijing, China; [3]University of Rochester, Rochester, NY*

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WP 488 **TGF-Beta Signaling in C. elegans Alters the Lipid Profile**; Ekta Tiwary[1]; Muhan Hu[2]; Landon Wilson[2]; Taylor Berryhill[2]; Michael A. Miller[2]; Jeevan K. Prasain[2]; *[1]University, Birmingham, AL; [2]University of Alabama at Birmingham, Birmingham, AL*

WP 489 **Lipidomic Profiling of Breast Cancer Extracellular Vesicles and Their Parental Cell Lines**; Erika J Dorado[1]; M Luisa Doria[1]; Anika Nagelkerke[2]; Thomas Whittaker[2]; Ulrike Kauscher[2]; R Charles Coombes[1]; Jeremy Nicholson[1]; Molly M Stevens[2]; Zoltan Takats[1]; *[1]Faculty of Medicine, Department of Surgery and Cancer, Imperial College London, London, UK; [2]Faculty of Engineering, Department of Materials/ Department of Bioengineering, Imperial College London, London, UK*

WP 490 **A Targeted Phospholipid Profiling Approach with PCA for Beans and Milks Using a Ready-To-Use MRM Method Package on LC/MS/MS**; Zhe Sun[1]; Udi Jumhawan[1]; Yu Jie Lee[2]; Nur Sadrina Binte Mohamed Shah[3]; Jie Xing[1]; Zhaoqi Zhan[1]; *[1]Shimadzu, Singapore, Singapore; [2]school of chemical and life sciences, Singapore polytechnic, Singapore, Singapore; [3]School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore, Singapore*

WP 491 **In Situdetecting Changes in Membrane Lipid Phenotypes of Macrophages Cultured in Different Microenvironments Using Mass Spectrometry**; Yupin Xu[1]; Mo Zhang[1]; Qing Wang[1]; Zhili Li[1]; *[1]Institute of Basic Medical Sciences, CAMS&PUMC, Beijing, China*

WP 492 **Quantitative Profiling and Pattern Analysis of Triacylglycerol in Oils by Using Supercritical Fluid Chromatography coupled with Triple Quadrupole MS detector**; Kyoko Yasuda[1]; Hirokazu Sawada[2]; *[1]Agilent Technologies Japan, Ltd, Suita, Osaka, Japan; [2]Agilent Technologies Japan, Ltd, Hachioji, Japan*

WP 493 **Live Single-Cell MS Analysis for Cellular Phospholipid Dynamics**; Hajime Mizuno[1]; Kenichiro Todoroki[2]; Naohiro Tsuyama[3]; Iwao Sakane[4]; Shinobu Kudoh[5]; *[1]School of Pharmaceutical Sciences, University of Shizuoka, Shizukoka, Japan; [2]School of Pharmaceutical Sciences, University of Shizuoka, Shizuoka, Japan; [3]School of Medicine, Fukushima Medical University, Fukushima, Japan; [4]Central Research Institute, ITO EN, Ltd., Makinohara, Japan; [5]Yokogawa Electric Corporation, Musashino, Japan*

WP 494 **Profiling Method of Constitutional Isomeric Phospholipids in MCF-7 Breast Cancer Cell Extracts by Hydrophilic Interaction Liquid Chromatography Coupled to ESI-MS/MS**; Christian Vosse[1]; Heiko Hayen[1]; *[1]Institute of Inorganic and Analytical Chemistry, Muenster, Germany*

WP 495 **Ultra-Performance Supercritical Fluid Chromatography Enable Separate Peripheral Free Fatty Acid in Four Minutes**; Kumari Ubhayasekera[1]; Santosh R. Acharya[1]; Rick Krom[1]; Jonas Bergquist[1]; *[1]Uppsala University, Uppsala, Sweden*

WP 496 **Application of SimLipid Software in Lipid Profiling of Secreted Lung Lipids by MSMSall Shotgun Lipidomics**; Ningombam Sanjib Meitei[1]; Himani Gupta[1]; Rajesh Pujari[1]; Arun Apte[2]; Hong Yin[3]; Vladimir Capka[3]; David Rowlands[3]; Sejal Patel[3]; Sandeep Daya[3]; Kate Choy[3]; *[1]PREMIER Biosoft, Indore, India; [2]PREMIER Biosoft International, San Francisco, CA; [3]Novartis Institutes for BioMedical Research, Inc., Cambridge, MA*

WP 497 **Functional Analysis of Lipidomic Alterations by Pathogenic Staphylococci S.Aureus (USA300)**; Naren Gajenthra Kumar[1]; Daniel Contaifer, Jr[2]; Paul Baker[3]; Kim Ekroos[4]; Kimberly K Jefferson[5]; Dayanjan Wijesinghe[2]; *[1]Virginia Commonwealth University, Richmond, VA; [2]Virginia Commonwealth University School of Pharmacy, Richmond, VA; [3]SCIEX, Concord, ON, Canada; [4]Lipidomics Consulting Ltd., FI-02230, Esbo, Finland; [5]Virginia Commonwealth University SOM, Richmond, VA*

WP 498 **Comparing Automatic Identifications in the Macro-Lipidomic Profiles of Human Whole Blood across UHPLC-MS/MS Platforms and Acquisition Modes**; Juan J Aristizabal Henao[1]; Ningombam Sanjib Meitei[2]; Dan Chalil[1]; Richard W Smith[1]; Ken D Stark[1]; *[1]University of Waterloo, Waterloo, ON, Canada; [2]PREMIER Biosoft, Palo Alto, CA*

WP 499 **Robust and Sensitive LC-MS/MS Based Plasma Lipid Profiling on a Thermo Scientific™ Q Exactive™ HF-X Mass Spectrometer**; Tabbiwang N. Array[1]; Elena Sokol[2]; Angela Criscuolo[1, 3, 4]; Claire Dauly[5]; Alexander Harder[1]; *[1]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [2]Thermo Fisher Scientific, Hemel Hempstead, UK; [3]Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, Universität Leipzig, Leipzig, Germany; [4]Center for Biotechnology and Biomedicine, Universität Leipzig, Leipzig, Germany; [5]Thermo Fisher Scientific, Courtaboeuf, France*

WP 500 **Comprehensive Analysis of Human Sebum Lipids by Using GCxGC–HRTOFMS**; John Dane[1]; Koji Okuda[1]; Robert B Cody[1]; *[1]JEOL USA, Inc., Peabody, MA*

WP 501 **Lipid Profiles of Gram-Negative Bacteria with Different Permeability Barriers and Active Efflux Efficiencies**; Vincent Bonifay[1]; Inga V Leus[1]; Ganesh Krishnamoorthy[1]; Helen I Zgurskaya[1]; *[1]University of Oklahoma, Norman, OK*

WP 502 **Lipid Profiling of Grape Samples Using Orbitrap Velos Pro Mass Spectrometer with SimLipid software**; Vladimir Shulaev[1, 2]; Giulia Chitarrini[1, 3]; Himani Gupta[4]; Rajesh Pujari[4]; Urska Vrhovsek[3]; Fulvio Mattivi[3, 5]; Ningombam Sanjib Meitei[4, 6]; *[1]Department of Biological Sciences, University of North Texas, Denton, TX; [2]Biodiscovery Institute, University of North Texas, Denton, TX; [3]Department of Food Quality and Nutrition, Research and Innovation Centre, Foundation Edmund Mach (FEM), San Michele all'Adige, Italy; [4]PREMIER Biosoft, Indore, India; [5]Center Agriculture Food Environment (CAFE), University of Trento, San Michele all'Adige, Italy; [6]PREMIER Biosoft, Palo Alto, CA*

WP 503 **Lipidomic Profiling of Cancer Cells Using High Resolution Orbitrap Mass Spectrometry with MS2/MS3**; Lin Tan[1]; Yulun Chiu[1]; Di Du[1]; Leona Martin[1]; John Weinstein[1]; Philip Lorenzi[1]; *[1]MD Anderson Cancer Center, Houston, TX*

WP 504 **Lipidomics to Examine the Role of ACC1 in GEMM Lymphatic Tumors using LC-MS/MS**; Min Liu[1]; Kristen E.N. Scott[1]; David C. Koomen[1]; John Koomen[1]; John L. Cleveland[1]; *[1]Moffitt Cancer Center, Tampa, FL*

LIPIDS: TARGETED AND QUANTITATIVE ANALYSIS II
505-520

WP 505 **Analysis of Endocannabinoids and N-Acylethanolamides in Biofluids, and Their Correlations with Female Infertility Using UPLC-MS/MS**; Mingquan Guo[1]; Mingquan Guo[2]; *[1]Wuhan Botanical Garden, Chinese Academy of Sciences ; The Sino-Africa Joint Research Center, Chinese Academy of Sciences, Wuhan, China; [2]Applied Bionanox, Alhambra, CA*

WP 506 **Verified HILIC LC-MS/MS Assay for High-Throughput Targeted Lipdomics Analysis**; Santosh Kapil Kumar Gorti[1]; Lijuan Fu[2]; Mackenzie J Pearson[2]; Baljit K. Ubhi[2]; Lei Xiong[2]; Paul Baker[2]; *[1]SCIEX, Framingham, MA; [2]Sciex, Redwood City, CA*

WP 507 **PEBP1 Enables 15-Lipoxygenase 1 to Generate Ferroptotic Cell Death Signals in Primary Human Airway Epithelial Cells. LC/MS study**; Yulia Tyurina[1]; Jinming Zhao[1]; Claudette St. Croix[1]; Simon Watkins[1]; Tyurin Vladimir[1]; Tamil Anthonymuthu[1]; Andrew Amoscato[1]; Haider Dar[1]; Joel Rosenbaum[1]; Andrew VanDemark[1]; Hülya Bayır[2]; Sally Wenzel[2]; Valerian Kagan[1]; *[1]University of Pittsburgh, Pittsburgh, PA; [2]University of Pittsburgh School of Medicine, Pittsburgh, PA*

WP 508 **Differential LC-MS Study of CLD1-Driven Diversification of Cardiolipins inΔ12-Desaturasetransfected Yeast Cells**; Vladimir Tyurin[1]; Hsiu-Chi Ting[1]; Wenjia Lou[2]; Christian A. Reynolds[2]; Yulia Y. Tyurina[1]; Wenxi Yu[2]; Zhuqing Liang[2]; Tamil S. Anthonymuthu[1]; Detcho A. Stoyanovsky[1]; Joel S. Greenberger[1]; Hülya Bayir[1]; Miriam L. Greenberg[2]; Valerian E. Kagan[1]; *[1]University of Pittsburgh, PA; [2]Wayne State University, Detroit , MI*

WP 509 **Novel LC-MS Method for the Quantitation of Short Chain Fatty Acids**; Ha Eun Song[1]; Su Jung Kim[1]; Hak Su Kim[2]; Jin Woo Song[2]; Hyun Ju Yoo[1]; *[1]Asan Institute for Life Sciences, Seoul, South Korea; [2]University of Ulsan College of Medicine, Seoul, South Korea*

WP 510 **13C Internal Standardization in Lipidomics – a Comparative Study on Different Quantification Methods**; Harald Schoeny[1, 2, 3]; Evelyn Rampler[1, 2, 3]; Yasin El Abiead[1]; Michaela Schwaiger[1]; Gerrit Hermann[1, 4]; Gunda Koellensperger[1, 2, 3]; *[1]University of Vienna, Vienna, Austria; [2]Vienna Metabolomics Center (VIME), University of Vienna, Vienna, Austria; [3]Chemistry Meets Microbiology, Vienna, Austria; [4]ISOtopic Solutions, Vienna, Austria*

WP 511 **Laser Capture Microdissection Coupled with Shotgun Profiling Reveals Full-Lipidome Zonation in Liver**; Olga Vvedenskaya[1]; Oskar Knittelfelder[1]; Sofia Traikov[1]; Andrej Shevchenko[1]; *[1]Max Planck Institute of Molecular Cell Biology and Genetics (MPI-CBG), Dresden, Germany*

WP 512 **Identification of Lipid Biomarkers in CAD Using a Targeted Liquid Chromatography Mass Spectrometry Approach**; Akash Kumar Bhaskar[1]; Swati Varshney[1]; Mainak Dutta[2]; Khushboo Adlakha[1]; Akanksha Singh[3]; Dipankar Malakar[3]; Manoj Pilla[3]; Shantanu Sengupta[1]; *[1]CSIR-Institute of Genomics and Integrative Biology, New Delhi, India; [2]Birla Institute of Technology Pilani, Dubai International Academic City, United Arab Emirates; [3]SCIEX, 121, Udyog Vihar, Phase IV, Gurgaon, India*

WP 513 **Lipid Analysis of Living Cyanobacteria by Easy Ambient Sonic-spray Ionization Mass Spectrometry**; Huwei Liu[1]; Jialing Zhang[1]; Yu Bai[1]; *[1]Peking University, Beijing, China*

WP 514 **Dried Blood Spot Quality Control Materials and a Multiplexed Assay for X-Linked Adrenoleukodystrophy and Metachromatic Leukodystrophy Newborn Screening**; Brandon M. Kenwood[1]; Christopher A. Haynes[1]; Konstantinos Petritis[1]; *[1]Centers for Disease Control and Prevention, Newborn Screening and Molecular Biology Branch, Atlanta, GA*

WP 515 **Discovery of Novel LPA-binding Proteins by A Chemical Proteomic Methodundefinedundefined**; Xuejiao Dong[1]; Yinsheng Wang[2]; *[1]UC Riverside, Riverside; [2]UC Riverside, Riverside, CA*

WP 516 **Comparing Phospholipid Profiles of Mitochondrial and Whole Cell Brain, Heart, Liver, and Kidney Tissues via Normal-Phase HPLC MS**; Cyrus E Kuschner[1]; Tai Yin Yin[2]; Junhwan Kim[1, 2]; *[1]Donald and Barbara Zucker School of Medicine at Hofstra/Northwell, Hempstead, NY; [2]Feinstein Institute for Medical Research, Manhasset, NY*

WP 517 **Quantification of a cationic lipid DOTMA in Human Plasma by LC-MS/MS**; Jintang He[1]; Wenfeng Xu[1]; Heinrich Haas[2]; Patricia Gomes[2]; Gautham Rao[1]; Surinder kaur[1]; Keyang Xu[1]; *[1]Genentech Inc., South San Francisco, CA; [2]BioNTech, Mainz, Germany*

WP 518 **Comparison of High Throughput UHPLC-MS/MS Methods for Lipid Class Totals with a Comprehensive DMS-MS/MS Targeted Lipidomics Method**; Michael S. Gardner[1]; Jon Rees[1]; Lisa G. McWilliams[1]; Antony K. Lehtikoski[1]; Gregory Reis[1]; Jennifer D. Kusovschi[1]; Rachel C. Shore[1]; Zsuzsanna Kuklenyik[1]; John R. Barr[1]; *[1]Centers for Disease Control and Prevention, Atlanta, GA*

WP 519 **Quantitative LC-MS/MS Analysis of Cortisol and Cortisone in Children's Hair. Comparison with Cortisol ELISA assay**; Karolina M. Krasinska[1]; Cynthia R. Rovnaghi[2]; Kanwaljeet J. S. Anand[2]; Allis S Chien[1]; *[1]SUMS, Stanford University, Palo Alto, CA; [2]Department of Pediatrics, Stanford University School of Medicine, Palo Alto, CA*

WP 520 **LipidCreator: A New Bridge between Targeted and Non-Targeted LC-MS/MS-Based Lipidomics**; Bing Peng[1]; Dominik Kopczynski[1]; Nils Hoffmann[1]; Brian Pratt[2]; Dominik Schwudke[3]; Christer S. Ejsing[4, 5]; Brendan MacLean[2]; Robert Ahrends[1]; *[1]ISAS, Dortmund, Germany; [2]University of Washington Genome Sciences, Seattle, WA; [3]Research Center Borstel, Leibniz-Center for Medicine and Biosciences, Borstel, Germany; [4]University of Southern Denmark, Odense, Denmark; [5]Cell Biology and Biophysics Unit, European Molecular Biology Laboratory, Heidelberg, Germany*

METABOLOMICS: GENERAL II
521-548

WP 521 **Metabolomic Analysis of the Effects of the Bioactive Grape Polyphenol Isorhapontigenin in Plasma Using GC-Triple Quadrupole MS**; Samuel C M Yeo[1]; Yu Dai[2]; Haishu Lin[2]; Lai Chin Loo[1]; *[1]Shimadzu, Singapore, Singapore; [2]Department of Pharmacy, National University of Singapore, Singapore, Singapore*

WP 522 **Differential Mobility Separation (DMS)-Based Separation of Bile Acid Isomers**; Joerg Dojahn[1]; Cyrus Papan[1]; Dietrich Merkel[1]; *[1]SCIEX, Darmstadt, Germany*

WP 523 **A Wellness Study Using Microflow Targeted Metabolomics to Investigate the Effects of Diet and Exercise on the Metabolome**; Khatereh Motamedchaboki[1]; Baljit Ubhi[1]; *[1]Sciex, Redwood City, CA*

WP 524 **Metabolite profiling of Single Cells by a Sheathless Capillary Electrophoresis- Mass Spectrometer System**; Rabia Raza[1]; Yu Bai[1]; Huwei Liu[1]; *[1]Peking University, Beijing, China*

WP 525 **The Effect of Synthetic Cystic Fibrosis Sputum Media on Pseudomonas Aeruginosasecondary Metabolism**; Rachel L Neve[1]; Vanessa V. Phelan[1]; *[1]University of Colorado - Denver | Anschutz Medical Campus, Aurora, CO*

WP 526 **Improved LC/MS Methods for the Analysis of Anionic Analytes**; Jordy J Hsiao[1]; Oscar G Potter[1]; Genevieve C Van de Bittner[1]; Te-Wei Chu[1]; Hongfeng Yin[1]; *[1]Agilent Technologies, Santa Clara, CA*

WP 527 **Investigation of the Stability of Human Saliva Metabolites Using Gas Chromatography-Triple Quadrupole MS with Widely-targeted Profiling Approach**; Samuel C M Yeo[1]; Elgin G W Ting[1]; Jia Wen Ding[2]; Si Ying Lim[3]; Lai Chin Loo[1]; *[1]Shimadzu Asia Pacific, Singapore, Singapore; [2]School of Physical & Mathematical Sciences, Nanyang Technological University, Singapore, Singapore; [3]Department of Chemistry, National University of Singapore, Singapore, Singapore*

WP 528 **Establishment IROA Methodology for Comparative Profiling of ccRCC-Kidney Pairs Metabolome Using *in vivo* Produced Heavy Isotope Labeled Standards**; Collin Wetzel[1]; Kelly N. Ennis[2]; Brian Johnson[2]; Nicholas J. Talbot[2]; Chris Beecher[3]; Felice A. De Jong[3]; Tom Cunningham[2]; David R. Plas[2]; Maria F. Czyzyk-Kreska[2]; *[1]University of Cincinnati, Cincinnati, OH; [2]University of Cincinnati, Department of Cancer Biology, Cincinnati, OH; [3]IROA Technologies, Bolton, MA*

WP 529 **Development of Online SFE-LC/MS System for Analysis of Metabilites in Microbial Cells**; Yuka Fujito[1]; Yoshimi Hori[2]; Masao Mochizuki[2]; Takanobu Yoshida[2]; Tomohisa Hasunuma[2]; Yoshihiro Hayakawa[1]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]Kobe University Graduate school of Science, Technology and Innovation, Kobe-shi, Japan*

WP 530 **Metabolomic Study and Functional Correlation between Bipolar Disorder and Circadian Clock**; Yu Bai[1]; Li Yang[1]; Huwei Liu[1]; *[1]College of Chemistry, Peking University, Beijing, China*

WP 531 **Generation of a Collisional Cross Section Library for Plant Metabolomics Using Trapped Ion Mobility Spectrometry (TIMS)**; Mark J Schroeder[1]; Sven W Meyer[2]; Aiko Barsch[2]; Lloyd W. Sumner[1]; *[1]University of Missouri-Columbia, Columbia, MO; [2]Bruker Daltonik GmbH, Bremen, Germany*

WP 532 **Correlation of Cytokinins in Maize Leaves as a Measure of Stay Green Effect**; Suresh Annangudi[1]; Daniel Gachotte[1]; Beth Blakeslee[1]; Scott Greenwalt[1]; John Davies[1]; Debby Camper[1]; Jeffrey Gilbert[1]; *[1]Dow AgroSciences, Indianapolis, IN*

WP 533 **Withdrawn**

WP 534 **Metabolic Reprogramming in Esophageal Squamous Cell Carcinoma Revealed by Combined Tissue Metabolomics and Proteomics Analysis**; Yanjun Hong[1, 2]; Zhiyi Yang[1]; Guodong Cao[1]; Xuan Li[1]; Zhenyu Guo[1]; Zhongjian Chen[3]; Zongwei Cai[1]; *[1]Hong Kong Baptist University, Hong Kong, Hong Kong; [2]HKBU Institute for Research and Continuing Education, Shenzhen, China; [3]Key Laboratory Diagnosis and Treatment Technology on Thoracic Oncology of Zhejiang Province, Hangzhou, Zhejiang, China*

WP 535 **Direct Determination of Glucosamine including Separation from Epimers in Mouse Plasma by LC-MS/MS**; Kazuo Kanaya; *Ono Pharmaceutical Co., Ltd., Osaka, Japan*

WP 536 **Application of Novel HILIC Column Configurations to Improve LC/ESI/MS Sensitivity of Metabolites**; Anne Mack[1]; William Long[1]; Mia Summers[1]; Adam Bivens[1]; *[1]Agilent Technologies, Inc., Wilmington, DE*

WP 537 **Complementary Analysis and Quantitation of Metabolites by MALDI- and Silicon Nanopost Array-LDI-MS**; Andrew Korte[1]; Akos Vertes[1]; *[1]George Washington University, Washington, DC*

WP 538 **Quantifying the Biomass Composition of Mammalian Cells Using Stable Isotope Internal Standards**; Mya Steadman[1]; Victor Chubukov[1]; *[1]Agios Pharmaceuticals, Cambridge, MA*

WP 539 **Drug Metabolite Identification: Increasing the Separation Power of LC-MS with Differential Mobility Spectrometry and Chemical Modifiers**; Richard P. Schneider[1]; Keith Goodman[2]; Robert Proos[2]; J. Larry Campbell[3]; J. C. Yves Le Blanc[3]; *[1]Pfizer, Groton; [2]Sciex, Framingham, MA; [3]SCIEX, Concord, ON, Canada*

WP 540 **A Compound-Centric Flux Metabolomics Workflow for Labeled and Unlabeled LC-MS Data**; Phillip Seitzer[1]; Susan Ludwigsen[1]; Brian C. Searle[1, 2]; Bradley Evans[3]; *[1]Proteome Software Inc., Portland, OR; [2]University of Washington Genome Sciences, Seattle, WA; [3]Danforth Center, St. Louis, MO*

WP 541 **The Effect of Exercise on Plasma and Muscle in a BALB/c Mouse Model: A Time-Course Study via UHPLC-HRMS**; Michelle Reid[1]; Atiye Ahmadireskety[1]; Yunping Qiu[2]; Irwin Kurland[2]; Timothy J. Garrett[1, 3]; Richard A. Yost[1, 3]; *[1]University of Florida, Department of Chemistry, Gainesville, FL; [2]Albert Einstein College of Medicine, New York, NY; [3]University of Florida, Department of Pathology, Immunology and Laboratory Medicine, Gainesville, FL*

WP 542 **Targeted Metabolomic Profiling of Low and High Grade Serous Epithelial Ovarian Cancer Tissues**; Ali Yilmaz[1]; Gunjal Garg[2]; Praveen Kumar[3]; Onur Turkoglu[3]; David G. Mutch[4]; Matthew A. Powell[4]; Barry Rosen[3]; Ray O. Bahado-Singh[3]; Stewart F. Graham[3]; *[1]Research Scientist, Royal Oak, MI; [2]Karmanos Cancer Institute, Mclaren Flint, Michigan; [3]Beaumont Health, Royal Oak, MI; [4]Washington University School of Medicine, St Louis, MO*

WP 543 **Expanding Mass Spectrometric Metabolomics Coverage of Polar Carbohydrates in Nectar Without Derivatization Using NMR and LC-PAD**; Jeffrey Morre[1]; Claire Lande[1]; Bob Durst[1]; Patrick Reardon[1]; Gracie Galindo[1]; Julie Kirby[1]; Jan Frederik Stevens[1]; Sujaya Rao[2]; *[1]Oregon State University, Corvallis, OR; [2]University of Minnesota, St. Paul, MN*

WP 544 **Metabolite Profile Signatures Associated with Accelerated Aging and Functional Deficiency of Succinate Dehydrogenase in S. Cerevisiae**; Marjorie Jones[1]; Haley Albright[1]; Michael Fitch[1]; Felice de Jong[2]; Tim Garrett[3]; Chris Beecher[2]; John L Hartman IV[1]; *[1]University of Alabama at Birmingham, Birmingham, AL; [2]IROA Technologies LLC, Bolton, MA; [3]University of Florida, Gainesville, FL*

WP 545 **iTree: MSn Mass Spectral Tree Library of Plant Natural Products**; Bennett Haffner[1]; Arpana Vaniya[1]; Sajjan S Mehta[1]; Dinesh Barupal[1]; Oliver Fiehn[1]; *[1]NIH West Coast Metabolomics Center, University of California, Davis, CA, Davis, CA*

WP 546 **Micromolar Phosphate Improves Hydrophilic Interaction Liquid Chromatography Peak Quality without Ion Suppression and Expands Metabolome Coverage**; Jonathan L. Spalding[1, 2]; Fuad J Naser[1]; Stephen L. Johnson[2]; Gary J Patti[1, 2]; *[1]Washington University in St. Louis, Saint Louis, MO; [2]Washington University School of Medicine, St Louis, MO*

WP 547 **Reduction of Interferences for IROA Pattern Detection by Use of SelexION Ion Mobility at Unit Dalton Resolution**; Yunping Qiu[1]; Felice de Jong[2]; Chris Beecher[2]; Irwin Kurland[1]; *[1]Department of Medicine, Albert Einstein College of Medicine, New York City, New York; [2]IROA Technologies LLC, Bolton, MA*

WP 548 **Untargeted Metabolomics Using High-Resolution Mass Spectrometry to Optimize Methods for Dried Blood Spots Analysis**; Vilinh Tran[1]; Dean P Jones[1]; *[1]Emory University School of Medicine, Atlanta, GA*

METABOLOMICS: TARGETED AND QUANTITATIVE ANALYSIS II
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WP 549 **Bioenergy Metabolite Profile in mCRPC Preclinical Models Using Triple Quadrupole Mass Spectrometry and Hyperpolarized Magnetic Resonance Imaging**; Sumankalai Ramachandran[1]; Niki Zacharias[1, 2, 3]; Jaehyuk Lee[3]; Sriram Shanmugavelandy[3]; James McHenry[3]; Prasanta Dutta[3]; Steven Millward[3]; Seth Gammon[3]; Minas Sakellakis[1]; Eleni Efstathiou[1]; Patricia Troncoso[4]; Daniel Frigo[3]; David Piwnica-Worms[3]; Christopher J Logothetis[1, 5]; Sankar N Maity[1]; Pratip Bhattacharya[3]; Mark A Titus[1]; *[1]Department of Genitourinary Medical Oncology, The University of Texas MD Anderson Cancer Center, houston, TX; [2]Department of Bioengineering, Rice University, Houston, TX; [3]Cancer Systems Imaging, The University of Texas MD Anderson Cancer Center, Houston, TX; [4]Department of Pathology, The University of Texas M.D. Anderson Cancer Center, Houston, tx; [5]Department of Clinical Therapeutics, University of Athens, Athens, Greece*

WP 550 **Simultaneous Separation and Quantitation of Branched amino acids (BCAAs) and Corresponding Ketoacids (BCKAs) by a Single LCMS Method**; Zhongyuan Sun[1]; Gang Xing[1]; Eliza Bollinger[1]; Matthew Peloquin[1]; Shashi Bhushan[1]; Rachel Roth Flach[1]; Michelle F. Clasquin[1]; *[1]Pfizer, Cambridge, MA*

WP 551 **Folate Quantification from Wild Lentil (Lens Spp.) Seeds Using Liquid Chromatography Mass Spectrometry**; Haixia Zhang[1]; Randy W. Purves[1]; Hamid Khazaei[1]; Ambuj B. Jha[1]; Thomas D. Warkentin[1]; Albert Vandenberg[1]; *[1]University of Saskatchewan, Saskatoon, SK, Canada*

WP 552 **Baseline Separation of Intracellular Sugar Phosphates by GC-NCI-MS and its Application to 13C-Metabolic Flux Analysis of Cancer Cells**; Nobuyuki Okahashi[1]; Kousuke Maeda[1]; Shuichi Kawana[2]; Hiroshi Shimizu[1]; Junko Iida[2, 3]; Fumio Matsuda[1]; *[1]Osaka University, Suita, Japan; [2]Shimadzu corp., Kyoto, Japan; [3]Osaka University Shimadzu Analytical Innovation Research Laboratory, Osaka University, Suita-shi, Japan*

WP 553 **Fast Track to Metabolic Biomarker Signatures Using the UPLC/MS-based AbsoluteIDQ p180 Kit**; Sri Ramya Donepudi[1]; Vasanta Putluri[1]; Venkatrao Vantaku[1]; Chandrali Shekar Ambati[1]; Arun Sreekumar[1]; Nagireddy Putluri[1]; *[1]Baylor College of Medicine, Houston, TX*

WP 554 **Sensitive and Quantitative Analysis of Phosphorylated Primary Metabolites Using Selective Metal Oxide Enrichment and GC-MS/MS**; Hung Le Si[1]; Tim Causon[1]; Christina Troyer[1]; Stephan Hann[1]; *[1]Division of Analytical Chemistry, Department of Chemistry, University of Natural Resources and Life Sciences (BOKU), Vienna, Austria*

WP 555 **DMABC Derivatization and LC-PRM MS for Measuring Estrogen Metabolites in Human Urine**; Lancia N.F. Darville-Bowleg[1]; John Koomen[1]; Carrie Rozmeski[1]; Yessica Martinez-Monta[1]; Shannan Rich[2]; Lusine Yaghjyan[2]; Kathleen Egan[1]; *[1]Moffitt Cancer Center, Tampa, FL; [2]University of Florida, Gainesville, FL*

WP 556 **A multiplexed LC-SRM assay to investigate steroid hormones in women during pregnancy and early postpartum period**; Serena Di Palma[1]; Pearl La Marca-Ghaemmaghami[2]; Ulrike Ehlert[2]; Firouzeh Farahmand[2]; Roland Zimmermann[3]; Endre Laczko[1]; *[1]Functional Genomics Center Zurich, Zurich, Switzerland; [2]Clinical Psychology and Psychotherapy, Zurich, Switzerland; [3]Obstetrics at the University Hospital Zurich, Zurich, Switzerland*

WP 557 **A Refined LC-MS/MS Method Targeting Bile Acids from the Gut Microbiome**; Mark Sartain[1]; Ariel R Brumbaugh[2]; Michael A Fischbach[2]; *[1]Agilent Technologies, Santa Clara, CA; [2]Department of Bioengineering, Stanford University, Palo Alto, CA*

WP 558 **GFP-guided Single-Cell Microchemical Analysis of Drosophila Melanogaster Neurons from Intact Brains**; Susanne Neupert; *University of Cologne, Cologne, Germany*

WP 559 **Targeted Metabolomics for Characterization of Marine Microbes**; Winifred M. Johnson[1]; Gregory A. Ellis[2]; Erin E. Kelly[1]; Dagmar H. Leary[2]; Gary J. Vora[2]; *[1]National Research Council (NRC) Postdoctoral Fellow, Washington, DC; [2]Naval Research Laboratory, Washington, DC*

WP 560 **Improving Precision in Plasma Amino Acid Analysis for Large Clinical Cohort Studies Using Stable Isotope Internal Standards**; Ying Zhang[1]; Nathaniel Grimes[1]; Brian DeFelice[1]; Jingying Zhao[2]; Oliver Fiehn[1, 3]; *[1]NIH West Coast Metabolomics Center, University of California, Davis, CA, Davis, CA; [2]Department of Epidemiology, University of Florida, Gainesville, FL, Gainesville, FL; [3]Biochemistry Department, King Abdulaziz University, Jeddah, Saudi Arabia, Jeddah, Saudi Arabia*

WP 561 **Metabolic Profiling of Central Carbon Metabolism Pathways in Engineered Microorganisms**; Bryan Fonslow[1]; Bradley B. Schneider[2]; Loren Olson[3]; Baljit K. Ubhi[3]; Julia Khandurina[1]; *[1]Genomatica, San Diego, CA; [2]SCIEX, Concord, ON, Canada; [3]SCIEX, Redwood City, CA*

WP 562 **Fucosyl Monosialoganglioside: Quantitative Analysis of Potential Biomarkers of Lung Cancer Using Immuno-Affinity Enrichment /High Resolution Mass Spectrometry**; Asoka Ranasinghe[1]; Eugene Ciccimaro[2]; Celia D'Arienzo[3]; Serhiy Hnatyshyn[3]; Paul Ponath[4]; Timothy Olah[3]; *[1]Bristol-Myers Squibb Company, Princeton, NJ; [2]Bristol Myers Squibb, Princeton, NJ; [3]Bristol-Myers Squibb Co., Princeton, NJ; [4]Bristol Myers Squibb, Redwood City, CA*

WP 563 **A Rapid Method for Profiling Endogenous Estrogen Metabolites in Human Plasma Using Ultra-Performance Convergence Chromatography-Tandem Mass Spectrometry (UPC2-MS/MS)**; Santosh Raman Acharya[1]; Kumari Ubhayasekera[1]; Jonas Bergquist[1]; *[1]Uppsala University, Uppsala, Sweden*

WP 564 **Quantifying Oxidative Stress Related Biomarkers and Metabolites in Biological Samples Using AccQ-Tag Derivatization followed by UPLC-ESI-MS**; Rajeswari Lakshmanan[1]; Zhao Zhou[1]; Tadimeti Rao[1]; Jiejun Wu[1]; *[1]Janssen Research & Development, LLC, San Diego, CA*

WP 565 **Plasticity of pyrimidine nucleotide metabolism in cancer revealed by multiplexed MRM assays**; Anthony E Cabebe[1]; Wesley R. Armstrong[1]; Joseph R. Capri[1]; Thuc M. Le[1]; Caius G. Radu[1]; *[1]UCLA, Los Angeles, CA*

METABOLOMICS: UNTARGETED METABOLITE PROFILING III
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WP 566 **Metabolomics/Biomarker Discovery Studies: Untargeted analysis by UPLC/High Resolution Mass Spectrometry combined with TWI/MSE-Techniques**; Hannes Dörfler[1]; Stefan Blech[2]; Ralf Laux[1]; *[1]Boehringer-Ingelheim Pharma GmbH & CO KG, Biberach, Germany; [2]Boehringer-Ingelheim Pharma GmbH & Co.KG, Biberach, Germany*

WP 567 **Investigating Metabolic Changes of Radioresistant Breast Cancer Cell Line Using Untargeted Metabolomics**; Zhihao Yu[1]; Ming Huang[2]; Brian H Clowers[1]; *[1]Washington State University, Pullman, WA; [2]University of California, Riverside, CA*

WP 568 **Personal Care Products Alter Skin Chemistry and Microbiome**; Amina Bouslimani[1]; Ricardo da Silva[1]; Tomasz Kosciolek[2]; Stefan Janssen[2]; Amnon Amir[2]; Chris Callewaert[2]; Kathleen Dorrestein[1]; Livia Zaramela[2]; Ji-Nu Kim[2]; Tara Schwartz[2]; Karenina Sanders[2]; Caitriona Brennan[2]; Alexey V. Melnik[1]; Tal Luzzatto-Knaan[1]; Gail Ackermann[2]; Karsten Zengler[2]; Rob Knight[2, 3, 4]; Pieter C. Dorrestein[1, 3, 5]; *[1]University of California San Diego, Skaggs School of Pharmacy and Pharmaceutical Sciences, La Jolla, CA; [2]University of California San Diego, Department of Pediatrics, La Jolla, CA; [3]Center for Microbiome Innovation, University of California San Diego, La Jolla, CA; [4]University of California San Diego, Department of Computer Science and Engineering, La Jolla, CA; [5]University of California San Diego, Department of Pharmacology, La Jolla, CA*

WP 569 **Development of a Metabo-Redoxome Platform to Assess the Oxidative Stress in the Lower Respiratory Tract caused by Smoking and HIV-Infection**; Miriam Sindelar[1]; Darya V Akimova[1]; Sarah L O'Beirne[1]; Ronald G Crystal[1]; Steven S. Gross[1]; *[1]Weill Cornell Medical College, New York, New York*

WP 570 **LC/MS-Based Metabolomic Approach to the Effect of Co-Administration of Fenofibrate with Atorvastatin in Hyperlipidemic Patients**; Ji Soo Han; Geum-Sook Hwang; Sang Hak Lee *Korea Basic Science Institute, Seoul, South Korea*

WP 571 **Nanoparticle Microarray for High-Throughput Metabolomics of Turkey Gut Microbiome Using Matrix-Assisted Laser Desorption/Ionization-Mass Spectrometry (MALDI-MS)**; Rebecca Hansen[1]; Maria Emilia Dueñas[1]; Torey Looft[2]; Young-Jin Lee[1]; *[1]Iowa State University, Ames, IA; [2]USDA-ARS, National Animal Disease Center, Ames, Iowa*

WP 572 **Mass Spectrometry-Based Metabolomics for the Investigation of Lung Cancer Susceptibility in Smokers from Two Ethnic Groups**; Romel Dator[1]; Peter W. Villalta[1]; Laura A. Maertens[1]; Joni A. Jensen[2]; Sharon E. Murphy[1]; Irina Stepanov[1]; Dorothy K. Hatsukami[1, 2]; Benedikt Warth[3, 4]; Silvia Balbo[1]; *[1]Masonic Cancer Center, University of Minnesota, Minneapolis, Minnesota; [2]Department of Psychiatry, University of Minnesota, Minneapolis, Minnesota; [3]University of Vienna, Faculty of Chemistry, Department of Food Chemistry and Toxicology, Währinger Straße 38, Austria; [4]Scripps Center for Metabolomics, The Scripps Research Institute, La Jolla, CA*

WP 573 **A Multi-Omics Approach to Reveal the Effects of Chemical- and Salmonella-induced Inflammation on Murine Intestines**; Jikang Wu[1]; Mikayla Borton[1]; Anice Sabag-Daigle[1]; Brian Ahmer[1]; Kelly Wrighton[1]; Vicki Wysocki[1]; *[1]The Ohio State University, Columbus, OH*

WP 574 **HILIC-LC-MS/MS Provides a Powerful Approach for the Non-Targeted Characterization of a Wide Range of Gut Microbiome Metabolites**; David T. Reeves[1, 2]; J. Alfredo Blakeley-Ruiz[2, 3]; Mallory P. Ladd[1, 2]; Robert L. Hettich[1, 2]; *[1]Bredesen Center for Interdisciplinary Research and Graduate Education, University of Tennessee, Knoxville, TN; [2]Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN; [3]Genome Science and Technology Program, University of Tennessee, Knoxville, Tennessee*

WP 575 **Comprehensive Chemical Characterization of Complex Matrices through Integration of Multiple Analytical Modes and Databases for LC-HRAM-MS-Based Non-Targeted Screening**; Christian Wachsmuth[1]; Daniel Arndt[1]; Elyette Martin[1]; Christoph Buchholz[1]; Mark Bentley[1]; *[1]PMI R&D, Philip Morris Products S.A., Neuchâtel, Switzerland*

WP 576 **Interrogating the Effect of Sleep Disruption on the Mouse Metabolome via Un-Targeted and Targeted LC/MS**; Fernando Vargas[1]; Samuel James Bowers[2]; Antonio González[3]; Rob Knight[3]; Fred Turek[2]; Martha Hotz Vitaterna[2]; Pieter C. Dorrestein[1]; *[1]Skaggs School of Pharmacy & Pharmaceutical Sciences, University of California, San Diego, CA; [2]Department of Neurobiology, Northwestern University, Evanston, IL; [3]Department of Pediatrics, University of California, La Jolla, CA*

WP 577 **Large-Scale Longitudinal Metabolomics Study Reveals Major Metabolic Alterations during Gestational Diabetes Mellitus**; Hongzhi Zhao[1]; Shunqing Xu[2]; Zongwei Cai[1]; *[1]State Key Laboratory of Environmental and Biological Analysis, Department of Chemistry, Hong Kong Baptist University, Hong Kong, Hong Kong; [2]State Key Laboratory of Environmental Health (Incubation), School of Public Health, Tongji Medical College, Huazhong University of Science and Technology, Wuhan, China*

WP 578 **Serum Metabolic Profiling of a High-Grade Serous Ovarian Cancer (HGSOC) Mouse Model: Insights into Disease Progression**; Danning Huang[1]; Yong-Hyun Shin[2]; David A. Gaul[1]; Jaeyeon Kim[2]; Facundo M. Fernandez[1]; *[1]Georgia Institute of Technology, Atlanta, GA; [2]Indiana University School of Medicine, Indianapolis, Indiana*

WP 579 **Metabolomics Nanostructure Imaging Mass Spectrometry (NIMS) with Perfluorinated Gold Nanoparticles**; Amelia Palermo[1]; Erica M Forsberg[2]; Benedikt Warth[3]; Aries E Aisporna[1]; Paul H Benton[1]; Gary Siuzdak[1, 4]; *[1]Scripps Center for Metabolomics, The Scripps Research Institute, 10550 North Torrey Pines Rd., La Jolla, California; [2]Department of Chemistry and Biochemistry, San Diego State University, 5500 Campanile Dr., San Diego, California; [3]Department of Food Chemistry and Toxicology, Faculty of Chemistry, University of Vienna, Waehringerstrasse 38, Austria; [4]Departments of Chemistry, Molecular, and Computational Biology, The Scripps Research Institute, 10550 North Torrey Pines Road, La Jolla, California*

WP 580 **High-Throughput Metabolite Profiling of Yeast and Plant Material Using Flow Injection Electrospray High-Resolution Mass Spectrometry (FIE-HRMS)**; João B. Mokochinski[1]; Roland Tengölics[1]; Balázs Szappanos[1]; Anikó Galambos[1]; Balázs Papp[1]; Szilvia Z. Tóth[1]; *[1]Biological Research Centre, Szeged, Hungary*

WP 581 **Direct Injection FTICR-Mass Spectrometry for Deep Metabotyping in Microbiome Related Research**; Philippe Schmitt-Kopplin[1]; Franco Moritz[1]; Marianna Lucio[1]; Alesia Walker[1]; Daniel Hemmler[1]; Nina Silner[1]; Sara Forcisi[1]; *[1]Helmholtz-Zentrum München (BGC, analytical BioGeoChemistry), München, Germany*

WP 582 **Intelligent MSn-Based Untargeted Metabolomics Workflow for Biomarker Discovery in Crohn's Disease**; Ioanna Ntai[1]; Amanda L. Souza[1]; Ralf Tautenhahn[1]; Gina Tan[1]; Andreas FR Huhmer[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

WP 583 **Strategies for Integrating Metabolomic Results with Other Omics Datasets – A Study of Methotrexate on Human Promyelocytic Leukemia Cells**; Randi Gant-Branum[1]; Stacy D. Sherrod[2, 3]; Simona G. Codreanu[2, 3]; Alexandra C. Rutledge[2, 3]; Danielle B. Gutierrez[4]; James C. Pino[2]; Michael Ripperger[2]; Tina Tsui[4]; Melissa Farrow[2]; Carlos F. Lopez[2]; Richard M. Caprioli[2, 4, 5]; John A. McLean[2, 3, 6]; *[1]Vanderbilt University, Greenbrier; [2]Vanderbilt University, Nashville; [3]Center for Innovative Technology, Vanderbilt University, Nashville, TN; [4]Vanderbilt Mass Spectrometry Research Center and Department of Biochemistry, Vanderbilt University School of Medicine, Nashville, TN; [5]Vanderbilt University Medical Center, Nashville, TN; [6]Vanderbilt Institute for Integrative Biosystems Research and Education, Nashville, TN*

WP 584 **Parallel Metabolomics Profiling of Human Cerebrospinal Fluid and Serum for Discovering Biomarkers to Assess Severity of Acute Spinal Cord Injury**; Minglei Zhu[1]; Xinyun Gu[1]; Hao Li[1]; Wei Han[1]; Brian Kwon[2]; Liang Li[1]; *[1]University of Alberta, Edmonton, AB, Canada; [2]University of British Columbia, Vancouver, BC, Canada*

WP 585 **Assessing Structural Diversity in Large-Scale LC-MS/MS Data Sets by Creating Informative Chemical maps based on molecular family and substructure recognition**; Justin J.J. van der Hooft[1, 2, 3]; Madeleine Ernst[2, 4]; Ricardo da Silva[2, 3]; Kyo Bin Kang[2, 5]; Joe Wandy[6]; Mingxun Wang[2, 3]; Marnix H. Medema[1]; Simon Rogers[6]; Pieter C. Dorrestein[2, 3, 7]; *[1]Bioinformatics Group, Department of Plant Sciences, Wageningen University, Wageningen, Netherlands; [2]Collaborative Mass Spectrometry Innovation Center, Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA; [3]Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California, San Diego, La Jolla, California; [4]Skaggs School of Pharmacy & Pharmaceutical Sciences, University of California San Diego, San Diego, CA; [5]College of Pharmacy and Research Institute of Pharmaceutical Sciences, Seoul National University, Seoul, South Korea; [6]Glasgow Polyomics, University of Glasgow, Glasgow, UK; [7]Center for Microbiome Innovation, University of California San Diego, La Jolla, CA*

WP 586 **Untargeted Metabolomics Analysis of Equine Synovial Fluid Reveals Association of Osteoarthritis with Environmental Toxins and Anti-Inflammatory Regulators**; Maria Elena Diaz Rubio[1]; Elizabeth T. Anderson[1]; Jin Su[2]; Heidi L. Reesink[2]; Sheng Zhang[1]; *[1]Institute of Biotechnology, Cornell University, Ithaca, NY; [2]College of Veterinary Medicine, Cornell University, Ithaca, NY*

WP 587 **The Microbiomes and Metabolomes of the Toxin-Producing Microalgae Pseudo-Nitzschia**; Irina Koester[1]; Daniel Petras[2]; John K. Brunson[1, 3]; Louis-Félix Nothias[2]; Margot E. White[1]; Kai Dührkop[4]; Sebastian Böcker[4]; Farooq Azam[1]; Rob Knight[5]; Andrew E. Allen[1, 3]; Pieter C. Dorrestein[2]; Lihini I. Aluwihare[1]; *[1]Scripps Insitution of Oceanography, La Jolla; [2]Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California, San Diego, La Jolla, California; [3]J. Craig Venter Institute, La Jolla, CA; [4]Friedrich-Schiller-University Jena, Jena, Germany; [5]Departments of Pediatrics and Computer Science & Engineering, University of California San Diego, La Jolla, CA*

WP 588 **Metabolomics of Solanum Lycopersicum Infected by Phytophthora Infestans Lead to Late Blight Detection and Reveals Metabolic Differences in Infection Times.**; Paula Liliana Galeano[1, 2]; Fábio Neves dos Santos[3]; Marcos Nogueira Eberlin[3]; Chiara Carazzone[4]; *[1]Laboratory of Advanced Analytical Techniques in Natural Products, Universidad de los Andes, Bogotá, Colombia; [2]Facultad de Ciencias Básicas, Universidad de la Amazonia, Florencia, Colombia; [3]ThoMSon Mass Spectrometry Laboratory, University of Campinas, Campinas, Brazil; [4]Laboratory of Advanced Analytical Techniques in Natural Products. Universidad de los Andes, Bogotá, Colombia*

WP 589 **Untargeted LC-MS Analysis of 3D Cell Cultures Exposed to Cigarette Smoke and Aerosol from a Novel Tobacco Vapor Product**; Yuichiro Takanami[1]; Nobumasa Kitamura[1]; Shigeaki Ito[1]; *[1]Japan Tobacco Inc., Yokohama, Japan*

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WP 590 **A High Resolution/Accurate Mass Data Dependent-Constant Neutral Loss-MS3 (DDA-CNL/MS3) DNA Adductomic Method for the Investigation of Alcohol-Related DNA Damage**; Valeria Guidolin[1, 2]; Andrea Carra'[2]; Erik S. Carlson[2]; Peter W. Villalta[2]; Silvia Balbo[1, 2]; *[1]Division of Environmental Health Sciences, University of Minnesota, Minneapolis, MN; [2]Masonic Cancer Center, University of Minnesota, Minneapolis, MN*

WP 591 **Differentiating Positional Isomers of Nucleoside Modifications by Higher-Energy Collisional Dissociation Mass Spectrometry**; Manasses Jora[1]; Balasubrahmanyam Addepalli[1]; Peter Lobue[1]; Robert Ross[1]; Patrick A. Limbach[1]; *[1]University of Cincinnati, Cincinnati, OH*

WP 592 **Unraveling the Radiation Resistance Network of Cryptococcus Neoformans by Genome Wide Transcriptome Analysis and Mass Spectrometry**; Mellie Paulines[1]; Patrick A. Limbach[1]; *[1]University of Cincinnati, Cincinnati, OH*

WP 593 ***In vitro* Metabolism Study of 2'-Ribose Unmodified and Modified Phosphorothioate Oligonucleotides for the Design of Antisense Therapeutics Using LC-MS/MS**; Jaeah Kim[1]; Michael G Bartlett[1]; *[1]University of Georgia, Athens, GA*

WP 594 **Identification of Box C/D sRNA-Guided 2'-O-Methylation at Position 34 of Sulfolobus acidocaldariustRNAs by Liquid Chromatography Tandem Mass Spectrometry**; Ningxi Yu[1]; Patrick A Limbach[2]; *[1]University of Cincinnati, Cincinnati; [2]University of Cincinnati, Cincinnati, OH*

WP 595 **Degradation Profiles and Kinetics of Phosphorothioate Oligonucleotides Using Liquid Chromatography Mass Spectrometry**; Noha Morsy Elzahar[1]; Nancy Magdy[2]; Amira M El-Kosasy[2]; Michael G Bartlett[1]; *[1]University of Georgia, Athens, GA; [2]Pharmaceutical Analytical Chemistry Department, Faculty of Pharmacy, Ain Shams University, Cairo, Egypt*

WP 596 **Forced Degradation of an Oligonucleotide – Impurity Identification and Quantitation**; Carolyn F Rosewall[1]; Jie Ding[1]; Bonnie E Gulley[1]; *[1]PPD Laboratories, Middleton, WI*

WP 597 **Cytotoxic and Mutagenic Properties of O6-Alkyl-2'-deoxyguanosine Lesions in Escherichia coli Cells**; Pengcheng Wang[1]; Yinsheng Wang[1]; *[1]Department of Chemistry, University of California, Riverside, Riverside, CA*

WP 598 **Elucidation of Paromomycin Binding Sites in an a Site Model of the 16S Ribosomal RNA by Native Top-Down MS**; Jovana Vusurovic[1]; Kathrin Breuker[1]; *[1]University of Innsbruck, Innsbruck, Austria*

WP 599 **Novel Aspects on Chemical Protein-RNA Cross-Linking Coupled with Mass Spectrometry**; Alexander Wulf[1]; Luisa M. Welp[1]; Seychelle Vos[1]; Alexandra Stützer[1]; Patrick Cramer[1]; Henning Urlaub[1]; *[1]Max Planck Institute for biophysical chemistry, Göttingen, Germany*

WP 600 **Interrogating the Conformation of HIV-1 Gag and the Stoichiometry of which it Binds Genomic RNAs with Native Mass Spectrometry**; Samantha H Sarni[1]; Erik D Olson[1]; Karin Musier-Forsyth[1]; Vicki Wysocki[1]; *[1]The Ohio State University, Columbus, OH*

WP 601 **A Novel Analytical Approach for Measuring Oxidative Stress in Cells**; Ranran Wu[1]; Kevin Janssen[1]; Benjamin A Garcia[1]; *[1]University of Pennsylvania, Philadelphia, PA*

WP 602 **Quantification of Tobacco-Specific Nitrosamine-Induced DNA Adducts in Mammalian Cells by LC-MS/MS**; Su Guo[1]; Jiapeng Leng[1]; Yinsheng Wang[1]; *[1]University of California, Riverside, Riverside, CA*

WP 603 **An Adductomic Approach for Assessing the Regulation of Epitranscriptome**; Gwendolyn Gonzalez[1]; David Bade[1]; Yinsheng Wang[2]; *[1]University of California Riverside, Riverside, CA; [2]University of California, Riverside, Riverside, CA*

WP 604 **A Software Tool for Characterizing Modified Oligonucleotides Using Highly-Accurate Tandem Mass Spectrometry Data**; Hiroshi Nakayama[1]; Masami Koike[1]; Masato Taoka[2]; Nobuhiro Takahashi[3]; Toshiaki Isobe[2]; *[1]RIKEN Center for Sustainable Resource Science, Wako, Japan; [2]Tokyo Metropolitan University, Tokyo, Japan; [3]Tokyo University of Agriculture and Technology, Fuchu, Japan*

WP 605 **Characterization of Oligonucleotide Biotransformation Using Ion-Paring Reverse-Phase Liquid Chromatography Coupled with High Resolution Mass Spectrometry**; Fang Xie[1]; Babak Basiri[1]; Julie Lade[1]; Mai Thayer[1]; David Doherty[1]; Omar Barnaby[2]; Brooke Rock[1]; *[1]Amgen, South San Francisco; [2]Amgen, Inc., Thousand Oaks, CA*

WP 606 **Replication Studies of N2-Alkylguanine Lesions in Human Cells**; Jun Wu[1]; Yinsheng Wang[1]; *[1]UCR, Riverside, CA*

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WP 607 **Data-Independent Acquisition Mass Spectrometry to Localize Phosphosites**; Qing-Run Li[1]; Shi-Sheng Wang[1]; Hong-Wen Zhu[1]; Fang-Ying Xia[1]; Jia-Rui Wu[1]; Rong Zeng[1]; *[1]Institute of Biochemistry and Cell Biology, Chinese Academy of Sciences, Shanghai, China*

WP 608 **Discovery of N-linked and O-linked Glycosylation in Neuropeptides in the Crustacean Nervous System**; Qinjingwen Cao[1]; Qing Yu[2]; Yang Liu[1]; Zhengwei Chen[1]; Lingjun Li[1, 2]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [2]School of Pharmacy, University of Wisconsin-Madison, Madison, WI*

WP 609 **Photochemical Reduction of Disulfide Bond Facilitates Structural Analysis of Disulfide Rich Peptides and Proteins**; Sarju Adhikari[1]; Xiaoyue Yang[2]; Yu Xia[1, 2]; *[1]Purdue University, West Lafayette, IN; [2]Tsinghua University, Beijing, China*

WP 610 **Exposing Structural Influences on Peptide Deamidation and Isomer Production**; Dylan L. Riggs[1]; Sonia V. Gomez[1]; Ryan R. Julian[1]; *[1]University of California, Riverside, CA*

WP 611 **Identifying Membrane Protein Phosphorylation Sites by Mass Spectrometry Using *in vitro* Translation into Nanodiscs**; Brian Conti; *UW Biotech Center, Madison, WI*

WP 612 **Elucidating the Various Multi-Phosphorylation Statuses of Proteins Functional Regions by Ultraviolet Photodissociation**; Zheyi Liu[1]; You Jiang[2]; Chunlei Xiao[1]; Xingchuang Xiong[2]; Xiang Fang[2]; Fangjun Wang[1]; Xueming Yang[1]; *[1]Dalian Institute of chemical physics, Chinese Academy of Sciences, Dalian, China; [2]National Institute of Metrology, Beijing, China*

WP 613 **Experimental Investigations of Serine Racemization Mechanism**; Ran Qiu[1]; Ryan R. Julian[1]; *[1]UC Riverside, Riverside, CA*

WP 614 **Identification of Citrullination Sites in Human Neutrophils by Accurate Annotation of Mass Spectrometry Data**; Raghothama Chaerkady[1]; Matthew Glover[1]; Chelsea Boo[1]; Kristen Lekstrom[1]; Wen Yu[1]; Yebin Zhou[1]; Nanette Mittereder[1]; Gary P Sims[1]; Sonja Hess[1]; *[1]MedImmune, Gaithersburg*

WP 615 **Systematic Proteomic Analysis of Protein Methylation in Prokaryotes and Eukaryotes Revealed Distinct Substrate Specificity**; Min Zhang[1]; Minjia Tan[1]; *[1]Shanghai Institute of Materia Medica, Shanghai, China*

WP 616 **Tryptic Peptides Bearing C-Terminal Dimethyllysine need be Considered during the Analysis of Lysine Dimethylation in Proteomic Study**; Minjia Tan[1]; Min Zhang[1]; Ming Chen[1]; Linhui Zhai[1]; *[1]Shanghai Institute of Materia Medica, Shanghai, China*

WP 617 **Analysis of Hydroxyproline-Containing Tryptic Peptide in Alpha1 Collagen Chain from Porcine Using UHPLC/QTOF MS**; Akio Hayashi[1]; Hiroshi Sezaki[2]; *[1]Agilent Technologies, Suita, Japan; [2]Agilent Technologies Japan, Ltd, Hachioji, Japan*

WP 618 **Characterization of Novel Triple Oxidation of Cysteine in an Insulin Analog under Oxidative Stress Using Mass Spectrometry**; Chunyan Gu; *Merck, Kenilworth, NJ*

WP 619 **Systematic Characterization of the Chromatographic and Mass Spectrometric Properties of 21 Post-Translational Modifications Using Synthetic Peptides**; Daniel P Zolg[1]; Mathias Wilhelm[1]; Siegfried Gessulat[1, 2]; Tobias Schmidt[1]; Patroklos Samaras[1]; Karsten Schnatbaum[3]; Johannes Zerweck[3]; Tobias Knaute[3]; Ulf Reimer[3]; Hans-Christian Ehrlich[2]; Stephan Aiche[2]; Pedro Navarro[4]; Bernard Delanghe[4]; Andreas Huhmer[5]; Bernhard Kuster[1, 6, 7]; *[1]Technical University Munich, Chair of Proteomics and Bioanalytics, Freising, Germany; [2]SAP SE, Potsdam, Germany; [3]JPT Peptide Technologies GmbH, Berlin, Germany; [4]Thermo Fisher Scientific, Bremen, Germany; [5]Thermo Fisher Scientific, San Jose, CA; [6]Center for Integrated Protein Science (CIPSM), Munich, Germany; [7]Bavarian Center for Biomolecular Mass Spectrometry, Freising, Germany*

WP 620 **Multiple Acquisition Methods on the Orbitrap Fusion Lumos Detect PARP14-Dependent Adp-Ribosylation**; Hideyuki Higashi[1]; Takashi Maejima[1]; Lang Ho Lee[1]; Yukiyoshi Yamazaki[1]; Masanori Aikawa[1, 2]; Sasha Singh[1]; *[1]Center for Interdisciplinary Cardiovascular Sciences, Brigham and Women's Hospital, Harvard Medical School, Boston, MA; [2]Center for Excellence in Vascular Biology, Cardiovascular Division, Brigham and Women's Hospital, Harvard Medical School, Boston, MA*

WP 621 **Differentiation of Aspartic and Iso-Aspartic Acid in Peptides by UVPD**; Aarti Bashyal[1]; John Hui[2]; Tawny Flick[3]; Andrew Dykstra[3]; Qingchun Zhang[4]; Iain D. G. Campuzano[2]; Jennifer S Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX; [2]Discovery Attribute Sciences, Amgen, Thousand Oaks, CA; [3]Pivotal Attribute Sciences, Amgen, Thousand Oaks, CA; [4]Biological Relevance and Characterization, Amgen, Thousand Oaks, CA*

WP 622 **Chemical Modification and Mass Spectrometry Analysis for Delineating Deacetylase-specific Acetylome**; Hsin-Yi Wu[1]; Hsin-Yi Lin[2]; Chuan-Fa Chang[3]; Yu-Ju Chen[2]; Pang-Hung Hsu[4]; *[1]Mass Spectrometry Division, Instrumentation Center, College of Science, National Taiwan University, Taipei, Taiwan; [2]Institute of Chemistry, Academia Sinica, Taipei, Taiwan; [3]Department of Medical Laboratory Science and Biotechnology, College of Medicine, National Cheng Kung University, Tainan, Taiwan; [4]Department of Bioscience and Biotechnology, National Taiwan Ocean University, Keelung, Taiwan*

PEPTIDES: TARGETED AND QUANTITATIVE ANALYSIS II
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WP 623 **Mouse Phenotyping by Quantification of Plasma Proteins Using 500 Multiplexed MRM Assays**; Sarah A. Michaud[1]; Nicholas J.T. Sinclair[1]; Helena Pětrošová[1]; Andrea L. Palmer[1]; Yassene Mohammed[1, 2]; Azad Eshghi[1]; Vincent R. Richard[3]; Albert Sickmann[4]; Christoph H. Borchers[1, 3, 5, 6]; *[1]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [2]Center for Proteomics and Metabolomics, Leiden University, Leiden, Netherlands; [3]Jewish General Hospital Proteomics Centre, McGill University, Montreal, QC, Canada; [4]Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Dortmund, Germany; [5]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada; [6]Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC, Canada*

WP 624 **Quantification of Pre-fusion Hemagglutinin in Potentially Pandemic H7N9 Influenza Vaccines Using a Limited Tryptic Digestion-Isotope Dilution Mass Spectrometry Method**; Keith R Morgenstern[1]; Tracie L Williams[1]; Yingxia Wen[2]; Giuseppe Palladino[2]; Yuhong Xie[2]; Ethan C Settembre[2]; John R Barr[1]; *[1]CDC, Atlanta, GA; [2]Seqirus, Cambridge, MA*

WP 625 **Challenges in the Development of Sensitive Methods and Stability Assessments of an Incretin Peptide in Rat, Monkey Plasma Using LC-MS/MS**; Cynthia M. Chavez-Eng[1]; Huaibing He[1]; Weixun Wang[1]; Dina Goykhman[1]; Lucinda Hittle[1]; Punam Sandhu[1]; *[1]Merck Research Laboratories, Kenilworth, NJ*

WP 626 **Strategies to Improve Sensitivity and Reduce Carryover in Therapeutic Peptide Bioanalysis by LC-MS/MS: A Case Study of Liraglutide**; Ying Peng[1]; Moo-Young Kim[1]; Rand Jenkins[2]; Fumin Li[1]; *[1]PPD labs, Middleton, WI; [2]PPD labs, Richmond, VA*

WP 627 **Therapeutic Teriparatide Peptide Impurities by Liquid Chromatography High Resolution Mass Spectrometry**; Kui Zeng[1]; Ilan Geerlof-Vidavsky[1]; Xiaoshi Wang[2]; Sarah Rogstad[3]; Eric pang[3]; David Keire[1]; *[1]FDA Division of Pharmaceutical Analysis, St Louis, MO; [2]FDA Division of Pharmaceutical Analysis, Silver Spring, MD; [3]FDA, Silver Spring, MD*

WP 628 **A Targeted Proteomics Workflow Employing 15-Plex Isobaric Reagents and Sample Multiplexing**; Craig Braun[1, 2]; Brian K. Erickson[2, 3]; Steven P. Gygi[3]; *[1]Havard Medical School, Boston, MA; [2]IQ Proteomics LLC, Cambridge, Massachusetts; [3]Harvard Medical School, Boston, MA*

WP 629 **Using Electrokinetic Injection to Increase throughput and Improve Sensitivity in the Detection of Proteins by CE-MS**; Stephen J. Lock[1]; Esme Candish[2]; Edna Betgovargez[3]; Christopher Loessnner[4]; *[1]SCIEX, Warrington, UK; [2]Sciex, Framingham, MA; [3]SCIEX, Brea, California; [4]SCIEX, Darmstadt, Germany*

WP 630 **Comparison of Peptide Parallel Reaction Monitoring via MS2 and MS3 Methods**; Philip M Remes[1]; Romain Huguet[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

WP 631 **Development of an MRM Assay to Distinguish Active and Latent TGF-β**; Chelsea C. Boo[1]; Raghothama Chaerkady[1]; Sonja Hess[1]; *[1]MedImmune, Gaithersburg, MD*

WP 632 **Rapid and Improved Assay of Surfactins from Bacillus subtilis, 203R via LC-ESI-MS.**; David M Wright[1]; Nadja B. Cech[1]; Daniel A. Todd[1]; *[1]University of NC - Greensboro, Greensboro, NC*

WP 633 **Development and Validation of a sensitive UPLC-MS/MS Method for the Quantitation of Liraglutide in Human Plasma**; Hui Hong[1]; Fei Wang[1]; Jianhong Lu[1]; Changming Yang[1]; Wenzhong Liang[1]; Xin Zhang[1]; *[1]WuXi Apptec, Shanghai, China*

WP 634 **Development of Highly Sensitive HPLC/MS/MS Method for the Concurrent Quantitation of Insulin and Insulin Analogs in Human Plasma**; Siethoff Christoph[1]; Manisha Saxena[1]; David Benda[1]; Werner Döbelin[2]; *[1]Swiss BioQuant, Reinach, Switzerland; [2]Prolab Instruments GmbH, Reinach, Switzerland*

WP 635 **Evaluating Bias in MS-based Light:Heavy Peptide Ratio Measurement**; David M Bunk; *NIST, Gaithersburg, MD*

WP 636 **Identification and Quantitation of Intact Antibody Mixtures**; Olivier Mozziconacci[1]; Elizabeth Pierson[1]; Sarita N. Mittal[2]; George Svitel[2]; Jason Cheung[2]; Roy Helmy[1]; *[1]Merck & Co., Inc., Rahway, NJ; [2]Merck & Co., Inc., Kenilworth, NJ*

WP 637 **HDAC6 Deacetylase does not Modulate Acetylation or Phosphorylation on Tau KIGS Motifs in PS19 Mice**; Bekim Bajrami[1]; Veronica Bieber[1]; Rachelle Driscoll[1]; H. Moore Arnold[1]; Frank Rigo[2]; Karen Ling[2]; Heike Hering[1]; Peter Juhasz[1]; Ru Wei[1]; *[1]Biogen, Cambridge, MA; [2]Ionis Pharmaceuticals, Inc., Carlsbad, CA*

WP 638 **Quantification of cobalamin sensitive proteins in marine microbial communities under changing environmental conditions. What's in a bucket of seawater?**; Elden Rowland[1]; Kira More[1]; Tor Kitching[1]; Erin M. Bertrand[1]; *[1]Dalhousie University, Halifax, NS*

WP 639 **Revealing the DPP4 Proteome: Discovery of Novel Substrates Using N-terminal Proteomics**; Shen Zhang[1]; Erin Mulvihill[1, 2]; Brett Larsen[1]; Karen Colwill[1]; Anne-Claude Gingras[1]; Daniel Drucker[1]; *[1]Lunenfeld-Tanenbaum Research Institute at Mount Sinai Hospital, Toronto; [2]University of Ottawa Heart Institute, Ottawa, ON, Canada*

WP 640 **Extraction of Microcystins from Plasma and Serum and their Quantification by LC-ESI-orbitrap-MS and LC-ESI-QqQ-MS/MS**; Dilrukshika S. W. Palagama[1]; David Baliu-Rodriguez[2]; Apurva Chandrakant Lad[2]; Bruce S Levison[2]; David J Kennedy[1]; Steven T Haller[2]; Judy Westrick[3]; Kenneth Hensley[4]; Dragan Isailovic[2]; *[1]University of Toledo, Toledo, OH; [2]The University of Toledo, Toledo, OH; [3]Wayne State University, Detroit , MI; [4]Arkansas College of Osteopathic Medicine, Fort Smith, Arkansas*

WP 641 **Development of a Liquid Chromatography Tandem Mass Spectrometry (LC-MS/MS) Method for the Quantification of C3adesArg in Human Serum**; James Vannicola[1]; Elizabeth Hyer[1]; Bob Xiong[1]; *[1]ICON, Whitesboro, NY 13492*

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WP 642 **Development of a Hybrid Immunoaffinity-LC-MS/MS Bioanalytical Method for the Highly Sensitive Quantification of Active Infliximab and Adalimumab**; Caitlin M. Dunning[1]; Mary E Lame[1]; Steven R. Calciano[1]; *[1]Waters Technologies Corporation, Milford, MA*

WP 643 **Development of a Quantitative Mass Spectrometry-based Multiple-Attribute Method (MAM) for Fast Quality Control Testing and Characterization of Fusion Protein Etanercept**; Daniel Michael Waldera-Lupa[1]; Gerhard Körting[1]; Yvonne Jasper[1]; Julia Brückner[1]; Heiner Falkenberg[1]; Anke Schnabel[1]; Roland Moussa[1]; *[1]Protagen Protein Services, Dortmund, Germany*

WP 644 **At-Line Mass Spectrometry-Based Process Analytical Technology for Linking Amino Acid Concentrations and Bioreactor Product Quality**; David Naoki Powers[1]; Sai Rashmika Velugula[1]; Nicholas Trunfio[1]; Phillip Angart[1]; Anneliese Faustino[1]; Cyrus Agarabi[1]; *[1]FDA, Silver Spring, MD*

WP 645 **Quantitation of Omalizumab from Human Plasma Using Nano-Surface and Molecular-Orientation Limited (nSMOL) Proteolysis and LC-MS/MS**; Deepti Bhandarkar[1]; Rashi Kochhar[1]; Shailendra Rane[1]; Shailesh Damale[1]; Purushottam Sutar[1]; Anant Lohar[1]; Ashutosh Shelar[1]; Navin Devadiga[1]; Bhaumik H Trivedi[1]; Jitendra Kelkar[1]; Pratap Rasam[1]; Ajit Datar[1]; Toshiya Matsubara[2]; *[1]Shimadzu Analytical (India) PVT LTD, Mumbai, India; [2]Shimadzu Corporation, Kyoto, Japan*

WP 646 **Applying Parallel Reaction Monitoring (PRM) for Multi-Attribute Method (MAM) in Late Stage Biotherapeutic Development**; Hao Zhang[1]; Ryan Petitt[1]; Ramsey Saleem[1]; Alla Polozova[1]; *[1]Amgen, Cambridge, MA*

WP 647 **A General IgG-Based Therapeutic mAb Quantification Method Using Protein G Purification and a Two Internal Standard Calibration Strategy**; Huai-Hsuan Chiu[1]; Hsiao-Wei Liao[1]; Yu-Yun Shao[2]; Yen-Shen Lu[2]; Ching-Hung Lin[2, 3]; I-Lin Tsai[4]; Ching-Hua Kuo[5]; *[1]School of Pharmacy, College of Medicine, National Taiwan University, Taipei, Taiwan; [2]Department of Oncology, National Taiwan University Hospital, Taiwan, Taipei, Taiwan; [3]Department of Internal Medicine, National Taiwan University Hospital, Taiwan, Taipei, Taiwan; [4]Department of Biochemistry and Molecular Cell Biology, School of Medicine, College of Medicine, Taipei Medical University, Taipei, Taiwan, Taipei, Taiwan; [5]School of Pharmacy, College of Medicine, National Taiwan University, Taipei, Taiwan, Taipei, Taiwan*

WP 648 **What Sample Preparation to Choose for MS based mAbs Quantification in Human Serum?**; Jerome Vialaret[1]; Sophie broutin[2]; Celia Puginier[1]; Sophie Santelé[1]; Aurore Jaffuel[3]; Alan Barnes[4]; Laurent Tiers[1]; Laurent Pelletier[5]; Sylvain Lehmann[1]; Angelo Paci[6]; Christophe Hirtz[1]; *[1]University of Montpellier, LBPC- IRMB, CHU Montpellier, Montpellier, France; [2]Service de pharmacologie, Département de Biologie et Pathologie Médicales, Gustave Roussy et Université Paris Saclay, Villejuif, France; [3]Shimadzu Corporation, Marne-la-Vallée, France; [4]Shimadzu Corporation, Manchester, UK; [5]Grenoble Institut des Neurosciences, grenoble, France; [6]2 Service de pharmacologie, Département de Biologie et Pathologie Médicales, Gustave Roussy et Université Paris Saclay, Villejuif, France*

WP 649 **A Novel and Universally-Applicable Antibody Free Multiple-Mechanism Peptide Level Enrichment Strategy for High Sensitive Target Protein Quantification**; Jie Pu[1]; Bo An[1]; Ming Zhang[1]; Yang Qu[1]; Jun Qu[1]; *[1]SUNY, at Buffalo, Buffalo, NY*

WP 650 **Evaluation of Monoclonal Antibody Subunit Analysis and High Resolution Accurate Mass for Quantitative Analysis**; Keeley Murphy[1]; Jonathan Josephs[2]; Stephane Houel[2]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Scientific, San Jose, CA*

WP 651 **Rapid Screening of Polysorbates in Biotherapeutics by High Resolution Mass Spectrometry and Kendrick Mass Defect Analysis**; Kui Yang[1]; Asha Hewarathna[1]; Ilan Geerlof-Vidavsky[1]; Ashutosh Rao[2]; Connie Ruzicka[1]; David Keire[1]; *[1]FDA Division of Pharmaceutical Analysis, St Louis, MO; [2]FDA, Silver Spring, MD*

WP 652 **Improving the Efficiency of Immunoaffinity Purification and Enzymatic Digestion of Monoclonal Antibodies Using Capturem Technology**; Michelle R. Robinson[1]; Lisa A. O'Callaghan[1]; Daniel S. Spellman[1]; *[1]Merck Research Labs, West Point, PA*

WP 653 **An Accurate and Sensitive Method for Determination of Insulin Analogues Using the TSQ Altis Triple Quadrupole Mass Spectrometer**; Neloni R Wijeratne[1]; Eric Huang[1]; Mary Blackburn[1]; Claudia P. B. Martins[1]; Antwi Kwasi[2]; Eric Niederkofler[2]; *[1]Thermo Fisher Scientific, San Jose, California; [2]2.Thermo Fisher Scientific, Tempe, AZ*

WP 654 **A Fast, Robust, and Generic IA-LC-MS/MS Method for Quantification of Monoclonal Antibody Therapeutics: Optimizing Immunocapture, Proteolytic Digest, and LC Conditions**; Shuyu Hou[1]; Kevin Pei[1]; Mark Kai Leung Ho[1]; Susan Carr Zondlo[1]; John Kolman[1]; *[1]QPS, LLC, Newark, DE*

WP 655 **Chip-Based Capillary Zone Electrophoresis Mass Spectrometry (CZE/MS) for Rapid Resolution and Quantitation of Critical Sequence Variants**; Tawnya Flick[1]; Andrew Dykstra[1]; Laura Blue[1]; Burton Lee[1]; *[1]Amgen Inc., Thousand Oaks, CA*

WP 656 **LC/MS based Quantitation of Intact Therapeutic Protein in Plasma Matrix**; Yihan Li[1]; Ian Moore[2]; Fan Zhang[3]; Sahana Mollah[4]; *[1]SCIEX, Redwood City, CA; [2]SCIEX, Concord, ON, Canada; [3]Sciex, Redwood City, CA; [4]SCIEX, Redwood City, California*

WP 657 **Host Cell Protein Analysis of Biopharmaceuticals Using Automated Sample Preparation and LC-MS/MS**; Linfeng Wu[1]; Shuai Wu[1]; Te-Wei Chu[1]; *[1]Agilent Technologies, Santa Clara, CA*

WP 658 **A 2D LC-MS/MS Method for Sensitive and Reliable Detection of Residual Host Cell Proteins in Biopharmaceutical Products**; Feng Yang[1]; Don E. Walker[1]; Jeannine Schoenfelder[2]; Joseph Carver[1]; Alice zhang[1]; Delia Li[1]; reed Harris[1]; David A. Michels[1]; Christopher X. Yu[1]; *[1]Genentech Inc., South San Francisco, CA; [2]Roche, Basel, Switzerland*

WP 659 **Mass Spectrometry Immunoassay Coupled with Peptide Enrichment to Detect Thyroglobulin by Capillary Flow LC/MS/MS**; Kerry Hassell[1]; Joshua J. Nicklay[2]; *[1]ThermoFisher Scientific, Somerset, NJ; [2]Thermo Fisher Scientific, Somerset, NJ*

WP 660 **Hight Throughput Multi-Attribute Method (MAM) Analysis of Fc-Fusion Biotherapeutics**; Yuko Ogata[1]; Richard S Rogers[1]; Nancy S Nightlinger[1]; *[1]Just Biotherapeutics, Seattle, WA*

WP 661 **Top-Down Proteomics Discovery of Factor Xa Anticoagulant Bioactive Proteins Derived from Scorpion Venom**; Meng Li[1]; Yuko P. Y. Lam[1]; Peng Chen[2]; Remy Gavard[1]; Cookson K. C. Chiu[1]; Qiong Wu[2]; Christopher A. Wootton[1]; Mark P. Barrow[1]; Hongzheng Fu[2]; Peter B. O'Connor[1]; *[1]University of Warwick, Coventry, UK; [2]Peking University, Beijing, China*

WP 662 **An Improved, Selective Trapping Micro-LC/MS for Ultra-Sensitive, Robust and High-Throughput Quantification of Biotherapeutics and Biomarkers in Plasma and Tissues**; Ming Zhang[1]; Bo An[1]; Jun Qu[1]; *[1]SUNY at Buffalo, Buffalo, NY*

WP 663 **Quantitation of Specific Product Quality Attributes by Platform Multi-Attribute Method**; Xiaoyan Guan[1]; Le Zhang[1]; Da Ren[1]; Tamer Eris[1]; *[1]Amgen, Inc., Thousand Oaks, CA*

WP 664 **Acceleration and Automation of Peptide Mapping Reporting in Biopharmaceutical Development**; David R Bush[1]; John McCarter[2]; Albert van Wyck[3]; Peter Haberl[4]; Joe Shambaugh[2]; Dominik Mertens[5]; Cassandra Wigmore[5]; Chung Ping Chow[5]; Aude Tartiere[2]; Arnd Brandenburg[5]; *[1]Genedata USA, Inc, Lexington, MA; [2]Genedata, Inc., Lexington, MA; [3]Genedata Ltd, Duxford, UK; [4]Genedata GmbH, Munich, Germany; [5]Genedata AG, Basel, Switzerland*

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WP 665 **Deciphering a Therapeutic Monoclonal Antibody with High Viscosity by Microdialysis-Hydrogen/Deuterium Exchange Mass Spectrometry**; Xiaobin Xu[1]; Aming Zhang[1]; Stephen Cale[1]; Yuan Cao[1]; Haibo Qiu[1]; Dingjiang Liu[1]; Ning Li[1]; *[1]Regeneron, Tarrytown, NY*

WP 666 **Site-Specific Antibody-Polymer Conjugates for Theranostic Radioimmunoconjugates**; Penny J. Le[1]; Shane Miersch[2]; Yije Lu[1]; Matthew W Forbes[1]; Sachdev S. Sidhu[2]; Raymond M. Reilly[3]; Mitch A. Winnik[1]; *[1]Department of Chemistry, University of Toronto, Toronto, ON, Canada; [2]Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, ON, Canada; [3]Leslie Dan Faculty of Pharmacy, University of Toronto, Toronto, ON, Canada*

WP 667 **Identification of Lysine Glycation Sites in Monoclonal Antibodies by HCD-Product-Dependent-ETD Using Orbitrap Fusion Lumos Mass Spectrometer**; Lei Wang[1]; Mei M Zhu[1]; Charles Nwosu[1]; *[1]Takeda, Cambridge, MA*

WP 668 **Use of LC/MS to Study Chemical Activation and Protein Conjugation for Conjugate Vaccines**; Paul W. Brown[1]; Jin Xie[1]; Steve A Kolodziej[1]; John F Baldus[1]; Nataliya Parahuz[1]; Alexei Demchenko[2]; Nathan Lacher[1]; Jason C Rouse[3]; Olga V Friese[1]; *[1]Pfizer, St. Louis, MO; [2]University of Missouri-St. Louis, St Louis, MO; [3]Pfizer, Andover, MA*

WP 669 **Physicochemical Characterization of an Original and Biosimilar Imiglucerase by Mass Spectrometry Methods**; Maksim Degterev[1]; Maksim Smolov[1]; Rakhim Shukurov[1]; Alexander Vishnevskiy[1]; Vyacheslav Leonov[1]; *[1]IBC Generium, Volginskiy, Russia*

WP 670 **Diethylpyrocarbonate Labeling and Mass Spectrometry Reveal Subtle Higher Order Structural Changes for Antibody Therapeutics**; Patanachai (Kong) Limpikirati[1]; John E. Hale[2]; Eric M. Graban[2]; Mahdieh Yazdani[1]; Robert C. Vaughan[3]; Richard W. Vachet[1, 4]; *[1]Department of Chemistry, University of Massachusetts Amherst, Amherst, Massachusetts; [2]QuarryBio, Bloomington, Indiana; [3]Department of Molecular and Cellular Biochemistry, Indiana University, Bloomington, Indiana; [4]Molecular and Cellular Biology Program, University of Massachusetts Amherst, Amherst, Massachusetts*

WP 671 **Rapid Characterization of Biotherapeutics Using Capillary Electrophoresis Mass Spectrometry**; Bo Yan[1]; Chris M. Chumsae[1]; Nathan J. Brown[1]; Taro Fujimori[1]; *[1]AbbVie, Worcester, MA*

WP 672 **In-Depth Biotherapeutical Antibody Characterization by Intact Mass Analysis Using a Novel Two-Dimensional Deconvolution Algorithm**; Peter Haberl[1]; Joe Shambaugh[2]; David Bush[2]; Dominik Mertens[3]; Cassandra Wigmore[3]; Chung Ping Chow[3]; John McCarter[2]; Aude Tartiere[2]; Albert van Wyk[4]; Arnd Brandenburg[3]; *[1]Genedata GmbH, München, Germany; [2]Genedata, Inc., Lexington, MA; [3]Genedata AG, Basel, Switzerland; [4]Genedata Ltd, Duxford, UK*

WP 673 **Tandem UHPLC Operation for High-Throughput LC-MS Peptide Mapping Analyses**; Martin Samonig[1]; Sabrina Patzelt[1]; Carsten Paul[1]; Martin Ruehl[1]; Remco Swart[1]; *[1]Thermo Fisher Scientific, Germering, Germany*

WP 674 **High Affinity Epitopes of Aptamer Complexes of the Multi-domain Protein C-Met Revealed by Proteolytic Excision Mass Spectrometry and Biosensor Analysis**; Loredana Mirela Lupu[1]; Hendrik Rusche[2]; Francesca Rinaldi[2]; Yannick Baschung[2]; Maxim Berezovski[3]; Michael Przybylski[2]; *[1]Steinbeis Center for Biopolymer Analysis and Biomedical Mass Spectrometry, Rüsselsheim, Germany; [2]Steinbeis Centre for Biopolymer Analysis and Biomedical Mass Spectrometry, Rüsselsheim am Main, Germany; [3]University of Ottawa, Department of Chemistry and Biomolecular Sciences, Ottawa, Canada*

WP 675 **Middle-Down Analyses of Unmodified and Stressed Monoclonal Antibodies Using an Orbitrap Fusion Lumos Tribrid Mass Spectrometer**; Stephane Houel[1]; Romain Huguet[2]; Jennifer Sutton[2]; Aaron Bailey[2]; Vlad Zabrouskov[2]; Jonathan Josephs[2]; *[1]Thermo Fisher Scientific, Cambridge, MA; [2]Thermo Fisher Scientific, San Jose, CA*

WP 676 **Monitoring Critical Quality Attributes: Core Fucosylation of N-glycans Using an Integrated Subunit LC/MS Workflow Method**; Nilini S Ranbaduge[1]; Henry Y Shion[1]; Ying Qing Yu[1]; Weibin Chen[1]; *[1]Waters Corporation, Milford, MA*

WP 677 **Identification of N-terminal Heterogeneities in Proteins Including low Abundant Proteolysis Products through ETD Fragmentation of TMPP-Tagged Proteins**; Dhanashri Bagal[1]; Bradford W Gibson[2]; *[1]Amgen, South San Francisco, CA; [2]Amgen, South San Francisco*

WP 678 **In-depth Characterization of the Heterogeneous Dimerization Interfaces of A Monoclonal Antibody: from Subdomain Level to Residue Level**; Yuetian Yan[1]; Shunhai Wang[1]; Thomas Daly[1]; Ning Li[1]; *[1]Regeneron Pharmaceuticals, Tarrytown, NY*

WP 679 **Characterization of Multivalent Antibody/Receptor Interactions: A Comparison of Native ESI and Light Scattering as On-Line Detection Tools for SEC**; Cedric Bobst[1]; Jake W Pawlowski[1]; Igor A. Kaltashov[1]; *[1]University of Massachusetts Amherst, Amherst, MA*

WP 680 **Implementation of the Q Exactive Plus BioPharma System in the BioCMC Laboratory**; Gregory W Sword[1]; Christa M Snyder[1]; Jeff S Patrick[1]; Aaron O Bailey[2]; Jonathan L Josephs[2]; Andrew Clark[2]; *[1]Covance, Greenfield, IN; [2]Thermo Fisher Scientific, San Jose, CA*

WP 681 **Developing a Quantitative LC/MS/MS Method for High-Throughput Characterization of the Structural Integrity of Protein Therapeutics During Biomanufacturing**; M. Cyndell Gracieux[1]; Jackson Struble[1]; Devon Poynter[1]; Jack Thomas[1]; Elizabeth Cogdell[1]; Kevin Blackburn[1]; Michael B. Goshe[1]; *[1]North Carolina State University, Raleigh, NC*

WP 682 **Intact Mass Analysis of a Large Therapeutic PEG-Fab Conjugate Using Native Ion Exchange and Ultra-High Mass Range Orbitrap MS**; Aaron O Bailey[1]; Guanghui Han[2]; Maria Reinhardt-Szyba[3]; Eugen Damoc[3]; Jonathan L Josephs[1]; Wendy Sandoval[2]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Genentech Inc., South San Francisco, CA; [3]Thermo Fisher Scientific, Bremen, Germany*

WP 683 **Electrospray Ion Mobility of Biomanufactured Macromolecule Higher Order Structure: Antibodies & Polysaccharides**; Henry Benner[1]; Mike Bogan[1]; *[1]Ion Dx, Monterey, CA*

WP 684 **Mapping an Antibody Binding Epitope Using Carbene Footprinting**; Jason Hogan[1]; Susan Wong[1]; Jia Dong[1]; Gavin Dollinger[1]; Arvind Rajpal[1]; *[1]Bristol-Myers Squibb, Redwood City, CA*

WP 685 **Discovery and Characterization of Histidine Oxidation Initiated Cross-links in an IgG1 Monoclonal Antibody**; Chongfeng Xu[1]; Rachel Chen[1]; Linda Yi[1]; Zoran Sosic[1]; Li Zang[1]; *[1]Biogen, Cambridge, MA*

WP 686 **An Online Four-Dimensional HICxSEC-IMxMS Methodology for Proof-of-Concept Characterization of Antibody Drug Conjugates**; Anthony Ehkirch[1]; Valentina D'Atri[2]; Florent Rouviere[3]; Oscar Hernandez-Alba[1]; Alexandre Goyon[2]; Olivier Colas[4]; Morgan Sarrut[3]; Alain Beck[4]; Davy Guillarme[2]; Sabine Heinisch[3]; Sarah Cianferani[1]; *[1]Laboratoire de Spectrométrie de Masse BioOrganique, Universié de Strasbourg, CNRS, IPHC UMR 7178, Strasbourg, France; [2]School of Pharmaceutical Sciences, University of Geneva, University of Lausanne, Geneva, Switzerland; [3]Université de Lyon, Institut des Sciences Analytiques, CNRS UMR5280, Villeurbanne, France; [4]IRPF - Centre d'Immunologie Pierre-Fabre (CIPF), Saint-Julien-en-Genevois, France*

WP 687 **Site-Specific Characterization and Occupancy Analysis of Proteins Conjugated with 5 and 20 kDa Poly(ethylene glycol) by Hyphenated Mass Spectrometry Techniques**; Selim Gerislioglu[1]; Addie Keating[1]; Chrys Wesdemiotis[1]; *[1]The University of Akron, Akron, OH*

WP 688 **Conformational Assessment of Adnectin and Adnectin-drug Conjugate by Hydrogen/Deuterium Exchange Mass Spectrometry**; Richard Yu-Cheng Huang[1]; Dasa Lipovsek[1]; Guodong Chen[1]; *[1]Bristol-Myers Squibb, Princeton, NJ*

WP 689 **ProteinCleavage: A Software Tool for Fast Identifying Protein Cleavage Degradation in LC-MS Analysis of Therapeutic Monoclonal Antibody**; Zhongping Liao[1]; Jason X Tang[1]; *[1]Eli Lilly and Company, Indianapolis, IN*

WP 690 **Profiling Biologic Drug Interactions with Small Molecules Using Both Native-MS and HDX-MS**; Xiaomei (Annie) He[1]; Siyang (Peter) Li[1]; Yue (Emma) Zhang[1]; Wanlu Qu[1]; Chen Li[1]; Shiaw-Lin (Billy) Wu[1]; *[1]BioAnalytix, Cambridge, MA*

WP 691 **LC-MS Characterization of Complex Glycoproteins**; Amber Peariso[1]; Jason X. Tang[1]; *[1]Eli Lilly & Company, Indianapolis, IN*

WP 692 **Rapid Identity Assays for mAb Development, Production Control and Release**; Anja Resemann[1]; Waltraud Evers[1]; Yue Ju[2]; Guillaume Tremintin[2]; Detlev Suckau[1]; *[1]Bruker Daltonics, Bremen, Germany; [2]Bruker Daltonics, Billerica, MA*

WP 693 **Understanding the Propensity of Sequence Variants During Cell Line and Culture Process Development**; Lisa A. Marzilli[1]; Tzihsuan Lin[1]; Mellisa Ly[1]; Karin Anderson[1]; Olga V Friese[2]; Bruno Figueroa[1]; Jason C Rouse[1]; *[1]Pfizer, Andover, MA; [2]Pfizer, Chesterfield, MO*

WP 694 **Lost in Translation: On the Formation of Protein Sequence Variants**; Zhongqi Zhang[1]; H. Edward Wong[1]; Chung-Jr Huang[1]; *[1]Amgen, Thousand Oaks, CA*

WP 695 **Investigating Structural Integrity of H1ssF, A Universal Influenza Vaccine Candidate, by LC-MS Analysis**; Nicole A. Schneck[1]; Vera B. Ivleva[1]; Frank Arnold[1]; Jonathan W. Cooper[1]; Q. Paula Lei[1]; *[1]NIH/NIAID/VPPL, Gaithersburg, MD*

WP 696 **Protein Conformers Characterization by Top-Down HDX Using a Standard Chromatographic System, and Coupled to ETD Fragmentation and Ion Mobility Spectroscopy**; Jérôme Haustant[1]; Frédéric Rosu[2]; Valérie Gabelica[3]; Cédric Mesmin[4]; *[1]Merck Biodevelopment, Martillac, France; [2]CNRS, INSERM & University of Bordeaux (IECB), Pessac, France; [3]INSERM, CNRS & University of Bordeaux (ARNA laboratory), Pessac, France; [4]Merck Biodevelopment, Martillac, France*

WP 697 **Epitope Mapping of Anti-CTLA4 Therapeutic Antibody by HDX-MS**; Grigori P Ermakov[1]; Edward J Hsieh[1]; Paul L Miller[1]; Maribel Beaumont[1]; *[1]Merck, Palo Alto, CA*

WP 698 **Applications of HDX-MS in Molecule Assessment for Protein Therapeutics**; Jun Zhang[1]; Devrishi Goswami[1]; Michael Treuheit[1]; Ping Yeh[1]; *[1]Amgen Inc., Thousand Oaks, CA*

WP 699 **Towards Overcoming the Challenges of Implementing Accurate Mass MS for Routine Biotherapeutic Analysis**; Henry Shion[1]; Jonathan Pugh[2]; Robert Lewis[2]; Ying Qing Yu[1]; John Gebler[1]; Scott Berger[1]; Weibin Chen[1]; *[1]Waters Corporation, Milford, MA; [2]Waters Corporation, Wilmslow, UK*

WP 700 **Understanding HCP-mAb Interactions in Biopharmaceutical Manufacturing with Crosslinking and Mass Spectrometry**; Romina Hofele[1]; Swarnim Ranjan[2]; Jenny Heidbrink-Thompson[3]; Wai-Keen Chung[3]; David Robbins[3]; Steven P. Cramer[2]; *[1]Medimmune, Gaithersburg, MD; [2]Rensselaer Polytechnic Institute, Troy, NY; [3]MedImmune, Gaithersburg, MD*

WP 701 **Selectivity Manipulation for LC/MS Analysis of Protein Variants**; Benjamin Libert[1]; Stephanie Schuster[1]; Brian Wagner[1]; William Miles[1]; Barry Boyes[1]; *[1]Advanced Materials Technology, Wilmington, DE*

WP 702 **Evaluation of Q-Exactive Plus BioPharma for Characterization of a Range of Different Biologic Formats**; Gregory W. Sword[1]; Christa M. Snyder[1]; Jeff S. Patrick[1]; Aaron O. Bailey[2]; Jonathan L. Josephs[2]; Andrew Clark[2]; *[1]Covance, Greenfield, IN; [2]Thermo Fisher Scientific, San Jose, CA*

WP 703 **Evaluation of CQAs Between ADCs and the Associated mAbs Under Mulitple Conditions Using a Thermo Q Exactive BioPharma Plus**; Gregory W. Sword[1]; Christa M. Snyder[1]; Jeff S. Patrick[1]; Aaron O. Bailey[2]; Jonathan L. Josephs[2]; Andrew Clark[2]; *[1]Covance, Greenfield, IN; [2]Thermo Fisher Scientific, San Jose, CA*

WP 704 **Quantitative Site Occupancy of Unusually O-Glycosylated mAbs**; Harsha Gunawardena[1]; Peter Haytko[1]; Alexander Barnakov[1]; Eric Beil[1]; Andrew Mahan[1]; Darryl Davis[1]; Hirsh Nanda[1]; Subinay Ganguly[1]; *[1]Janssen Research & Development, Spring House, PA*

WP 705 **Assessing Biosimilarity by Monitoring Multiple Critical Quality Attributes of an Intact Monoclonal Antibody Drug Using Orbitrap Native LC-MS**; Aaron O. Bailey[1]; Michael Blank[1]; Terry Zhang[1]; Stephane Houel[1]; Shanhua Lin[2]; Guanghui Han[3]; Roberto Gamez[1]; Katie S. Peterson[1]; Wendy Sandoval[3]; Jonathan L. Josephs[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Sunnyvale, CA; [3]Genentech, Inc., South San Francisco, CA*

WP 706 **Identification of Dimeric Variants of Human Growth Hormone Connected by Mismatched Disulfide Bonds between Different Monomers**; Eun Young Choi[1]; Jung-Keun Suh[1]; *[1]Seoul Media Institute of Technology, Seoul, South Korea*

WP 707 **Withdrawn**

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WP 708 **Proteome-Wide SUMOylation in Kidney Collecting Duct Epithelial Cells**; Qi Wu[1]; Takwa S. Aroankins[1]; Lei Cheng[1]; Robert A. Fenton[1]; *[1]Aarhus University, Aarhus, Denmark*

WP 709 **The Post-Translationally Modified Heart Proteome Reveals Potential Markers of Myocardial Infarction Injury**; Celia Castans[1]; Aleksandra Binek[1]; Navratan Bagwan[1]; Inmaculada Jorge[1, 2]; Elena Bonzón-Kulichenko[1, 2]; Rodrigo Fernández-Jiménez[1, 2]; Carlos Galán-Arriola[1, 2]; Borja Ibáñez[1, 2]; Jesús Vázquez[1, 2]; *[1]CNIC, Madrid, Spain; [2]Cibercv, Madrid, Spain*

WP 710 **Comprehensive Profiling of Lysine 2-Hydroxyisobutyrylated Proteins in Proteus Mirabilis**; Kai Zhang[1]; Hanyang Dong[1]; Zhenchang Guo[1]; Guijin Zhai[1]; Shanshan Tian[1]; Xue Bai[1]; *[1]Tianjin Medical University, Tianjin, China*

WP 711 **Development of a Robust and Reproducible Method for Detection of Citrullination for Complex Samples**; Daniel Nyberg Larsen[1]; Peter Højrup[1]; Jakub Z. Kaczmarek[1, 2]; Jan Potempa[3, 4]; *[1]SDU, Odense, Denmark; [2]Sanovo Biotech, Odense, Denmark; [3]Jagiellonian University, Kraków, Poland; [4]University of Louisville, KY*

WP 712 **N-GlcNAc or O-GlcNAc Post-Translational Modification of Cathepsin H Expressed in SF9 Insect Cells**; Christopher Spahr[1]; Yue Hao[2]; Hao Chen[2]; Kui Chen[1]; Yan Gu[2]; Xin Huang[2]; Allen Sickmier[2]; *[1]Amgen Inc., Thousand Oaks, CA; [2]Amgen, Cambridge, MA*

WP 713 **Mapping Disulfide Linkages Without Detecting Disulfide-linked Peptides**; Tommy K. Cheung[1]; Twyla Lombana[1]; Marissa Matsumoto[1]; David Arnott[1]; *[1]Genentech Inc., South San Francisco, CA*

WP 714 **Elucidation of Phosphoribose Bridged Ubiquitination**; Florian Bonn[1]; Thomas Colby[2]; Sagar Bhogaraju[1, 3]; Sissy Kalayil[1, 3]; Ivan Matic[2]; Ivan Dikic[1, 3]; *[1]Institute of Biochemistry 2, Goethe University School of Medicine, Frankfurt, Germany; [2]Max Planck Institute for Biology of Ageing, Cologne, Germany; [3]Buchmann Institute for Molecular Life Sciences, Goethe University, Frankfurt, Germany*

WP 715 **Understanding E3 Ligase Ube3a Substrates and Pathophysiology in Angelman Syndrome**; Nikhil Janak Pandya[1, 2]; Yasmina Marti-Gil[1, 3]; Veronica Costa[1, 4]; Martin Ebeling[1, 2]; Marco Berrera[1, 2]; Gonzalo Duran Pacheco[1, 2]; Balazs Banfai[1, 2]; Christoph Patsch[1, 4]; Marius Hoener[1, 3]; Tobias Bergauer[1, 2]; Joerg Hipp[1, 3]; Meghan Thorne-Miller[1, 3]; Soren Rasmussen[1, 4]; Axel Ducret[1, 2]; Manuel Tzouros[1, 2]; Tom Dunkley[1, 2]; Ravi Jagasia[1, 3]; *[1]Roche Pharma Research and Early Development, Roche Innovation Center Basel, Hoffmann-La Roche Ltd, Grenzacherstrasse 124, 4070 Basel, Switzerland; [2]Pharmaceutical Sciences, Basel, Switzerland; [3]Neuroscience Ophthalmology and Rare Diseases Discovery and Translational Area, Basel, Switzerland; [4]Therapeutic Modalities, Basel, Switzerland*

WP 716 **Mass Spectrometry Reveals Differential Ubiquitin Signals on Depolarized Mitochondria**; Yi Zeng[1]; Lilian Phu[1]; Baris Bingo[1]; Erik Verschueren[1]; Donald S. Kirkpatrick[1]; *[1]Genentech Inc., South San Francisco, CA*

WP 717 **Thiolomics of Mouse Aortic Endothelial Cells Under Hypoxia**; Xinggui Shen[1]; Pardue Sibile[1]; Christopher B. Pattillo[2]; Hyung W. Nam[3]; Christopher Kevil[1]; *[1]Department of Pathology and Translational Pathobiology, LSU Health-Shreveport, LA; [2]Department of Department of Molecular and Cellular Physiology, LSU Health-Shreveport, LA; [3]Department of Pharmacology, Toxicology and Neuroscience, LSU Health-Shreveport, Shreveport, LA*

WP 718 **A Vendor-Neutral MAM Workflow for Accelerated PTMs Profiling Analysis**; Ben Niu[1]; St John Skilton[2]; Ilker Sen[2]; Jihong Wang[1]; *[1]MedImmune, Gaithersburg, MD; [2]Protein Metrics Inc., San Carlos, CA*

WP 719 **A Proteomics Strategy for Endogenous, *in vivo*, and Site-Specific Characterization of SUMOylation**; Ivo A. Hendriks[1]; David Lyon[1]; Dan Su[1]; Jeremy A. Daniel[1]; Lars J. Jensen[1]; Michael L. Nielsen[1]; *[1]Novo Nordisk Foundation Center for Protein Research, København, Denmark*

WP 720 **Interplay between Oxygen Sensors and The Cell Cycle: Identification of Novel PHD-Dependent, Cell Cycle-Regulated Protein Targets**; Dalila Bensaddek[1]; Alejandro Brenes-Murillo[1]; Sonia Rocha[2]; Jason Swedlow[1]; Angus Lamond[1]; *[1]University of Dundee, UK; [2]University Of Liverpool, UK*

WP 721 **Utilizing LCMS and UVPD for Mapping Non-native Disulfide Bonds in Crystallin Proteins**; James Bonner[1]; Yana Lyon[1]; Tyler Lambeth[1]; Ryan R. Julian[1]; *[1]UCR, Riverside, CA*

WP 722 **Lysine Benzoylation is a New Type of Histone Mark Regulated by SIRT2**; He Huang[1]; Di Zhang[1]; Mathew Perez-Neut[1]; Yingming Zhao[1]; *[1]University of Chicago, IL*

WP 723 **Quantitative Elution of Biotinylated Peptides and Proteins from Streptavidin Complexes**; Martina Schnölzer[1]; Johannes Hartmann[1]; Alexander Lohr[1]; Uwe Warnken[1]; *[1]DKFZ Heidelberg, Heidelberg, Germany*

WP 724 **Revealing Synergistic Effects of Posttranslational Modifications and Ligand Binding to Membrane Proteins Using High-Resolution Native MS**; Idlir Liko[1]; Jonathan T.S. Hopper[1]; Hsin-Yung Yen[1]; Timothy M. Allison[2]; Joseph Gault[2]; Carol V. Robinson[2]; *[1]OMass Technologies Ltd., Oxford, UK; [2]University of Oxford, UK*

WP 725 **Analyzing the Mechanism of Interferon Regulation in pDCs Using Phospho and Ubiquitin Remnant Motif Proteomics**; Dirk Walther[1]; Alex Pellerin[1]; Kejie Li[1]; Dania Rabah[1]; Peter Juhasz[1]; *[1]Biogen, Cambridge, MA*

WP 726 **Simple, Scalable, and Ultra-Sensitive Tip-Based Identification of Protease Substrates Using Mass Spectrometry**; Gerta Shema[1]; Minh T.N. Nguyen[1]; Fiorella A. Solari[1]; Stefan Loroch[2]; A. Saskia Venne[1]; Laxmikanth Kollipara[1]; Albert Sickmann[1, 3, 4]; Steven H.L. Verhelst[1, 5]; René Zahedi[6, 7]; *[1]Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Dortmund, Germany; [2]Leibniz-Institut für Analytische Wissenschaften – ISAS*

– e.V., Dortmund, Germany; [3]Medizinisches Proteom-Center, Ruhr-Universität, Bochum, Germany; [4]Department of Chemistry, College of Physical Sciences, University of Aberdeen, Aberdeen, UK; [5]Department of Cellular and Molecular Medicine, KU Leuven – University of Leuven, Leuven, Belgium; [6]Jewish General Hospital Proteomics Centre, McGill University, Montreal, QC, Canada; [7]Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC, Canada

WP 727 **Identification of Post-Translational Modifications (PTMs) on CDK9 and CDK9-Associated Hsp90 and Cdc37 Proteins and HIV Reactivation**; Benlian Wang[1]; Uri R. Mbonye[2]; Sichun Yang[1]; Giridharan Gokulrangan[1, 3]; Wuxian Shi[1]; Jonathan Karn[2]; Mark R. Chance[1]; *[1]Center for Proteomics and Bioinformatics, Cleveland, OH; [2]Department of Molecular Biology and Microbiology, Case Western Reserve University School of Medicine,, Cleveland, OH; [3]Bristol-Myers Squibb, Wallingford, CT*

WP 728 **Elucidating the Structural Implications of Isomerization and Epimerization in α-Crystallins from Cataractous Human Lenses**; Yana A. Lyon[1]; Dylan L. Riggs[1]; Miranda P. Collier[2]; Matteo T. Degiacomi[3]; Justin L. P. Benesch[2]; Ryan R. Julian[1]; *[1]University of California, Riverside, CA; [2]University of Oxford, UK; [3]Durham University, UK*

WP 729 **Identification and Functional Characterization of Novel Proteins Involved in Protein α-N-Demethylation**; David Bade[1]; Lin Li[2]; Xiaoxia Dai[2]; Yinsheng Wang[1, 2]; *[1]Environmental Toxicology Graduate Program, University of California, Riverside, California; [2]Department of Chemistry, University of California, Riverside, CA*

WP 730 **Role of Acetylation in Hepatic Mitochondrial Proteome Stability in Nonalcoholic Fatty Liver Disease**; Kwangwon Lee[1]; Sergey Ilchenko[1]; Ahmad Borzou[2]; Rovshan Sadygov[2]; Takhar Kasumov[1]; *[1]Neomed, Rootstown, OH; [2]UTMB, Galveston, TX*

WP 731 **Proteomic Analysis of the Role of Thiol Switches in the Metabolic Transition Between Aerobic and Anaerobic Conditions in E. Coli**; Mohammed Refai[1]; Dana Kramer[1]; Nina Paris[1]; Paul Greico[1]; Brian Bothner[1]; *[1]Montana State University, Bozeman, MT*

WP 732 **When a Protein Post-Translational Modification is a Metabolite-Mass-Spectrometry-Based Quantification of Protein-Bound Fatty Acid Synthesis Intermediates in Escherichia Coli.**; Marek J. Noga[1]; Niels van der Broek[1]; Gregory Bokinsky[1]; *[1]Delft University of Technology, Delft, Netherlands*

WP 733 **Quantitation of the S-glutathionylated Proteome Using TMT-Isotope Labeling and LC-MS/MS Mass Spectrometry in the Development of Obese Allergic Airway Disease**; Allison M. Manuel[1]; Shi Biao Chia[1]; Dylan Casey[1]; Cheryl Van De Wetering[1]; Reem Aboushousha[1]; Yvonne Janssen-Heininger[1]; *[1]University of Vermont College of Medicine, Burlington, VT*

PROTEOMICS: CLINICAL APPLICATIONS I
734-750

WP 734 **Can Cytokine and IDMS Measurements Provide Clearer Risk Stratification for Type II Diabetics?**; Bryan Parks[1]; Michael S. Gardner[2]; Lisa G. McWilliams[2]; Zsuzsanna Kuklenyik[2]; John R. Barr[2]; *[1]Centers for Disease Control and Prevention, Atlanta, GA; [2]Centers for Disease Control and Prevention, Atlanta, GA*

WP 735 **Single Nephron Proteomes Connect Morphology and Function in Heterogenous Kidney Diseases**; Markus Rinschen[1]; Martin Höhne[1]; Christian Frese[2]; *[1]University Hospital Cologne, Germany; [2]CECAD Research Center/ University of Cologne, Köln, Germany*

WP 736 **Developing Proteomics Platforms to Study Lipid Pathways in Alzheimer's Disease**; Kaitlyn Stepler[1]; Renã A. S. Robinson[1]; *[1]Vanderbilt University, Nashville, TN*

WP 737 **Proteins Associated with Olanzapine Effectiveness in the Blood Plasma of Schizophrenia Patients**; Sheila Garcia-Rosa[1]; Johann Steiner[2]; Valeria de Almeida[1]; Daniel Martins-de-Souza[1]; *[1]University of Campinas, Dept. of Biochemistry, Laboratory of Neuroproteomics, Campinas, Brazil; [2]University of Magdeburg, Department of Psychiatry, Magdeburg, Germany*

WP 738 **Intracellular Metabolic and Structural Transportation System Drives Chemotherapeutic Resistance in Breast Cancer: New Insight to Overcome Drug Resistance**; Min Ji Song[1]; Dohyun Han[1]; Kwangsoo Kim[1]; Han Suk Ryu[1]; *[1]Seoul National University Hospital, Seoul, South Korea*

WP 739 **MDS Analysis of Bottom-Up Proteomics Subdivides Preeclampsia HELLP Samples**; Sten Heinze[1]; Hongwu Jing[2]; Guomao Zhao[1]; Catalin S. Buhimschi[2]; Irina A Buhimschi[1]; Vicki H. Wysocki[2]; *[1]Nationwide Children's Hospital, Columbus, OH; [2]The Ohio State University, Columbus*

WP 740 **A Novel RNA-Affinity Proteogenomic Technique that Overcomes Tumor Heterogeneity and Distinguishes Markers for Precise Prediction of Cancer Patient Prognosis**; Li Wang[1]; John A. Wrobel[1]; Ling Xie[1]; Dongxu Li[1]; Giada Zurlo[1]; Qing Zhang[1]; Xian Chen[1]; *[1]UNC-Chapel Hill, NC*

WP 741 **Evaluation of NCI-7 Cell Line Panel as a Reference Material for Clinical Proteomics**; David Clark[1]; Yingwei Hu[1]; William Bocik[2]; Lijun Chen[1]; Michael Schnaubelt[1]; Rhonda Roberts[2]; Punit Shah[1]; Gordon R. Whiteley[2]; Hui Zhang[1]; *[1]The Johns Hopkins University, Baltimore, MD; [2]NCI-Frederick/Leidos, Inc., Frederick, MD*

WP 742 **Microproteomic Profiling of Cervical High-Grade Squamous Intraepithelial Lesions**; Charles Pottier[1]; Mark Kriegsmann[2]; Nicolas Smargiasso[1]; Dominique Baiwir[1]; Gabriel Mazzucchelli[1]; Rita Casadonte[3]; Edwin De Pauw[1]; Rémi Longuespée[2]; *[1]Mass Spectrometry Laboratory, University of Liège, Liège, Belgium; [2]University of Heidelberg, Institute of pathology, Heidelberg, Germany; [3]Proteopath GmbH, Trier, Germany*

WP 743 **Clinical Shotgun Proteomics Assay Identifies DNAJB9 as a Pathogenic Protein in Fibrillary Glomerulonephritis**; Jason D. Theis[1]; Surendra Dasari[1]; Julie A. Vrana[1]; Paul J. Kurtin[1]; Ellen D. McPhail[1]; Mariam P. Alexander[1]; Samih H. Nasr[1]; *[1]Mayo Clinic, Rochester, MN*

WP 744 **Biomarker for Platelet Function**; Christin Lorenz[1]; Christina Loosse[1]; Sebastian Malchow[1]; Albert Sickmann[1]; *[1]Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Dortmund, Germany*

WP 745 **Mitra® Microsampling Devices in Remote, Longitudinal Monitoring of Apolipoprotein B/Apolipoprotein A-I in Patients at Risk for Cardiac Events**; Mitra Mastali[1]; Kelly Mouapi[1]; Irene van den Broek[1]; Qin Fu[1]; Chrisandra Shufelt[2]; Brennan Spiegel[3]; Noel Bairey Merz[2]; Jennifer Van Eyk[1, 2]; *[1]Advanced Clinical Biosystems Research Institute, Heart Institute, Cedars Sinai Medical Center, Los Angeles, CA; [2]Barbra Streisand Women's Heart Center, The Heart Institute, Cedars-Sinai Medical Center, Los Angeles, California; [3]Cedars-Sinai Center for Outcomes Research and Education (CS-CORE), Cedars-Sinai Medical Center, Los Angeles, California*

WP 746 **Proteomic Analysis of the Clinical Induced Colistin-Resistant Acinetobacter Baumannii**; Cheng-Kang Chiang[1]; Chia-Wei Chang[2]; Anren Hu[2]; Kai-Chih Chang[2]; *[1]Department of Chemistry, National Dong Hwa University, Shou-Feng, Hualien, Taiwan; [2]Department of Laboratory Medicine and Biotechnology, Tzu Chi University, Hualien County, Taiwan*

WP 747 **A Proteomics Approach for the Early Clinical Identification of Axial Spondyloarthritis: A Study of First Degree Relatives**; Tess Kelly[1]; Brooke Thompson[1]; Paulos Chumala[1]; Udoka Okpalauwaekwe[1]; Brenna

Bath[1]; Catherine Trask[1]; Regina Taylor-Gjevre[1]; David Leswick[1]; Haron Obaid[1]; Melanie Bussey[2]; Bindu Nair[1]; Stephan Milosavljevic[1]; George S. Katselis[1]; *[1]University of Saskatchewan, Saskatoon, SK, Canada; [2]University of Otago, Dunedin, New Zealand*

WP 748 **Utilizing Carrier Reference Proteins in TMT to Push the Detection Limit of nLC-MS Towards Single-Cell Proteomics**; Chuanzi Ouyang[1]; Hui Zhang[1]; *[1]Johns Hopkins School of Medicine, Baltimore, MD*

WP 749 **Resistance to Mek and PI3K Inhibitors in Pancreatic Cancer Cells: A Proteomic Exploration**; Ana Javier-García[1]; Juan F. Martínez-Aguilar[2]; *[1]Universidad de la Cañada, Oaxaca, Mexico; [2]Red de Apoyo a la Investigación-CIC-INCMNSZ, National Autonomous University of Mexico, Mexico City, Mexico*

WP 750 **Version:1.0 StartHTML:0000000168 EndHTML:0000000760 StartFragment:0000 Epitope Peptides Revealed by Biosensor- MS Effectively Neutralize Pathophysiological Antibodies in Clinical Lysosomal Enzyme Therapy**; Michael Przybylski[1]; Stefan Maeser[2]; Zdenek Kukacka[2]; Loredana Mirela Lupu[2]; Fabio Borri[3]; Hendrik Rusche[2]; Lorenzo Altamore[3]; Julia Hennermann[4]; Anna Maria Papini[3]; *[1]Steinbeis Centre Biopolymer Analysis and Biomedical Mass Spectrometry, Ruesselsheim, Germany; [2]Steinbeis Centre for Biopolymer Analysis and Biomedical Mass Spectrometry, Rüsselsheim am Main, Germany; [3]University of Florence, Italy; [4]Universitätsmedizin Mainz, Zentrum Fuer Kinder- Und Jugendmedizin, Mainz, Germany*

PROTEOMICS: QUANTITATIVE III
751-775

WP 751 **Relative Quantification of Proteome via Partial Metabolic Heavy Water Labeling**; Jonghyun Kim[1]; Ho Hee Jang[2]; Tae-Young Kim[1]; *[1]School of Earth Sciences and Environmental Engineering, Gwangju Institute of Science and Technology, Gwangju, South Korea; [2]Department of Biochemistry, College of Medicine, Lee Gil Ya Cancer and Diabetes Institute, Gachon University, Incheon, South Korea*

WP 752 **Extracting Sub-Proteomes from Neurons: From Newly-Synthesized Proteome Dynamics in Synaptic Plasticity to Cell Type-Specific Labeling *in vivo*.**; Christoph T. Schanzenbächer[1]; Beatriz Alavarez-Castelao[1]; Erin M. Schuman[1]; Julian Langer[1, 2]; *[1]MPI for Brain Research, Frankfurt am Main, Germany; [2]MPI of Biophysics, Frankfurt Am Main, Germany*

WP 753 **High Speed, High Sensitivity and Highly Reproducible and Accurate Label Free Quantification Using the PASEF Method on a TIMS QTOF**; Gary Kruppa[1]; Markus Lubeck[2]; Heiner Koch[2]; Paul Shan[3]; Jürgen Cox[4]; Scarlet Koch[2]; *[1]Bruker Daltonics, Billerica, MA; [2]Bruker Daltonik GmbH, Bremen, Germany; [3]Bioinformatics Solutions Inc, Waterloo, ON, Canada; [4]Max Planck Institute of Biochemistry, Martinsried, Germany*

WP 754 **Comprehensive Proteomic Analysis of Ibrutinib Mediated Changes on Proteins and PTMs in Malignant Human B Cells**; Reinhild Rösler[1]; Sascha Endres[1, 2]; Jennifer Haas[2]; Martin Wist[2]; Claudia Walliser[2]; Heike Wiese[2]; Peter Gierschik[2]; Sebastian Wiese[1]; *[1]Core Unit Mass Spectrometry and Proteomics, Ulm University, Ulm, Germany; [2]Institute of Pharmacology and Toxicology, Ulm University, Ulm, Germany*

WP 755 **Interrogating Functional Consequences of Cancer-Associated Mutations Using a BioID-Magnetic Bead Workflow**; Cassandra Wong[1]; Zhen-Yuan Lin[1]; Brett Larsen[1]; Anne-Claude Gingras[1, 2]; *[1]Lunenfeld-Tanenbaum Research Institute at Mount Sinai Hospital, Toronto; [2]Department of Molecular Genetics at University of Toronto, Toronto, ON, Canada*

WP 756 **Missing Data Approaches for Label-Free Quantitative Proteomics Data**; Gina D'Angelo[1]; Pin Ren[1]; Wen Yu[1]; Raghothama Chaerkady[1]; Wei Zhao[1]; Lorin Roskos[1]; Sudhish Sharma[2]; Sunjay Kaushal[2]; Sonja Hess[1]; Harry Yang[1]; *[1]MedImmune, Gaithersburg, MD; [2]University of Maryland School of Medicine, Baltimore, MD*

WP 757 **Development of a Robust, Routine, and Highly Multiplexed Plasma Profiling Method Using UHPLC-SRM Assays**; Kerry Hassell[1]; Debadeep Bhattacharyya[2]; *[1]ThermoFisher Scientific, Somerset, NJ; [2]Thermo Scientific, Cambridge, MA*

WP 758 **Chemical Proteomic Characterization of a Covalent KRASG12C Inhibitor**; Aruna Wijeratne[1]; Junpeng Xiao[1]; Christopher Reutter[1]; Kelly W. Furness[1]; Mohammad Zia-Ebrahimi[1]; John M. Strelow[1]; Sheng-Bin Peng[1]; Thomas A. Engler[1]; David A. Barda[1]; Michael Chalmers[1]; *[1]Eli Lilly and Company, Indianapolis, IN*

WP 759 **Fast Photochemical Oxidation of Proteins Coupled with Ligand Titration Determines Protein-Ligand Binding Affinities at the Peptide Level**; Roger (Xiaoran) Liu[1]; Don L. Rempel[1]; Michael L. Gross[1]; *[1]Washington University in St. Louis, MO*

WP 760 **Quantitative Proteomic Profiling Reveals Key Pathways in Anti-Cancer Action of Novel Natural Product derivatives**; Catherine C Going[1]; Vineet Kumar[2]; Dhanir Tailor[2]; Alisha Birk[1]; Sanjay Malhotra[2]; Sharon J. Pitteri[1]; *[1]Canary Center at Stanford for Cancer Early Detection, Department of Radiology, Stanford University School of Medicine, Palo Alto, CA; [2]Department of Radiation Oncology, Stanford University School of Medicine, Palo Alto, CA*

WP 761 **SWATH-Based Comparative Proteomic Analysis of Leaf Color Mutant in Oryza Stativa**; Hung-Shu Tsai[1]; Chan-Sen Wan[2]; Chien-Chen Lai*[1]; *[1]Institute of Molecular Biology, National Chung Hsing University, Taichung, Taiwan; [2]Department of Agronomy, National Chung Hsing University, Taichung, Taiwan*

WP 762 **Development of a Quality Control Standard for Tandem Mass Tags (TMT) Workflows**; Jae Choi[1]; Aaron M. Robitaille[2]; Tabiwang Arrey[3]; Rosa Viner[2]; Andreas Huhmer[2]; John C. Rogers[1]; *[1]Thermo Fisher Scientific, Rockford, IL; [2]Thermo Fisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific, Bremen, Germany*

WP 763 **Quantitative Proteomics of Lethal Thrombosis Model Mice by SWATH Analysis**; Mina Kawamura[1]; Seiya Kawahara[1]; Fumihiko Nagano[1]; Kei-Ichiro Iwaki[1]; Mai Sakai[1]; Fumitaka Tani[1]; Mie Shimizu[1]; Tomohiro Mizuno[1]; Ken-ichi Harada[1]; Susumu Y. Imanishi[1]; *[1]Meijo University, Nagoya, Japan*

WP 764 **Microflow Bottom-Up Proteomics in the Low Microgram Range Using Ion-Mobility Enhanced Data-Independent Acquisition**; Ute Distler[1]; Jörg Kuharev[1]; Markus Wanninger[2]; Stefan Tenzer[1]; *[1]University of Mainz, Mainz, Germany; [2]Waters Corporation, Milford, MA*

WP 765 **Proteomic Analysis of "Oriental Beauty" Oolong Tea Leaves with Different Degrees of Leafhopper Infestation.**; Han-Ju Chien[1]; Pei-Chien Sung[2]; Chia-Chang Wu[3]; Man-Miao Yang[4]; Chien-Chen Lai*[1, 5]; *[1]Institute of Molecular Biology, National Chung Hsing University, Taichung City, Taiwan; [2]National Chung-Hsing University, Taichung City, Taiwan; [3]Taichung‧Lishan Fushoushan Farm, Taichung County, Taiwan; [4]Department of Entomology, National Chung Hsing University, Taichung City, Taiwan; [5]Graduate Institute of Chinese Medical Science, China Medical University, Taichung city, Taiwan*

WP 766 **Proximity-Based Proteomic Profiling of DNA Double-Strand Break Repair Proteins Identifies Shieldin Complex as Novel Regulator of NHEJ**; Rajat Gupta[1]; Kumar Somyajit[2]; Takeo Narita[1]; Elina Maskey[1]; Magdalena Kremer[3]; Andre Stanlie[4]; Dimitris Typas[2]; Michael Lammers[3];

Niels Mailand[2]; Andre Nussenzweig[4]; Jiri Lukas[2]; Chunaram Choudhary[1]; *[1]Proteomics Program, the Novo Nordisk Foundation Center for Protein Research, Faculty of Health and Medical Sciences, University of Copenhagen, Copenhagen, Denmark; [2]Protein Signaling Program, the Novo Nordisk Foundation Center for Protein Research, Faculty of Health and Medical Sciences, University of Copenhagen, Copenhagen, Denmark; [3]Institute for Genetics and Cologne Excellence Cluster on Cellular Stress Responses in Aging-Associated Diseases (CECAD), University of Cologne, Cologne, Germany; [4]Laboratory of Genome Integrity, National Institutes of Health, Bethesda, Maryland*

WP 767 **Ion Interference in Isobaric Labelling Experiments: A Knock-Out Case Study**; Julien Peltier[1]; Michael A. Cousin[2]; Matthias Trost[1]; *[1]Institute for Cell and Molecular Biosciences, Newcastle University, UK; [2]Centre for Integrative Physiology, Hugh Robson Building, George Square, University of Edinburgh, UK*

WP 768 **Protein Turnover in Neurons and its Regulation during Homeostatic Synaptic Scaling**; Aline R. Dörrbaum[1]; Erin M. Schuman[1]; Julian D. Langer[1, 2]; *[1]Max Planck Institute for Brain Research, Frankfurt Main, Germany; [2]Max Planck Institute of Biophysics, Frankfurt, Germany*

WP 769 **Absolute Quantification of the Lysosomal Proteome by QConCats and Multiple Reaction Monitoring**; Peter Mosen[1]; Roman Sakson[2]; Thomas Ruppert[2]; Volkmar Gieselmann[1]; Dominic Winter[1]; *[1]Institute for Biochemistry and Molecular Biology, Bonn, Germany; [2]Zentrum für Molekulare Biologie, Heidelberg, Germany*

WP 770 **Evaluation of the Phase-Constrained Spectrum Deconvolution Method (ΦSDM) for Multiplex TMT Application**; Tabiwang N. Arrey[1]; Konstantin Aizikov[1]; Grinfeld Dmitry[1]; Arne Kreutzman[1]; Daniel Mourad[1]; Oliver Lange[1]; Alexander Makarov[1]; *[1]Thermo Fisher Scientific, Bremen, Germany*

WP 771 **Deep Proteome Characterization Reveals Mechanism for Platinum Resistance in Ovarian Cancer**; Qing Yu[1]; Catherine Huntoon[2]; Jacob Kennedy[3]; Lei Zhao[3]; Chenwei Lin[3]; Richard G. Ivey[3]; Xiaonan Hou[2]; Larry Karnitz[2]; Pei Wang[4]; Andy Hoofnagle[5]; Steven Skates[6]; Scott Kaufmann[2]; Saravut Weroha[2]; Jeffrey R. Whiteaker[3]; Amanda G. Paulovich[3]; Michael Birrer[7]; Steven P. Gygi[1]; *[1]Harvard Medical School, Boston, MA; [2]Mayo Clinic, Rochester, MN; [3]Fred Hutchinson CRC, Seattle, WA; [4]Icahn School of Medicine at Mount Sinai, New York, NY; [5]University of Washington, Seattle, WA; [6]Massachusetts General Hospital, Boston, MA; [7]University of Alabama at Birmingham, AL*

WP 772 **Large-Scale Quantitative Proteome Profiling in Yeast**; Christoph B. Messner[1]; Vadim Demichev[1, 2]; Kathryn S. Lilley[2]; Markus Ralser[1, 2]; *[1]Francis Crick Institute, London, UK; [2]Department of Biochemistry, University of Cambridge, UK*

WP 773 **Real-Time Statistical Analysis of Multiplexed, Quantitative Proteomics Samples Improves both Peptide Identification Rates and Quantitative Accuracy**; Devin Schweppe[1]; Edward Huttlin[1]; Jonathon O'Brien[1]; Brian K. Erickson[1]; Joao Paulo[1]; Steven P. Gygi[1]; *[1]Harvard Medical School, Boston, MA*

WP 774 **Cross-Species Comparison of Proteome Turnover Kinetics**; Kyle Swovick[1]; Kevin Welle[2]; Jennifer Hryhorenko[2]; Andrei Seluanov[1]; Vera Gorbunova[1]; Sina Ghaemmaghami[1, 2]; *[1]University of Rochester, NY; [2]University of Rochester Mass Spectrometry Resource Laboratory, NY*

WP 775 **'Immunoaffinity Enrichment Combined with Isobaric Labelling for Monitoring the Dynamics of Chromatin-associated Complexes'**; Evangelia K Papachristou[1]; Kamal Kishore[1]; Andrew N. Holding[1]; Kate Harvey[2]; Theodoros I Roumeliotis[3]; Chandra Sekhar Reddy Chilamakuri[1]; Soleilmane Omarjee[1]; Kee Ming Chia[2]; Alex Swarbrick[2, 4]; Elgene Lim[2, 4]; Florian Markowetz[1]; Matthew Eldridge[1]; Rasmus Siersbaek[1]; Clive S D'Santos[1]; Jason Carroll[1]; *[1]Cancer Research UK Cambridge Institute, University of cambridge, UK; [2]Garvan Institute of Medical Research, Sydney, Australia; [3]Wellcome Trust Sanger Institute, Cambridge, UK; [4]St Vincent's Clinical School, Sydney, Australia*

SMALL MOLECULES: QUANTITATIVE ANALYSIS II
776-808

WP 776 **Advanced Robotics Coupled with Tandem Mass-Spectrometry Platform for Clinical Studies, *in-vitro* Biopharmaceutical Analysis and Pharmaceutical Analysis to Support Regulatory Science**; Jinhui Zhang[1]; Celia N. Cruz[2]; Patrick J. Faustino[2]; *[1]FDA, Silver Spring, MD; [2]US Food and Drug Adminiatration, Silver Spring, MD*

WP 777 **AMicrosamplingAssay for Analysis of Cannabinoids in Human Whole Blood**; Ganesh S Moorthy[1]; Christina Vedar[1]; Harini Jogiraju[1]; Athena F. Zuppa[1]; *[1]The Children's Hospital of Philadelphia, PA*

WP 778 **An LC-MS/MS Method for the Quantification of the Endogenous Steroid Progesterone in Mouse Plasma Using the Surrogate Analyte Approach**; Amanda P. Schauer[1]; Craig Sykes[1]; S. Rahima Benhabbour[1]; Mackenzie L. Cottrell[1]; Angela DM Kashuba[1]; *[1]University of North Carolina at Chapel Hill, NC*

WP 779 **Quantitative Analyses of APEOs and AP in Textile Samples by SIM and MRM Methods on LC/MS/MS**; Jun Xiang Lee[1]; Jie Xing[1]; Shao Hua Chia[1]; Zhaoqi Zhan[1]; *[1]Shimadzu Asia Pacific, Singapore*

WP 780 **Use of Alkaline Mobile Phase to Achieve Good Peak Shape in the Rapid LC-MS/MS Analysis of Lisinopril in Human Plasma**; Alan Dzerk[1]; Patrick Miller[1]; Ridha Nachi[1]; Christine Kafonek[1]; Emina Sarajlic[1]; *[1]Celerion, Inc, Lincoln, NE*

WP 781 **Quantitation of Isomers by Multi-CV FAIMS-MS Scans**; Bennett Kalafut[1]; Rae Ana Snyder[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

WP 782 **High Sensitivity Method Validated to Quantify Estradiol in Human Plasma by LC–MS/MS**; Mônica Siqueira Ferreira[1]; André M.M. Arruda[2]; Giovanni T. Pepi[2]; Aline C. Martho[2]; Pâmela M Maximiano[2]; Lina S.O.B.O. Ricci[2]; Maria Francesca Riccio[2]; Ana Cláudia Noboli[2]; Pedro S. Júnior[2]; *[1]Centro Avançado de Estudos e Pesquisas, Campinas, Brazil; [2]Centro Avançado de Estudos e Pesquisas, Campinas, Brazil*

WP 783 **Validated LC-MS/MS Assay for Quantitation of TP-1287 and Alvocidib in Rat K2EDTA Plasma**; Robert Clegg[1]; Rachel Sun[1]; Jason Foulks[2]; *[1]BASi, West Lafayette, IN; [2]Tolero Pharmaceuticals, Inc., Lehi, UT*

WP 784 **Development and Validation of an Analytical Method for Bisphenol S in Rodent Plasma by UPLC-MS/MS**; Melanie A. Rehder Silinski [1]; Brenda L. Fletcher[1]; Reshan A. Fernando[1]; Veronica G. Robinson[2]; Suramya Waidyanatha[2]; *[1]RTI International, Research Triangle Park, NC; [2]Division of the National Toxicology Program, NIEHS, Research Triangle Park, NC*

WP 785 **Validation of Direct Method to Quantify Dexamethasone in Human Aqueous Humor by Ultra High-Performance Liquid Chromatography–Tandem Mass Spectrometry**; Mônica Siqueira Ferreira[1]; Cláudio Roberto Marquez[1]; Danieli Almeida dos Santos[1]; José Jorge Gabbai[1]; Aline Cristina Martho[1]; Amanda Hayashi Yamanouchi Brandão[1]; Kleyton Arlindo Barella[2]; Maria Francesca Riccio[1]; Ana Cláudia Noboli[1]; Pedro Serafim Júnior[1]; *[1]Centro Avançado de Estudos e Pesquisas, Campinas, Brazil; [2]Penido Burnier Institute, Campinas, Brazil*

WP 786 **The Development, Validation and Application of an Automated LC-MS/MS Method for the Quantitation of Nanoparticle-Released Drug Concentrations in Monkey Plasma**; Wei Song[1]; Joseph Tweed[1]; Zhenhua Gu[1]; Ravi Visswanathan[1]; Christopher L Holliman[1]; *[1]Pfizer Inc., Groton, CT*

WP 787 **Assay of Lovastatin in Dietary Supplement by LCMS/MS Under MRM Condition**; Fabio Mazzotti[1]; Leonardo Di Donna[1]; Lucia Bartella[1]; Anna Napoli[1]; Giovanni Sindona[1]; *[1]Dipartimento di Chimica e Tecnologie Chimiche Università della Calabria, Arcavacata Di Rende, Italy*

WP 788 **Stability Analysis of Prodrug Conversion to Treprostinil Using LC/MS**; Shawn Burton[1]; Troy Voelker[1]; Brandon Wilcock[1]; Blake Nielsen[1]; Anthony Sciammarella[1]; Laura Komenda[1]; Jessica Jorvig[1]; Ryan Adler[1]; Scott Reuschel[1]; Michael Scannell[2]; *[1]Covance, Millcreek, UT; [2]United Therapeutics Corp., Durham, NC*

WP 789 **Method Development and Validation for Menthone Glycerin Acetal in Plasma Using Chemical Derivatization with LC-MS/MS**; Yunlin Fu[1]; Ryan Anstatt[2]; Stephanie Graham[2]; Michael Herrera[2]; Panos Hatsis[1]; Wenkui Li[1]; Jimmy Flarakos[1]; *[1]Novartis Institutes for BioMedical Research, East Hanover, NJ; [2]MPI Research, Mattawan, MI*

WP 790 **A Multi-Detector Set-Up Comprising of UV/Vis, Charged Aerosol Detection and Single Quadrupole Mass Spectrometric Detection for Comprehensive Quantitative Sample Analysis**; Stephan Meding[1]; Katherine Lovejoy[1]; Martin Samonig[1]; Frank Hoefler[1]; Remco Swart[1]; Frank Steiner[1]; Martin Ruehl[1]; *[1]Thermo Fisher Scientific, Germering, Germany*

WP 791 **Rapid Determination of Bioactive Compounds in Salvia Miltiorrhiza Samples by UPLC-MS/MS**; Yu-Hsun Chen[1]; Ting-Sian Lin[1]; Hung-Yu Lin[1]; Chan-Sen Wang[2]; Chien-Chen Lai*[1]; *[1]Institute of Molecular Biology, National Chung Hsing University, Taichung, Taiwan; [2]Department of Agronomy, National Chung Hsing University, Taichung, Taiwan*

WP 792 **Analysis of Beta-Carbolines in Smokeless Tobacco Products by Liquid Chromatography-Tandem Mass-Spectrometry**; Vipin Jain[1]; Irina Stepanov[1]; *[1]University of Minnesota, Minneapolis, MN*

WP 793 **Highly Sensitive Quantitative Analysis of Vitamin K2-9 (Menaquinone-9) from Plasma Using LC-MS/MS**; Anant Lohar[1]; Shailesh Damale[1]; Ashutosh Shelar[1]; Shailendra Rane[1]; Rashi Kochhar[1]; Purushottam Sutar[1]; Navin Devadiga[1]; Bhaumik H. Trivedi[1]; Ajit Datar[1]; Pratap Rasam[1]; Jitendra Kelkar[1]; Deepti Bhandarkar[1]; *[1]Shimadzu Analytical PVT LTD, Mumbai, India*

WP 794 **Determination of Estrogens in Environmental Water by Temperature Controlled Liquid Phase Microextraction in-situ Derivatization Coupled to GC-MS/MS**; Yi-Yu Chen[1]; Chung-Yu Chen[1]; Maw-Rong Lee[2]; *[1]National Chung Hsing University, Department of Chemistry, Taichung City, Taiwan; [2]National Chung-Hsing University, Taichung, Taiwan*

WP 795 **Current Approaches and Challenges for Metabolite Mining of Oligonucleotidesusing Liquid Chromatography Coupled with High Resolution/Accurate Mass (HR/AM) Mass Spectrometry**; Nidhi Jaiswal[1]; Cassidy Hatch[1]; Spencer Williams[1]; Juan Rogness[1]; Scott Antonetti[1]; Scott Reuschel[1]; Troy Voelker[1]; *[1]Covance, Salt Lake City, UT*

WP 796 **LC-MS/MS Development and Validation for the Quantitation of 24 Antipsychotics and Their Metabolites in Urine**; Chris Riley[1]; Amber Awad[1]; Lawrence J. Andrade[1]; *[1]Dominion Diagnostics, North Kingstown, RI*

WP 797 **Decontamination of Pesticide-Exposed Clothing: Differential Effects of Washing and Drying Types Determined by GC MS/MS and LC MS/MS**; Claudia Boot[1]; Karolien Denef[1]; Jeff Edwards[2]; Thia Walker[1]; *[1]Colorado State University, Fort Collins, CO; [2]University of Wyoming, Laramie, WY*

WP 798 **A Novel Derivatization Method for Aromatic Compounds with Broad Applicability and Ease of Use to Enhance LC-MS Sensitivity**; Yiqi Ruben Luo[1]; Alan Wu[1]; Kara Lynch[1]; *[1]University of California San Francisco, San Francisco, CA*

WP 799 **Rapid Screening for Fentanyl in Urine Using a Compact Mass Spectrometer (CMS) with an Open Port Sampling Interface (OPSI)**; Changtong Hao[1]; Daniel Eikel[1]; Simon Prosser[1]; Jack D Henion[1]; *[1]Advion Inc., Ithaca, NY*

WP 800 **Fast Liquid Chromatography-Tandem Mass Spectrometry for Simultaneous Determination of Antiepileptic Drugs Using Polarity Switching and Timed Selected Reaction Monitoring**; Raghavendhar R. Kotha[1]; Jace W. Jones[1]; James E. Polli[1]; Maureen A. Kane[1]; *[1]University of Maryland Baltimore School of Pharmacy, Baltimore, MD*

WP 801 **Method Development for Four Explosive Compounds Using APCI –LC/MSMS**; Kelly H. Smith[1]; Kathleen J. Maistros[1]; Jonathan M. Oyler[1]; *[1]U.S. Army Medical Research Institute of Chemical Defense, APG, MD*

WP 802 **Developing a More Rugged and Efficient LC-MS/MS Method for Bioanalysis of E and Z-Isomers of Vitamin K1 in Human Plasma**; Jingguo Hou[1]; Cynthia Carrasco[2]; Edward Wells[2]; Thomas Lloyd[2]; Steve Unger[2]; *[1]Worldwide Clinical Trials, Austin, TX; [2]Worldwide Clinical Trials, Austin, TX*

WP 803 **Ultivo LC/TQ: Analytical Determination of Testosterone in Human Serum**; Yanan Yang[1]; Carrie Adler[1]; Victor Mondragon[2]; Peter Stone[1]; *[1]Agilent Technologies, Inc., Santa Clara, CA; [2]Agilent Technologies, Inc., Mexico City, Mexico*

WP 804 **Development of an Analytical Method for the Analysis of 13 Steroids in Serum by UPLC-MS/MS**; Samantha Blake[1]; Brenda Fletcher[1]; Melanie A. Rehder Silinski [1]; *[1]RTI International, Durham*

WP 805 **Capillary Electrophoresis-Mass Spectrometry (CE-MS) Platform Method for Quantitation of Mutagenic Impurities in Active Pharmaceutical Ingredients**; Helen Yan[1]; Laura Blue[2]; Tawnya Flick[2]; Jiemin Bao[2]; Burton Lee[2]; J. Scott Mellors[2]; *[1]Amgen Inc, Thousand Oaks, CA; [2]Amgen, Inc., Thousand Oaks, CA*

WP 806 **Use of Low Ionization Energy Direct Mass Spectrometry for On-Line Reaction Monitoring**; Chris Davis; *Dow Chemical Company, Carrollton, KY*

WP 807 **Self-Assembly of Discrete Micelle Populations Observed by Charge Detection Mass Spectrometry**; Nicholas Lyktey[1]; Martin F. Jarrold[1]; *[1]Indiana University, Bloomington, IN*

WP 808 **New Methodology for Comprehensive Quantitation of Volatile Organic Compounds Using Proton-Transfer-Reaction Mass Spectrometry (PTR-MS) and Molecular Properties**; Kanako Sekimoto[1, 2]; Shao-Meng Li[3]; Bin Yuan[1, 4]; Abigail Koss[1, 4]; Matthew Coggon[1, 4]; Carsten Warneke[1, 4]; Joost de Gouw[1, 4]; *[1]NOAA Earth System Research Laboratory, Boulder, CO; [2]Yokohama City Univ., Yokohama, Japan; [3]Environment and Climate Change Canada, Toronto, ON, Canada; [4]Cooperative Institute for Research in Environmental Sciences, Boulder, CO*

SYSTEMS BIOLOGY II
809-826

WP 809 **Single-Cell Proteomics and Metabolomics Using Microprobe CE-ESI-HRMS: Towards Single-Cell Systems Biology**; Camille Lombard-Banek[1]; Rosemary M. Onjiko[1]; David O. Plotnick[1]; Reem Q. Al Shabeeb[1]; Sally A. Moody[2]; Peter Nemes[1]; *[1]University of Maryland, College Park, MD; [2]The George Washington University, Washington, DC*

WP 810 **Proteomic Analysis of Signaling Specificity in Breast Cancer Cells**; Chiara Francavilla; *The University of Manchester, UK*

WP 811 **Network Biology for Advancing Drug Discovery and Human Health**; Mark Chance[1]; John Schenkel[2]; Sean Maxwell[1]; *[1]Case Western Reserve University School of Medicine, Cleveland, OH; [2]NeoProteomics, Inc., Cleveland, OH*

WP 812 **Comparing the Short-Term and Long-Term Impact of Host Chronic Restraint Stress to the Gut Microbial Population and Their Metabolic Activities**; Mengyang (Flora) Xu[1]; Chen Wang[1]; Kristen Krolick[1]; Jiangjiang Zhu[1]; Haifei Shi[1]; *[1]Miami University, Oxford, OH*

WP 813 **Dedicated Pipeline for Quantitative Proteomic Measurement of Rare Primary Cell Populations**; Joanna M. Kirkpatrick[1]; Nadja Gebert[1]; Svenja C. Schueler[1]; Simone Di Sanzo[1]; Bing Han[1]; Karl Lenhard Rudolph[1]; Julia von Maltzahn[1]; Alessandro Ori[1]; *[1]FLI - Leibniz Institute on Aging, Jena, Germany*

WP 814 **Metabolic Systems Analysis of Endothelial Dysfunction in Sepsis**; Ottar Rolfsson[1]; Sarah McGarrity[1]; Haraldur Halldórsson[1]; Per Johannsson[2]; *[1]University of Iceland, Reykjavik, Iceland; [2]University of Copenhagen, Copenhagen, Denmark*

WP 815 **Post-Translational Mass Spectral Analysis Guides Targeted Therapy for Traumatic Brain Injury**; Pavel N. Lizhnyak[1]; Demisha DL Porter[1]; Andrew K. Ottens[1]; *[1]Virginia Commonwealth University, Richmond, VA*

WP 816 **Comparative Analysis of Growth Factor Signaling Reveals the Differential Dynamics of Phosphorylation and Kinase Activities in Overlapping Regulatory Pathways**; Anthony S. Valente[1]; Robert T. Lawrence[1]; Judit Villén[1]; *[1]Genome Sciences, University of Washington, Seattle, WA*

WP 817 **Thermal Profiling as a Novel Tool to Analyze the Impact of Missense Mutants on the Proteome**; Sarah A. Peck[1]; Aruna B. Wijeratne[1]; Amber L. Mosley[1]; *[1]Indiana University School of Medicine, Indianapolis, IN*

WP 818 **Integrated Proteome, Acetylproteome, and Metabolome Analysis of Mouse Brown Fat During Adaptation to Cold Temperature**; Samuel Entwisle[1, 2]; Joan Sanchez-Gurmaches[3]; David A. Guertin[4]; Judit Villen[1, 2]; *[1]University of Washington Genome Sciences, Seattle, WA; [2]University of Washington Molecular and Cellular Biology Program, Seattle, WA; [3]Cincinnati Children's Hospital Medical Center, Cincinnati, OH; [4]University of Massachusetts Medical School, Worcester, MA*

WP 819 **Iron as a Global Proteome Modifier in Saccharomyces Cerevisiae.**; Jose Navarrete-Perea[1]; Joao A. Paulo[1]; Steven P. Gygi[1]; *[1]Department of Cell Biology, Harvard Medical School, Boston, MA*

WP 820 **Blocking Estrogen Receptor (ER) Coregulator Signaling Enhances CDK4/6 Inhibitor Palbociclib Therapy in ER-Positive Advanced Breast Cancer**; Suryavathi Viswanadhapalli[1]; Sammy Pardo[1]; Dana Molleur[1]; Susan T. Weintraub[1]; Jacob Lippincott[2]; Sareddy Gangadhara Reddy[1]; Xihui Liu[3]; Ganesh Raj[3]; Ratna Vadlamudi[1]; *[1]Univ. of Texas HSC, San Antonio, TX; [2]Proteome Software, Portland, OR; [3]UT Southwestern Medical Center, Dallas, TX*

WP 821 **An Integrated Omics Approach to Define the Molecular Mechanisms of Galactic Cosmic Ray Induced Hepatocellular Carcinoma**; Brooke Barnette[1]; Anna M. Nia[1]; Shinji K. Strain[1]; Cheryl F. Lichti[2]; Yu Yongjia[1]; Robert L. Ullrich[1]; Mark R. Emmett[1]; *[1]UTMB, Galveston, TX; [2]Washington University School of Medicine, St Louis, MO*

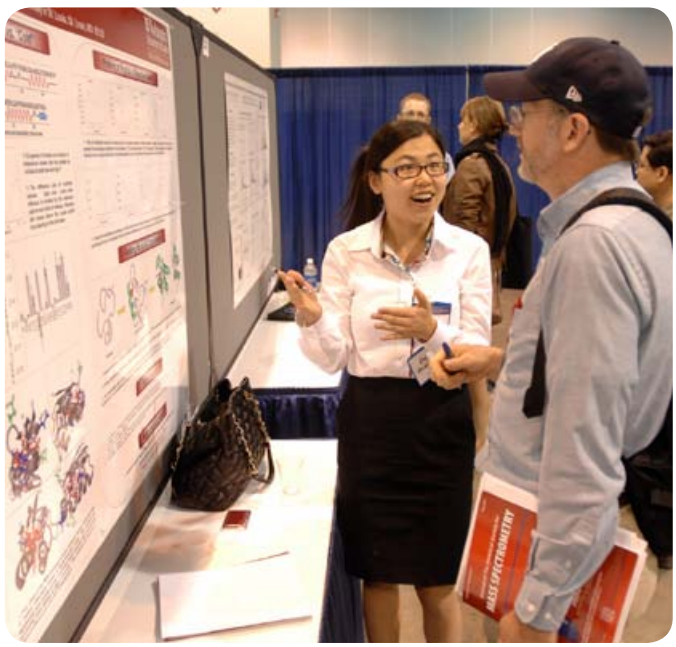
WP 822 **Dynamic Proteome Remodeling Induced by Oncogene Activation Revealed by Comprehensive Analyses of Protein Abundance and Turnover**; Tony Ly[1]; Aki Endo[2]; Alejandro Brenes-Murillo[3]; Marek Gierlinski[3]; Angus Lamond[3]; *[1]Wellcome Centre for Cell Biology, Edinburgh, UK; [2]Tokyo Institute of Technology, Japan; [3]University of Dundee, UK*

WP 823 **Multifaceted Proteomics Evaluation of Lysosomal Dysfunction in iPSC-Derived Neuron Models of Neurodegeneration**; Ling Hao[1]; Michael Fernandopulle[1]; Ryan Prestil[1]; Amra Saric[1]; Yacheng Liao[2]; Jennifer Lippincott-Schwartz[2]; Richard Youle[1]; Michael Ward[1]; *[1]National Institute of Neurological Disorders and Stroke, National Institute of Health, Bethesda, MD; [2]Janelia Research Campus, Howard Hughes Medical Institute, Ashburn, VA*

WP 824 **Integrated Multi-Omics and Systems Biology Analysis of the Targeted Treatment of Obesity within Mouse Models**; Martijn van der Lienden[1]; Gertjan Kramer[2]; Nicholas Dekker[2]; Lee A. Gethings[3]; Johannes P.C. Vissers[3]; Carmen Argmann[4]; Jimmy Yuk[5]; Johannes M.F.G. Aerts[1]; Marco van Eijk[1, 2]; *[1]Department of Biochemistry, Leiden Institute of Chemistry, University of Leiden, Netherlands; [2]Academic Medical Centre, University of Amsterdam, Netherlands; [3]Waters Corporation, Wilmslow, UK; [4]Department of Genetics & Genomic Sciences, Ichan School of Medicine at Mount Sinai, New York, NY; [5]Waters Corporation, Milford, MA*

WP 825 **Global Acetylome Data Interpretation Challenges Associated with Effects of a Deacetylase Inhibitor on Ovarian Cancer Cells**; Aaron R. Goldman[1]; Shuai Wu[1]; Rugang Zhang[1]; David W. Speicher[1]; *[1]The Wistar Institute, Philadelphia, PA*

WP 826 **Integrative Proteomic/Phosphoproteomic, Epigenomic and Genomic Analyses Identify Novel Therapeutic Targets in Rhabdomyosarcoma**; Hong Wang[1]; Mingming Niu[2]; Vishwajeeth R. Pagala[3]; Anthony A. High[3]; Junmin Peng[2]; *[1]St.Jude Children's Research Hospital, Memphis, TN; [2]St. Jude Children's Research Hospital, Memphis, TN; [3]St. Jude Proteomics Facility, St. Jude Children's Research Hospital, Memphis, TN*



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

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

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

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

ANTIBODIES & ANTIBODY DRUG CONJUGATES III
001-028

ThP 001 **LC/MS-Based Structural Elucidation of a New Basic Species Observed by Imaged Capillary Electrophoresis from Forcibly Degraded Monoclonal Antibodies**; Andrew Saati[1]; Penelope Sharpe[1]; Matthew Thompson[1]; Jason C. Rouse[1]; Hugh Conlon[1]; *[1]Pfizer, Andover, MA*

ThP 002 **High-Order Structural Characterization of 10 Monoclonal Antibodies by Combination of Intact, Middle-Up and Bottom-Up Techniques Using Sheathless Capillary Electrophoresis-Mass Spectrometry**; Jérémie Giorgetti[1]; Nassur Said[1]; Rabah Gahoual[2]; Alain Beck[3]; Emmanuelle Leize-Wagner[1]; Yannis Nicolas Francois[1]; *[1]Laboratoire de Spectrométrie de Masse des Interactions et des Systèmes (LSMIS), CNRS – UMR7140, University of Strasbourg, Strasbourg, France; [2]Unité de Technologies Chimiques et Biologiques pour la Santé (UTCBS), Faculté de Pharmacie de Paris - Université Paris Descartes, Paris, France; [3]Centre d’immunologie Pierre Fabre, Saint-Julien-en-Genevois, France*

ThP 003 **LC-MS in Combination with Multiple Enzymatic Digestion for Sequence Variant Identification in Support of Cell Line Development**; Renpeng Liu[1]; Lintao Wang[1]; Alexandru C. Lazar[1]; *[1]ImmunoGen, Waltham, MA*

ThP 004 **Product Quality Attribute Assessment of a Bispecific Antibody Using Enhanced Mass Spectrometry**; Milady Ninonuevo[1]; Delia Li[1]; Alexander Kozintsev[1]; Dana McDaniel[1]; Judith Zhu Shimoni[1]; *[1]Genentech, a member of the Roche group, South San Francisco, CA*

ThP 005 **Comparison of Capillary Electrophoresis Electrospray Ionization Mass spectrometry and Liquid Chromatography Mass Spectrometry for Intact Mass Analysis of Monoclonal Antibody**; Dilipkumar Reddy Kandula[1]; Manoj Pillai[2]; *[1]Sciex, Gurugram, India; [2]Sciex India Pvt Ltd, Gurgaon, India*

ThP 006 **High-Throughput Mass Spectrometry for Antibodies**; Neha Srikumar[1]; Pamela Chan[1]; Yichin Liu[1]; John Tran[1]; *[1]Genentech Inc., San Francisco, CA*

ThP 007 **Multi-Attribute Monitoring (MAM) to Identify Differences in Trastuzumab from 2 Manufacturers**; Sibylle Heidelberger; *Sciex, Warrington, UK*

ThP 008 **BiopharmaViewTM for Fast and Efficient Monitoring of pH Induced Deamidation**; Ji Luo[1]; Sibylle Heidelberger[2]; Annu Uppal[3]; *[1]Sciex, Shanghai, China; [2]Sciex, Warrington, UK; [3]Sciex, Gurugram, India*

ThP 009 **Characterization of the Drug Conjugation Sites for Site-Specific Antibody Drug Conjugate Using UHPLC/ AdvanceBio 6545XT Q-TOF**; Leilei Xu[1]; Manyu Zhang[1]; Shan-An Chan[2]; *[1]Agilent Technologies, Shanghai, China; [2]Agilent Technology, Inc ., Taipei, Taiwan*

ThP 010 **Characterization of Product-Related Low Molecular Weight Impurities in Therapeutic Monoclonal Antibodies Using Hydrophilic Interaction Chromatography Coupled with Mass Spectrometry**; Shunhai Wang[1]; Anita Liu[1]; Yuetian Yan[1]; Thomas Daly[1]; Ning Li[1]; *[1]Regeneron Pharmaceuticals, Tarrytown, NY*

ThP 011 **Characterization of NIST Monoclonal Antibody on Intact, Subunit, and Peptide Level with Monitoring of CQA’s Attributes on the X500B**; Chris Nortcliffe[1]; Annu Uppal[2]; Sibylle Heidelberger[1]; *[1]Sciex, Warrington, UK; [2]Sciex India Pvt Ltd, Haryana, India*

ThP 012 **Development of a High-Throughput Workflow Using Middle Down Mass Spectrometry with Online Chromatography to Characterize Antibodies from Accelerated Stability Studies**; Michael Bacica[1]; Micheal Batt[1]; Jon Fitchett[1]; Bryan E. Jones[1]; *[1]Lilly Biotech Center, San Diego, CA*

ThP 013 **Strategies to Correctly Sequence Antibodies by Mass Spectrometry**; Keith W. Rickert[1]; Arnita Barnes[2]; Raghothama Chaerkady[2]; Sonja Hess[2]; *[1]Medimmune, Gaithersburg, MD; [2]MedImmune, Gaithersburg, MD*

ThP 014 **Impact Assessment of AEBSF, a Protease Inhibitor, Added to the Cell Culture Media as a Clipping Control Strategy for CAP256-VRC26.25**; Cindy Cai[1]; Nicole A. Schneck[1]; Vera B. Ivleva[1]; Weidong Zhao[1]; Daniel Blackstock[1]; Frank Arnold[1]; Jonathan W. Cooper[1]; Q. Paula Lei[1]; *[1]VPPL/VRC/NIAID/NIH, Gaithersburg, MD*

ThP 015 **Automated *de novo* Sequencing of Antibodies with Isoleucine/Leucine Differentiation by Using EThcD Fragmentation**; Wen Zhang[1]; Lin He[1]; Lei Xin[1]; Jonathan R. Krieger[2]; Paul Taylor[2]; Paul Shan[1]; *[1]Bioinformatics Solutions Inc., Waterloo, ON, Canada; [2]Hospital for Sick Children, Toronto, ON, Canada*

ThP 016 **LC-MS/MS Assay for the Quantification of the Total ADCfromMEDI1498 (Deacetylated MEDI4276) in Human Plasma**; Marlking Peay[1]; Morse Faria[1]; Moucan Yuan[1]; Eric Ma[1]; Michael Waldron[1]; William R. Mylott Jr.[1]; Meina Liang[2]; Anton I Rosenbaum[3]; Brandon Lam[3]; *[1]PPD Laboratories, Richmond, VA; [2]Medimmune, San Francisco,, CA; [3]MedImmune, LLC, San Francisco, CA*

ThP 017 **Consortium for Top-Down Proteomics Inter-Laboratory Study for Characterizing Monoclonal Antibodies (mAbs) by Top-Down Mass Spectrometry**; Kristina Srzentic[1]; Luca Fornelli[1]; Yury Tsybin[2]; Joseph Loo[3]; Jeffrey Agar[4]; Julia Chamot-Rooke[5]; Paul Danis[6]; Ying Ge[7]; David Goodlett[8]; Neil Kelleher[1]; Ljiljana Pasa Tolic[9]; Lloyd Smith[7]; Timothy Toby[1]; Konstantin Nagornov[2]; Jennifer Brodbelt[10]; Sylvester Greer[10]; Mathieu Dupré[5]; David Clarke[11]; Ziqing Lin[7]; Kim Haselmann[12]; Christopher Hendrickson[13]; Lidong He[13]; Donald Hunt[14]; Jared Shaw[9]; Wendy Sandoval[15]; Richa Sarin[16]; Detlev Suckau[17]; Yuri E.M. van der Burgt[18]; Norelle Wildburger[19]; Nicolas L. Young[20]; Alain Beck[21]; John Yates[22]; Jolene Diedric[22]; Sneha Chatterjee[23]; Frank Sobott[24]; Anton Kozhinov[2]; Alan G. Marshall[13]; Lissa C. Anderson[13]; Natalia Gasilova[25]; Laure Menin[25]; Neil Quebbenamm[3]; Sung Hwan Yoon[26]; Josh Hinkle[14]; Simone Nicolardi[18]; Matthew V. Holt[20]; Yunqiu Chen[16]; Nicholas Schmitt[4]; *[1]Northwestern University, Evanston, IL; [2]Spectroswiss Sàrl, Lausanne, Switzerland; [3]UCLA, Los Angeles, CA; [4]Northeastern University, Boston, MD; [5]Institute Pasteur, Paris, France; [6]Eastwoods Consulting, Boylston, MA; [7]University of Wisconsin, Madison, WI; [8]University of Maryland, Baltimore, ML; [9]PNNL, Richland, WA; [10]University of Texas at Austin, TX; [11]Edinburgh University, Edinburgh, UK; [12]Novo Nordisk, Malov, Denmark; [13]National High Magnetic Field Laboratory, Tallahassee, FL; [14]University of Virginia, Charlottesville, VA; [15]Genentech, Inc., South San Francisco, CA; [16]Biogen Inc, Cambridge, MA; [17]Bruker Daltonik GmbH, Bremen, Germany; [18]Leiden University Medical Centre, Leiden, Netherlands; [19]Washington University, St. Louis, MO; [20]Baylor College of Medicine, Houston, TX; [21]Centre d'immunologie Pierre Fabre, Saint-Julien-en-Genevois, France; [22]The Scripps Research Institute, La Jolla, CA; [23]University of Antwerp, Antwerp, Belgium; [24]University of Leeds, Leeds, UK; [25]Ecole Polytechnique Fédérale de Lausanne, Ch-1015 Lausanne, Switzerland; [26]University of Maryland, Baltimore, MD*

ThP 018 ***De novo* Sequencing of Antibodies by Mass Spectrometry of Sap9 Peptides**; Kira Vyatkina[1]; Kristina Srzentic[2]; Konstantin O. Nagornov[3]; Natalia Gasilova[4]; Laure Menin[4]; Yury O. Tsybin[3]; *[1]SPb Academic University, St Petersburg, Russian Federation; [2]Northwestern University, Evanston, IL; [3]Spectroswiss Sàrl, EPFL Innovation Park, Lausanne, Switzerland; [4]EPFL, Lausanne, Switzerland*

ThP 019 **Improved Sensitivity for LC-MS Quantitation of Trastuzumab Emtansine in Rat Plasma with Trap-and-Elute MicroLC Using a New Microflow Source**; Khatereh Motamedchaboki[1]; Remco Van Soest[1]; Ian Moore[2]; *[1]Sciex, Redwood City, California; [2]Sciex, Concord, ON, Canada*

ThP 020 **Structural Comparison and Epitope Mapping of Innovator and Biosimilar Therapeutic Antibodies**; Cristina Lento[1]; Kerene A. Brown[1]; Derek J. Wilson[1]; *[1]York University, Toronto, ON, Canada*

ThP 021 **Activated Ion-Electron Transfer Dissociation Allows Characterization of Intact Monoclonal Antibodies with High Sequence Coverage**; Kevin L Schauer[1]; Jean M Lodge[1]; Nicholas M. Riley[1, 2]; Michael S. Westphall[1]; Joshua J. Coon[1, 2, 3, 4]; *[1]Genome Center of Wisconsin, Madison, WI; [2]Department of Chemistry, University of Wisconsin, Madison, WI; [3]Department of Biomolecular Chemistry, University of Wisconsin, Madison, WI; [4]Morgridge Institute for Research, Madison, WI*

ThP 022 **Microflow LC-MS/MS Analysis of Signature Peptide Derived Frommonoclonal Antibody at ng/mL level with nSMOL proteolysis**; Masateru Oguri[1]; Toshiya Matsubara[1]; Atsuhiko Toyama[1, 2]; Wataru Fukui[1]; Takashi Shimada[1]; Shinya Imamura[1]; Scott Kuzdzal[3]; Kyoko Watanabe[1]; *[1]Shimadzu Corp., Kyoto, Japan; [2]Shimadzu, Singapore; [3]Shimadzu Scientific Instruments, Inc., Columbia, MD*

ThP 023 **Absolute Quantitation of N-linked Glycans Attached to Biotherapeutics with Isotopically Labeled Internal Standards**; Ron Orlando[1, 2]; Naglaa Sheiba[1]; Marla Popov[2]; Benjamin Libert[3]; Barry Boyes[2, 3]; *[1]University of Georgia, Athens, GA; [2]Glycoscientific, Athens, GA; [3]Advanced Materials Technology, Wilmington, DE*

ThP 024 **Investigation of the Fragmentation Pattern of a Fab Fragment at Non-Reducing Conditions Using the Omnitrap Platform**; Ioannis L. Karageorgos[1]; A. Michelle English[2]; St John Skilton[2]; Marshall Bern[2]; Jeffrey W Hudgens[1]; Malvina Papanastasiou[3]; Dimitris Papanastasiou[4]; *[1]NIST, Rockville, MD; [2]Protein Metrics, San Carlos, CA; [3]Broad Institute of MIT and Harvard, Cambridge, MA; [4]Fasmatech, Athens, Greece*

ThP 025 **A Novel Tool for Interpretation and Validation of Top-Down and Middle-Down Mass Spectrometry Data of Monoclonal Antibodies**; Kristina Srzentic[1]; Luca Fornelli[1]; Ryan Fellers[1]; Romain Huguet[2]; Stephane Houel[3]; Kenneth R. Durbin[4]; Neil Kelleher[1]; *[1]Northwestern University, Evanston, IL; [2]ThermoFisher, San Jose, CA; [3]Thermo Scientific, Cambridge, MA; [4]Proteinaceous, Inc., Evanston, IL-Illinois*

ThP 026 **Workflow Solution for the Characterization of Biosimilar Using Different Modes of Analytical Chromatography Techniques**; Atis Chakrabarti[1]; Papa Nii Asare-Okai[2]; Zhihua Yang[2]; *[1]Tosoh Bioscience LLC, King Of Prussia, PA; [2]University of Delaware, Newark, DE*

ThP 027 **Biotherapeutic Protein Analysis by MS-Compatible Size Exclusion Chromatography**; Veronica Qin[1]; Andrew Coffey[2]; Anne E Blackwell[1]; Suma Ramagiri[1]; *[1]Agilent Technologies, Inc., Wilmington, DE; [2]Agilent Technologies Inc., Brecknell, UK*

ThP 028 **Top- and Middle-Down CE-ESI-MS Analysis of Intact mAbs Using the ZipChip Coupled to a Fusion Lumos ETD Mass Spectrometer**; Tricia C. Ho[1]; Erik J. Soderblom[1]; Erin Redman[2]; Greg M. Waitt[1]; M. Arthur Moseley[1]; *[1]Duke University School of Medicine, Proteomics and Metabolomics Shared Resource, Durham, NC; [2]908 Devices, Inc., Carrboro, NC*

BIOMARKERS: DISCOVERY II
029-056

ThP 029 **Missing Protein Identification - the Translational Research Study of NKX1 Genes Related to Hepatocellular Carcinoma**; Ming-Hui Yang[1]; Yu-Chang Tyan[1]; *[1]Kaohsiung Medical University, Kaohsiung, Taiwan*

ThP 030 **Morphometric Analysis of Molecular Image: A New Process to Strengthen Biomarkers Discovery**; Rémi Coutant[1]; Rima Ait-Belkacem[1]; Fabien Pamelard[1]; Jonathan Stauber[1]; *[1]Imabiotech, Loos, France*

ThP 031 **Disease-Specific Haptoglobin βchainN-Glycosylation as Personalized Biomarkers to Differentiate Non-Small Cell Lung Cancer from Benign Lung Diseases**; Tianjing Chen[1]; Mo Zhang[1]; Yujie Liu[1]; Dan Zhang[1]; Zhili Li[1]; *[1]Institute of Basic Medical Sciences, Cams&Pumc, Beijing, China*

ThP 032 **Metabolomics Analysis of Hypoxic Preconditioning in *C. elegans***; Dongfang Wang[1]; Chun-Ling Sun[2]; Qiang Fei[2, 3]; Michael Crowder[2]; Sunny Lihua Chen[2]; Julia Yue Cui[2]; Daniel Raftery[2]; Haiwei Gu[4]; *[1]Chongqing Blood Center, Chongqing, China; [2]University of Washington, Seattle, WA; [3]Jilin University, Changchun, China; [4]Mayo Clinic, Scottsdale, Scottsdale, AZ*

ThP 033 **Protocetraric Acid Identification Using LC-ESI-MS/MS : an Excellent Lichen Secondary Metabolite with Redox Properties and Cytoprotective Actions**; Ila Shukla[1]; Lubna Azmi[2]; Shashi Kant Shukla[3]; Ch V Rao[2]; *[1]CSIR-NBRI, Lucknow, India; [2]CSIR-NBRI, Lucknow, India; [3]University of lucknow, Lucknow, India*

ThP 034 **Metabolic Signature to Predict Future Diabetes Susceptibility**; Yashwant Kumar[1]; Sonu Kumar Gupta[1]; *[1]Translational Health Science and Technology Institute, Faridabad, India*

ThP 035 **Lung Cancer Patient Derived Signature Proteins Based on Pattern Identification in Traditional Korean Medicine (TKM) in Human Plasma**; Wonryeon Cho[1]; Miseon Jeong[1]; Jihoon Shin[1]; Jinwook Lee[1]; Min-gyu Youn[1]; Junghoon Kang[1]; Youngwon Jung[2]; *[1]Wonkwang University, Iksan, South Korea; [2]Yonsei University, Seoul, South Korea*

ThP 036 **MDM2 Alterations Reprogram the Metabolic Functioning of Liposarcoma Cell Lines**; Andrew Patt[1]; Bryce Demoret[1]; Andrew Patterson[2]; Philip Smith[2]; Ewy Mathe[1]; James L Chen[1]; *[1]Ohio State University, Columbus, OH; [2]Penn State University, University Park, Pennsylvania*

ThP 037 **Development of a Comprehensive Affinity Matrix for Activity and Selectivity Screening Across the PARP Family Using Chemical Proteomics**; Fiona Pachl[1]; Andrew Zhang[1]; Piero Ricchiuto[2]; Elisabetta Leo[3]; Jeffrey Johannes[4]; Paola Castaldi[1]; *[1]Discovery Sciences, IMED Biotech Unit, Waltham, MA; [2]Discovery Sciences, IMED Biotech Unit, Waltham, MA; [3]Bioscience, Oncology, IMED Biotech Unit, Cambridge, UK; [4]Chemistry, IMED Biotech Unit, Waltham, MA*

ThP 038 **Identification of Novel Biomarkers for Ovarian Cancer**; Danting Liu[1]; Aimin Zhou[2]; *[1]Cleveland State University, ClevelaND, OH; [2]Cleveland State University, Cleveland, OH*

ThP 039 **Expression of Ganglioside GD2, Reprogram the Lipid Metabolism and EMT Phenotype in Bladder Cancer**; Chandra Shekar R Ambati[1]; Nagireddy Putluri[1]; *[1]Baylor College of Medicine, Houston, TX*

ThP 040 **LC-MS/MS Method for Quantitative Analysis of HDNCfromaegle Marmelosinrat Plasma and its Application in Pharmacokineticstudies**; Lubna Azmi[1, 2]; Ila Shukla[1]; Aniruddh Chaudhary[2]; Padam Kant[2]; Ch V Rao[1]; *[1]CSIR-NBRI, Lucknow, India; [2]University of lucknow, Lucknow, India*

ThP 041 **DNA Adductomics for the Screening of Anticancer Drug-Induced DNA Adducts as Biomarkers of Efficacy**; Alessia Stornetta[1]; Kristine Walters[2]; Romel Dator[1]; Valeria Guidolin[1, 3]; William R. Wilson[4]; Shana J. Sturla[5]; Peter W. Villalta[1]; Silvia Balbo[1, 3]; *[1]Masonic Cancer Center, University of Minnesota, Minneapolis, Minnesota; [2]University of Minnesota College of Veterinary Medicine, Minneapolis, Minnesota; [3]Division of Environmental Health Sciences, University of Minnesota, Minneapolis, Minnesota; [4]Auckland Cancer Society Research Center, School of Medical Sciences, the University of Auckland, Auckland, New Zealand; [5]Department of Health Sciences and Technology, ETH Zurich, Zurich, Switzerland*

ThP 042 **Proteomic Profiling Analysis of Extracellular Vesicles Derived from Glioblastoma Cell Lines**; Sabrina F. Comin[1]; Clarice Izumi[1]; Jose C. Rosa[1]; *[1]Medical School of Ribeirao Preto University of Sao Paulo, Ribeirao Preto, Brazil*

ThP 043 **Identification of Signature Metabolites of *Pseudomonas aeruginosain* Different Living Modes via Metabolomic Profiling**; Zhao Cai[1]; Micheal Givskov[1, 2]; Stephan C. Schuster[1, 3]; Liang Yang[1, 3]; *[1]Singapore Centre for Environmental Life Sciences Engineering (SCELSE), Nanyang Technological University, Singapore, Singapore; [2]Costerton Biofilm Center, Department of Immunology and Microbiology, University of Copenhagen, Denmark, Denmark; [3]School of Biological Sciences, Nanyang Technological University, Singapore, Singapore*

ThP 044 **Selection of *Dehalococcoides mccartyi* Protein Biomarkers for LC-MRM-MS Monitoring of Contaminated Groundwater**; Manuel I. Villalobos-Solis[1, 2]; Paul E. Abraham[3]; Cynthia M. Swift[2]; Karuna Chourey[3]; Frank E. Löffler[2]; Robert L. Hettich[2, 3]; *[1]Oak Ridge National Laboratory, Oakridge, TN; [2]University of Tennessee, Knoxville, TN; [3]Oak Ridge National Laboratory, Oak Ridge, TN*

ThP 045 **Identifying Putative Substrates of HtrA1 *in-vivo* Using TAILS**; Victoria Pham; *Genentech, San Francisco, CA*

ThP 046 **Mass Spectral Profiling to Identify Cerebrospinal Fluid Markers in Niemann-Pick Disease, Type C1**; Dylan Nicholas Tabang[1]; Alfred L. Yergey[2, 3]; Peter B. Harrington[4, 5, 6]; Forbes D. Porter[2, 3]; Stephanie M. Cologna[1]; *[1]Department of Chemistry, University of Illinois at Chicago, Chicago, IL; [2]Eunice Kennedy Shriver National Institute of Child Health and Human Development, Bethesda, MD; [3]National Institutes of Health, Bethesda, MD; [4]Center for Intelligent Chemical Instrumentation, Athens, OH; [5]Clippinger Laboratories, Athens, OH; [6]Department of Chemistry and Biochemistry, Ohio University, Athens, OH*

ThP 047 **Mass Spectrometry-Based Proteomics of Human Breast Milk by Two-Dimensional Polyacrylamide Gel Electrophoresis (2D-PAGE) to Assess Breast Cancer Risk**; Roshanak Aslebagh[1]; Devika Channaveerappa[1]; Kathleen F. Arcaro[2]; Costel C. Darie[1]; *[1]Clarkson University, Potsdam, NY; [2]University of Massachusetts Amherst, Amherst, MA*

ThP 048 **Development of Novel Diagnostic and Prognostic Peptide-Based Markers of Parkinson's Disease Using Machine Learning**; Giuseppe Infusini[1]; Laura F Dagley[1]; Andrew I. Webb[1]; *[1]Walter & Eliza Hall Institute, Parkville, Australia*

ThP 049 **Using a Machine-Learned Peptide Signature as a Plasma-Based Clinical Diagnostic Test for Acute Rheumatic Fever**; Laura F Dagley[1, 2]; Giuseppe Infusini[1, 2]; Andrew I Webb[1, 2]; *[1]The Walter and Eliza Hall Institute of Medical Research, Parkville, Australia; [2]Department of Medical Biology, The University of Melbourne, Parkville, Australia*

ThP 050 **Quantitative Proteomics Profiling for ABT-555 Treatment Biomarker Discovery Using Aged Rat Model**; Chenqi Hu[1]; Liang Jin[1]; Khader Awwad[2]; Janina Ried[2]; Elizabeth van der Kam[2]; Michael Schulz[2]; Edit Tarcsa[1]; Yu Tian[1]; *[1]AbbVie, Worcester, MA; [2]AbbVie, Ludwigshafen am Rhein, Germany*

ThP 051 **Increased Trans-Sulfuration and Glucose Metabolism Defines a Distinct Metabotype in Sporadic ALS Cases**; Qiuying Chen[1]; Davinder Sandhu[1]; Csaba Konrad[2]; Dipa Roychoudhury[3]; Benjamin Schwartz[2]; Giovannni Manfredi[1]; Steven M. Fischer[3]; Steven S. Gross[1]; *[1]Weill Cornell Medical College, New York, NY; [2]Weill Cornell Medical College, New York, NY; [3]Agilent Technologies, Santa Clara, CA*

ThP 052 **A Diagnostic Test for Sjogren's Syndrome Based on a Sjogren's-Specific Biomarker Discovered by Mass Spectrometry**; Earl L. White[1]; Kevin Dawson[1]; Goran Sabljic[1, 2]; *[1]MDx BioAnalytical Laboratory, Inc., College Station, TX; [2]Blinn College - Bryan Campus, Bryan, TX*

ThP 053 **Discovery and Characterization of Leukemia Chemotherapy-Related Neurotoxicity Biomarkers in Cerebrospinal Fluid Using Two Orthogonal Proteomics Strategies**; Qinying Yu[1]; Xiaofang Zhong[1]; Bingming Chen[1]; Yu Feng[1]; Chrysanthy Ikonomidou[1]; Lingjun Li[1]; *[1]University of Wisconsin, Madison, WI*

ThP 054 **Effective Phosphoproteome Capture and Analysis Procedure of Urinary Extracellular Vesicles**; Xiaofeng Wu[1]; Anton B Iliuk[2]; Andy W. Tao[1]; *[1]Purdue University, Lafayette, IN; [2]Tymora Analytical Operations, Lafayette, IN*

ThP 055 **Comparative Analysis of Level of Serum Protein Expression in Individual Patients with Large Artery Atherosclerotic Stroke and Healthy Subjects**; Sora Mun[1]; Jiyeong Lee[2]; Arum Park[1]; You-Rim Lee[1]; Ae Eun Seok[1]; Hyo-Jin Kim[1]; Yoo-Jin Lee[1]; Hee-Gyoo Kang[1, 2]; *[1]Department of Senior Healthcare, BK21 Plus Program, Graduate School, Eulji University, Daejeon, South Korea; [2]Department of Biomedical Laboratory Science, College of Health Sciences, Eulji University, Seongnam-si, Gyeonggi-do, South Korea*

ThP 056 **Analysis of Cerebrospinal Fluid by Data-Independent Acquisition Mass Spectrometry and Targeted Mass Spectrometry Reveals Biomarkers Specific for Parkinson's Disease**; Melissa Rotunno[1]; Monica Lane[1]; Pavlina Wolf[1]; Wenfei Zhang[1]; Petra Oliva[1]; Clemens Scherzer[2]; Lamya Shihabuddin[1]; Pablo Sardi[1]; Kate Zhang[1]; *[1]Sanofi, Framingham, MA; [2]Harvard Medical School, Boston, MA*

BIOMARKERS: QUANTITATIVE ANALYSIS III
057-087

ThP 057 **A Promising Biomarker for Chronic Obstructive Pulmonary Disease (COPD)**; Shuren Ma[1]; Xingjian Liu[1]; Yong Y. Lin[1]; Gerard M. Turino[1]; Jerome O. Cantor[2]; *[1]Mount Sinai, St. Luke's Hospital, New York, NY; [2]St. John's University, Queens, NY*

ThP 058 **Development of a Novel LC-ESI-MS/MS Method for Quantitative Determination of Endogenous Markers in Plasma for Evaluation of CYP3A Induction**; Yuki Taya[1]; Yusuke Aratsu[1]; Kota Asahina[1]; Mitsuru Takahashi[1]; Motohiro Kogayu[1]; *[1]Japan Tobacco Inc., Takatsuki Osaka, Japan*

ThP 059 **Quantitation of PI3K p110a, PTEN, and AKT 1+2 in Cancer-Cell Lysate and Tissue Samples Using Immuno-MALDI Mass Spectrometry (iMALDI)**; Bjorn Frohlich[1]; Robert Popp[1]; Rene Zahedi[2]; Andre LeBlanc[3]; Yassene Mohammed[1, 4]; Adriana Aguilar-Mahecha[3]; Oliver Poetz[5]; Mark Basik[6]; Gerald Batist[7]; Christoph H. Borchers[1, 3, 7, 8]; *[1]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [2]Proteogenomics Program, Segal Cancer Centre, Jewish General Hospital, Department of Oncology, McGill University, Montreal, QC, Canada; [3]Jewish General Hospital Proteomics Centre, McGill University, Montreal, QC, Canada; [4]Center for Proteomics and Metabolomics, Leiden University, Leiden, Netherlands; [5]Signatope GmbH, Reutlingen, Germany; [6]Departments of Surgery and Oncology, McGill University, Montreal, QC, Canada; [7]Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC, Canada; [8]Department of Biochemistry and Microbiology, University of Victoria, BC, Canada*

ThP 060 **Quantitation of LRRK2 Protein and S1292 Autophosphorylation Using LC-MS/MS**; Tao Ye[1]; Omar Mabrouk[1]; *[1]Biogen Inc, Cambridge, MA*

ThP 061 **Quantification of Lysosphingomyelin in Human K2EDTA Plasma by HPLC-MS/MS Method**; Xianai Wu[1]; Tian-Sheng Lu[1]; Joshua Froning[1]; Yong-Xi Li[1]; *[1]Medpace, Cincinnati, OH*

ThP 062 **Quantitative LC-EThcD-MS/MS Determination of Intact N-glycopeptides in Serum Haptoglobin between Heptocellular Carcinoma and Liver Cirrhosis**; Jianhui Zhu[1]; Zhengwei Chen[2]; Jie Zhang[1]; Mingrui An[1]; Jing Wu[1]; Marshall Bern[3]; Ilker Sen[3]; Brent Weatherly[3]; St John Skilton[3]; Lingjun Li[2]; David M. Lubman[1]; *[1]University of Michigan Medical Center, Ann Arbor, MI; [2]University of Wisconsin-Madison, Madison, WI; [3]Protein Metrics Inc., San Carlos, CA*

ThP 063 **Analysis of Bile Acids in Human Feces : Relationship betweFen Metabolic Disorders and Microbiota**; Claude-Paul Lafrance[1]; Maxim Maheux[1]; Mylène Brochu[1]; *[1]TransBIOTech, Levis, QC, Canada*

ThP 064 **Matrix Metalloproteinase-3 as a Potential Safety Biomarker in Glucocorticoid Treated Duchenne Muscular Dystrophy Patients**; Michael Ogundele[1]; Tchilabalo Alayi[1]; Mansi V Goswami[1]; Alison M Samsel[1]; Yetrib Hathout[1]; *[1]Binghamton University, Vestal, NY*

ThP 065 **Development of Mass Spectrometry (MS)-Based Proteomics Multiplex Assay to Monitor Blood Biomarkers in Duchenne Muscular Dystrophy**; Tchilabalo D Alayi[1]; Michael R Ziemba[1]; Michael Ogundele[1]; Alison M Samsel[1]; Yetrib Hathout[1]; *[1]Binghamton University State University of New York, Binghamton, NY*

ThP 066 **Development of a High Sensitivity Multiplexed Parallel-Reaction Monitoring Assay for Plasma Biomarkers of Cardiotoxicity Induced by Breast Cancer Therapy**; Pengyuan Liu[1]; Lynn Beer[1]; Bonnie Ky[2]; David W Speicher[1]; *[1]Wistar Institute, Philadelphia, PA; [2]Hospital of the University of Pennsylvania, Philadelphia, PA*

ThP 067 **Development of Robust and Sensitive Immuno-capture LC-MS/MS Assays for Free and Total IP-10 in Human Serum**; Huidong Gu[1]; Yue Zhao[1]; Hongwei Zhang[1]; Ian M. Catlett[1]; Petia Shipkova[1]; Jian Wang[1]; Yan Zhang[1]; Jianing Zeng[1]; *[1]Bristol-Myers Squibb Co., Princeton, NJ*

ThP 068 **Measurements of N1-Methylnicotinamide as an Endogenous Probe of Renal Transporters for Evaluation of Drug-Drug Interactions in First-In-Human Clinical Trial**; Lina Luo[1]; Ragu Ramanathan[1]; Jared Kay[1]; Christopher L Holliman[1]; David Rodrigues[1]; *[1]Pfizer, Groton*

ThP 069 **Analysis of Etheno-DNA Adducts in Human Oral Cells Using Liquid Chromatography-Nanoelectrospray Ionization-High Resolution Tandem Mass Spectrometry (LC-NSI-HRMS/MS)**; Viviana Paiano[1]; Jing Yang[1]; Peter W. Villalta[1]; Stephen S. Hecht[1]; *[1]University of Minnesota, Minneapolis, MN*

ThP 070 **High-Throughput LC–MS/MS Based Biomarker Analysis in Oncology Drug Discovery**; Hyun Woo[1]; Robert Forget[1]; Meiyao Wang[1]; Vincenzo Pucci[1]; *[1]Merck Research Labs, Boston, MA*

ThP 071 **LC-MS/MS Method for the Measurements of Circulating Oncometabolite 2-Hydroxygluturate, a Predictive Biomarker in IDH1 Mutant Xenograft Animal Model**; Meiyao Wang[1]; Vincenzo Pucci[2]; *[1]Merck Research Laboratory, Boston, MA; [2]Merck Research Labs, Boston, MA*

ThP 072 **A Targeted Top-Down Proteomics Methodology for the Discovery and Quantitative Study of Apolipoprotein Proteoforms**; Henrique Dos Santos Seckler[1]; Luca Fornelli[1]; R. Kannan Mutharasan[2]; C. Shad Thaxton[1]; Ryan Fellers[1]; Martha Daviglus[3]; Allan Sniderman[4]; Daniel Rader[5]; Neil Kelleher[1]; Donald. M. Lloyd-Jones[2]; Philip Compton[1]; John Wilkins[2]; *[1]Northwestern University, Evanston, IL; [2]Northwestern University, Chicago, IL; [3]University of Illinois at Chicago, IL; [4]McGill University, Montréal, QC, Canada; [5]University of Pennsylvania, Philadelphia, PA*

ThP 073 **Identification of Lysophosphatidylcholines as Skin Biomarkers Associated with Atopic Dermatitis**; Evgeny Berdyshev[1]; Elena Goleva[1]; Irina Bronova[1]; John Jung[1]; Max A. Seibold[1]; Donald LY Leung[1]; *[1]National Jewish Health, Denver, CO*

ThP 074 **Altered Profiles of L- and D-Amino Acids in Cultured Human Breast Cancer Cells**; Siqi Du; *University of Texas at Arlington, TX*

ThP 075 **Circulating Exosomes from Pancreatic Cancer Alter the Proteome of PanC-1 Cells**; Mingrui An[1]; Jianhui Zhu[1]; Jing Wu[1]; David M. Lubman[1]; *[1]University of Michigan, Ann Arbor, MI*

ThP 076 **Sensitive and Selective Quantification of Octreotide in Human Plasma by LC-MS/MS**; Jeff Jeppson[1]; Veniamin Lapko[1]; Christine Kafonek[1]; Ridha Nachi[1]; Curtis Sheldon[1]; *[1]Celerion, Lincoln, NE*

ThP 077 **Analysis of Hemoglobinopathy by 21 Tesla FT-ICR MS/MS**; Alan G Marshall[1, 2]; Lidong He[1]; Alan L Rockwood[1, 3]; Archana M Agarwal[4, 5]; Lissa C Anderson[2]; Christopher L Hendrickson[1, 2]; *[1]Florida State University, Tallahassee, FL; [2]National High Magnetic Field Laboratory, Tallahassee, FL; [3]Rockwood Scientific Consulting, Salt Lake City, UT; [4]University of Utah School of Medicine, Salt Lake City, UT; [5]ARUP Institute for Clinical and Experimental Pathology, Salt Lake City, UT*

ThP 078 **Method Development and Validation of High Throughput Quantitative Assay for Analysis of Phosphatidylinositols in Human Plasma by Negative Mode HILIC-MRM**; Anton I. Rosenbaum[1]; Lingyi Huang[2]; Swati Anand[1]; Yue Huang[1]; *[1]MedImmune, LLC, Mountain View, CA; [2]MedImmune, LLC, South San Francisco, CA*

ThP 079 **A Multiplex HRMS Assay for Quantifying Human Transporter Bile Acids Biomarkers**; Brian Rago[1]; Brendan Tierney[1]; Ragu Ramanathan[1]; Christopher L Holliman[1]; David Rodrigues[1]; *[1]Pfizer Inc., Groton, CT*

ThP 080 **Quantitative Method to Analyze the Effect of Acetaminophen on Bile Acids in Rat Plasma by LC-MRM**; Vivaldy Prinville[1]; Leanne Ohlund[1]; Lekha Sleno[1]; *[1]UQAM, Montreal, QC, Canada*

ThP 081 **Discovery of Urinary Glycan Markers to Predict Children with Vesicoureteral Reflux at Risk for Urinary Tract Infection and Renal Scarring**; Haiying Li[1]; John Froehlich[1]; Viral Patel[1]; Stephen A. Kostel[1]; Richard S. Lee[2]; *[1]Boston Children's Hospital, Boston, MA; [2]Boston Children's Hospital and Harvard Medical School, Boston, MA*

ThP 082 **A Novel Derivatization Strategy for the Characterization of Short-chain Fatty Acids and Their Hydroxylated Metabolites Using UHPLC-MS/MS**; Juntong Wei[1]; Li Xiang[1]; Xiaona Li[1]; Zongwei Cai[1]; *[1]Hong Kong Baptist University, Hong Kong, China*

ThP 083 **A New Sensitive LC-MS/MS Method for Separation and Quantification of Underivatized Aminobutyric Acid Isomers in Animal and Human Biological Fluids**; Zhiying Wang[1]; Liangqiao Bian[2]; Chenglin Mo[1]; Maciej Kukula[2]; Jauh Tzuoh Lee[3]; Marco Brotto[1]; *[1]College of Nursing and Health Innovation, The University of Texas, Arlington, TX; [2]SCAAC, the University of Texas, Arlington, TX; [3]AZYP LLC-Separation & Analytics, Arlington, TX*

ThP 084 **A Semi-Automated LC-MS Assay to Support Biomarker Discovery for Drug Induced Liver Injury**; Michelle R. Robinson[1]; Vivian Ke[1]; Raymond J. Gonzalez[1]; Kara Michelle Pearson[1]; Kevin P. Bateman[1]; Daniel S. Spellman[1]; *[1]Merck Research Labs, West Point, PA*

ThP 085 **LC-MS/MS Quantification of Intactinsulin-Like Growth Factor I (IGF-I) from Serum**; Nikunj Tanna[1]; Caitlin M. Dunning[1]; Mary E. Lame[1]; Mark Wrona[1]; Logan Umberger[2]; *[1]Waters Corporation, Milford, MA; [2]Waters Corp, Beverly, MA*

ThP 086 **Multiplexed Targeted Quantitation of Membrane-Integrated Receptors**; Simion Kreimer[1]; Peter M. Abadir[1]; Robert N. Cole[1]; *[1]Johns Hopkins School of Medicine, Baltimore, MD*

ThP 087 **New Method for Rapid LC-MS/MS Quantification of N1,N12-Diacetylspermine in a Wide-Range of Common Biofluids , Relevance in Cancer Biomarker Screening**; Brian C. DeFelice[1]; Oliver Fiehn[1]; *[1]University of California, Davis, CA*

BIOMOLECULAR STRUCTURE ANALYSIS: CHEMICAL CROSSLINKING AND COVALENT LABELING II
088-109

ThP 088 **Variation in FPOP Measurements is Primarily Caused by Poor Peptide Signal Intensity**; Niloofar Abolhasani Khaje[1]; Joshua S. Sharp[1]; *[1]University of Mississippi, MS*

ThP 089 **In-Cell Fast Photochemical Oxidation of Proteins for Proteome Wide Structural Biology**; Emily Hart[1]; Lisa M. Jones[1]; *[1]University of Maryland, Baltimore, MD*

ThP 090 **Fluorine-Containing Reagents for Soluble and Bio-orthogonal Membrane-Protein Footprinting**; Ming Cheng[1]; Chunyang Guo[2]; Weidong Cui[1]; Bojie Zhang[1]; Michael L. Gross[1]; *[1]Washington University, St. Louis, MO; [2]Washington University, Saint Louis, MO*

ThP 091 **IC-FPOP as a Tool for In-Cell Structural Biology: Calmodulin and Actin as Model Systems**; Danté T. Johnson[1]; Lisa M. Jones[1]; *[1]University of Maryland Baltimore School of Pharmacy, Baltimore, MD*

ThP 092 **Development of Fast Photochemical Oxidation of Proteins for *in vivo* Modification *inCaenorhabditis elegans***; Jessica Arlett Espino[1]; Lisa M. Jones[1]; *[1]University of Maryland Baltimore School of Pharmacy, Baltimore, MD*

ThP 093 **Application of In-Cell Fast Photochemical Oxidation of Proteins to Multiple Cell Lines**; Upneet Kaur[1]; Danté T Johnson[1]; Lisa M Jones[1]; *[1]University of Maryland Baltimore School of Pharmacy, Baltimore, MD*

ThP 094 **Improved Topographical Mapping of Large Protein Structures with Carbene-based Chemical Labeling Methods**; Daniel S. Ziemianowicz[1]; Vlad Sarpe[1]; David C. Schriemer[1]; *[1]University of Calgary, Calgary*

ThP 095 **Unraveling Coagulation Factor IX Allostericity via Footprinting Mass Spectrometry**; Nadia Freato[1]; Eduard HTM Ebberink[1]; Floris PJ van Alphen[1]; Carmen van der Zwaan[1]; Mariette Boon-Spijker[1]; Alexander B Meijer[1, 2]; Maartje van den Biggelaar[1]; Koen Mertens[1, 2]; *[1]Sanquin, Amsterdam, Netherlands; [2]Utrecht University, Netherlands*

ThP 096 **Towards a Competitive Labelling Mechanism for FPOP**; Susan Ma[1]; Don L. Remple[1]; Michael L. Gross[1]; *[1]Washington University, St. Louis, MO*

ThP 097 **Optimization of HRFP for Observation of Highly Basic Regions**; Charles Mobley[1]; Pradeep Prabhakar[2]; Kelley Moremen[2]; Joshua Sharp[1]; *[1]University of Mississippi, MS; [2]University of Georgia, Athens, GA*

ThP 098 **Using Multiple Structural Proteomics Techniques to Determine the Structure of the α-Synuclein Oligomer and the Misfolding Mechanism**; Nicholas I. Brodie[1]; Konstantin I. Popov[2]; Evgeniy V. Petrotchenko[1]; Nikolay V. Dokholyan[2]; Christoph H. Borchers[1, 3, 4, 5]; *[1]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [2]University of North Carolina, School of Medicine, Chapel Hill, NC; [3]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada; [4]Jewish General Hospital Proteomics Centre, McGill University, Montreal, QC, Canada; [5]Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC, Canada*

ThP 099 **Structural Mass Spectrometry Reveals the Beauty of the Transcription factor/DNA Response Element Interaction**; Lukas Slavata[1, 2]; Ruzena Liskova[1, 2]; Michal Rosulek[1, 2]; Daniel Kavan[1, 2]; Karel Valis[1]; Josef Chmelik[1]; Petr Man[1, 2]; William McIntyre[3]; Daniel Fabris[3]; Petr Novak[1, 2]; *[1]Institute of Microbiology, Prague 4, Czech Republic; [2]Faculty of Science, Charles University, Prague 2, Czech Republic; [3]RNA Institute, University at Albany, Albany, NY*

ThP 100 **Towards High-Throughput Fast Photochemical Oxidation of Proteins: Quantifying Exposure in High Fluence Microtiter Plate Photolysis**; Mohammad Riaz[1]; Sandeep Misra[1]; Joshua S. Sharp[1]; *[1]University of Mississippi, MS*

ThP 101 **Covalent Labeling-Mass Spectrometry for Studying Protein-Ligand Binding Sites, Affinities, and Conformational Changes**; Tianying Liu[1]; Richard W. Vachet[1]; *[1]University of Massachusetts, Amherst, MA*

ThP 102 **Bench-Top Oxidative Protein Footprinting**; Jessica R Chapman[1, 2]; Max Paukner[3]; Micheal Leser[3]; Kevin Teng[2]; Shohei Koide[2]; Chris Becker[4]; Michael Brenowitz[3]; Beatrix M. Ueberheide[2]; *[1]MSKCC, New York, NY; [2]NYU School of Medicine, New York, NY; [3]Albert Einstein College of Medicine, New York, NY; [4]Protein Metrics, San Carlos, CA*

ThP 103 **Higher-Order Structure Influences the Kinetics of Diethylpyrocarbonate Covalent Labeling of Proteins**; Xiao Pan[1]; Richard W. Vachet[1]; *[1]University of Massachusetts, Amherst, MA*

ThP 104 **Determining the Dynamics of GRK5-β2AR Interaction Using X-ray Hydroxyl Radical Footprinting**; Awuri Asuru[1]; Jen Bohon[2, 3]; Liwen Wang[3]; Mark R Chance[2, 3]; David Lodowski[3]; *[1]Case Western Reserve, Cleveland, OH; [2]Brookhaven National Laboratory, Upton, NY; [3]Case Western Reserve University School of Medicine, Cleveland, OH*

ThP 105 **High-Resolution Hydroxyl Radical Protein Footprinting Introduction and Workflow**; Mark Chance[1]; John Schenkel[2]; Janna Kiselar[1]; *[1]Case Western Reserve University, Cleveland, OH; [2]NeoProteomics, Inc., Cleveland, OH*

ThP 106 **Dual FPOP Footprinting by Hydroxyl Radicals and Carbenes: 1+1 > 2 ?**; Bojie Zhang[1]; Ming Cheng[1]; Don L. Rempel[1]; Michael L. Gross[1]; *[1]Washington University in St. Louis, MO*

ThP 107 **Analysis of Bioorthogonally Modified Glycoproteins on Cell Membrane**; Yixuan Xie[1]; Qiongyu Li[1]; Gege Xu[1]; Ace G. Galermo[1]; Carlito B. Lebrilla[1]; *[1]University of California, Davis, CA*

ThP 108 **Isotope-Encoded Benzhydrazide for MS-Based Protein Conformational Study**; Chunyang Guo[1]; Ming Cheng[1]; Michael L Gross[1]; *[1]Washington University in St. Louis, MO*

ThP 109 **Enabling Robust Hydroxyl Radical Footprinting for Biotherapeutic Structural Characterization via an Internal Standard Reporter Peptide**; Natalie K. Garcia[1]; Galahad Deperalta[1]; Aaron Wecksler[1]; *[1]Genentech Inc., San Francisco, CA*

CLINICAL ANALYSIS II
110-135

ThP 110 **A Six Second Analytical Method for Quantitation of Tacrolimus in Whole Blood Using Laser Diode Thermal Desorption Tandem Mass Spectrometry**; Stephen D. Merrigan[1]; Kamisha L Johnson-Davis[1, 2]; *[1]ARUP Institute for Clinical and Experimental Pathology, Salt Lake City, UT; [2]University of Utah Health Sciences Center, Department of Pathology, Salt Lake City, UT*

ThP 111 **A Novel Mass Spectrometry Based Assay for the Diagnosis and Typing of Systemic Amyloidosis**; Paul J. Boersema[1]; Ting Huang[2]; Johan Bijzet[3]; Olga Vitek[2]; Bouke P.C. Hazenberg[3]; Paola Picotti[4]; *[1]ETH Zurich, Zurich, Switzerland; [2]Northeastern University, Boston, MA; [3]University Medical Center, Groningen, Netherlands; [4]ETH, Zurich, Switzerland*

ThP 112 **Molecular Identification of Tissue Types to Improve and Expedite Cervical Endocrine Surgery Using the MasSpec Pen**; Rachel J. DeHoog[1]; Jialing Zhang[1]; Elizabeth Alore[2]; John Q. Lin[1]; Wendong Yu[2]; Anton F Engelsman[3]; Stan B Sidhu[3]; James Suliburk[2]; Livia S Eberlin[1]; *[1]University of Texas at Austin, TX; [2]Baylor College of Medicine, Houston, TX; [3]University of Sydney, Australia*

ThP 113 **Rapid, Direct Mass Spectrometry of Fentanyl and Designer Opioid Analogs for Use in Harm Reduction Strategies**; Gregory W. Vandergrift[1, 2]; Joseph H. Kennedy[3]; Arden J. Hessels[1]; Erik T. Krogh[1, 2]; Jan Palaty[4]; Justin M. Wiseman[3]; Christopher G. Gill[1, 2, 5, 6]; *[1]Appl. Env. Res. Labs. (AERL), Nanaimo, BC, Canada; [2]Chemistry, University of Victoria, Victoria, BC, Canada; [3]Prosolia Inc., Indianapolis, IN; [4]LifeLabs, Burnaby, BC, Canada; [5]Chemistry, Simon Fraser University, Burnaby, BC, Canada; [6]University of Washington, Seattle, WA*

ThP 114 **Development of a Mass Spectrometric Reference Measurement Procedure for Parathyroid Hormone (PTH)**; Candice Z. Ulmer[1, 2]; Uliana Danilenko[2]; Hubert Vesper[2]; *[1]Battelle Memorial Institute, Atlanta, GA; [2]Centers for Disease Control and Prevention, Atlanta, GA*

ThP 115 **Differentiation of IGF-1 Protein Variants by Calculating the Center of Mass of the Isotopic Distribution**; Anthony Maus[1]; Jennifer Kemp[1]; Ravinder Singh[1]; Stefan Grebe[1]; *[1]Mayo Clinic, Rochester, MN*

ThP 116 **Multidimensional LC-MS/MS Method for the Quantification of Intact Human Insulin**; Daryl Kim Hor Hee[1]; Jun Liang Ong[1]; Zhi Wei Edwin Ting[2]; Jie Xing[2]; Lawrence Soon-U Lee[1]; Zhaoqi Zhan[2]; *[1]Department of Medicine Research Laboratories, National University of Singapore; [2]Application Development and Support Centre, Shimadzu (Asia Pacific) Pte Ltd, Singapore*

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ThP 184 **Contribution of the Ultra-High Resolution Mass Spectrometry for Microbiological Study of Contaminated Systems by Hydrocarbons on Ground-Sea Continuum**; Marie Hubert-Roux[1]; Florent Guillaumin[1]; Isabelle Schmitz-Afonso[1]; Anne Carbon[2]; Christine Cagnon[2]; Elise Chatillon[2]; François Rigal[2]; Catherine Lorgeoux[3]; Aurélie Cebron[3]; Pierre Faure[3]; Robert Duran[2]; Cristiana Cravo-Laureau[2]; Carlos Afonso[1]; *[1]University of Rouen, Mont Saint Aignan, France; [2]University of Pau and Pays de l'Adour, Pau, France; [3]University of Lorraine, Vandœuvre-lès-Nancy, France*

ThP 185 **Homologous Series to Find Hydrocarbon Surfactants in AFFFs and in AFFF-impacted Groundwater**; Raymmah Garcia[1]; Aurea Chiaia[2]; Pablo Lara-Martin[3]; Martin Loos[2]; Juliane Hollender[2]; Jennifer Field[1]; *[1]Oregon State University, Corvallis, OR; [2]Swiss Federal Institute of Aquatic Science and Technology, Dübendorf, Switzerland; [3]University of Cádiz, Andalusia, Spain*

ThP 186 **Fluorene-9-bisphenol (BHPF): The New BPA? An Investigation Into BHPF Extraction/Detection Methods in Common Consumer Products**; Gregory S. Rahn[1]; Ellen Chinchilli[1]; Catherine Ryczek[1]; *[1]Hamilton College, Clinton, NY*

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ThP 187 **Mapping of the Phosphorylation Patterns of the Low Complexity Domain of RNA Polymerase II**; Ignasi Forné Ferrer[1]; Roland Schüller[2]; Tobias Straub[3]; Axel Imhof[1]; Dirk Eick[2]; *[1]Biomedical Center Munich, Protein Analysis Unit, Planegg-Martinsried, Germany; [2]Department of Molecular Epigenetics, Helmholtz Center Munich and Center for Integrated Protein Science Munich (CIPSM), Munich, Germany; [3]Biomedical Center Munich, Bioinformatic Unit, Planegg-Martinsried, Germany*

ThP 188 **DIA-Based Proteomics Reveals Pathways of Heterochromatin Assembly and Propagation**; Tania Auchynnikava[1]; Piotr Grabowski[2]; Alison Pidoux[3]; Lauri Peil[4]; Juri Rappsilber[3]; Robin Allshire[3]; *[1]University of Edinburgh, UK; [2]Technical University Berlin, Germany; [3]Edinburgh University, UK; [4]The University of Tartu, Estonia*

ThP 189 **Development of Chlamydomonas Reinhardtii Histone Methyltransferase Activity Assays Using Enzymatic, Chromatographic and Mass Spectrometric Approaches**; Jada N. Walker[1]; Brittany J. Jensen[1]; Aliyya Khan[1]; Anthony T. Iavarone[2]; Gary H. Karpen[3]; James J. Pesavento[1]; *[1]Saint Mary's College of California, Moraga, CA; [2]QB3/Chemistry Mass Spectrometry Facility, Berkeley, CA; [3]Lawrence Berkeley Laboratory, Berkeley, CA*

ThP 190 **A Mass Spectrometric Method for the Detection and Quantitation of Symmetric and Asymmetric Dimethylation of Arginine Sites**; Craig Wagner[1]; Sarah Gerhart[1]; Olena Barbash[1]; Roland Annan[1]; Francesca Zappacosta[1]; *[1]GlaxoSmithKline, Collegeville, PA*

ThP 191 **Comparison of Deconvolution Algorithms for Middle-Down Analysis of Histone Peptides**; Michael J Sweredoski[1]; Roxana Eggleston-Rangel[1]; Annie Moradian[1]; *[1]Caltech, Pasadena, CA*

ThP 192 **Methods for Characterization of Arginine Methylation in Histones Using Parallel Reaction Monitoring (PRM) and Electron Transfer/Higher Energy Collision Dissociation (EThcD)**; Roxana Eggleston-Rangel[1]; Annie Moradian[2]; Michael J Sweredoski[2]; Sonja Hess[2, 3]; Cecilia Zurita-Lopez[1]; *[1]California State University, Los Angeles, Los Angeles, CA; [2]California Institute of Technology, Pasadena, CA; [3]MedImmune, Gaithersburg, MD*

ThP 193 **Use of an Orbitrap Fusion for *in vitro* Characterization of HDAC1 Deacetylation on Histone H3 Acetylated Peptides**; Shekufeh Zareian[1]; Roxana Eggleston-Rangel[1]; Michael J Sweredoski[1]; Jost G Vielmetter[1]; Michael Anaya[1]; Andrea R Kuipers[1]; Sonja Hess[1, 2]; Annie Moradian[1]; *[1]California Institute of Technology, Pasadena, CA; [2]MedImmune, Gaithersburg, MD*

ThP 194 **Deciphering Histone H2B Acetylation Dynamics in Fission Yeast Using High-Resolution LC-MS and Bioinformatic Algorithms**; Paul Drogaris[1]; Charles Homsi[1]; Alain Verreault[1]; Pierre Thibault[1]; *[1]IRIC – Université de Montréal, Montreal, QC, Canada*

ThP 195 **Quantitative Top Down Mass Spectrometry of Histone H4 Proteoforms Reveals the Immediate-Early Response Dynamics of Methyltransferase SUV4-20 Inhibition**; Tao Wang[1]; Matthew V. Holt[2]; Nicolas L. Young[1]; *[1]Baylor College of Medicine, Houston, TX; [2]Baylor College of Medicine, Houston, Texas*

ThP 196 **Histone Lysine Acetoacetylation a Novel Epigenetic Mark Regulated by the Ketogenic Pathway in T1DM**; Sunjoo Kim[1, 2]; Yingming Zhao[2]; Sangkyu Lee[3]; *[1]kyungpook national university, Daegu, South Korea; [2]University of Chicago, Chicago, IL; [3]Kyungpook National University, Daegu, South Korea*

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ThP 197 **The Determination of Mercury Concentration Distributions for Six Retail Finfish and the Implications for Exposure from Consumption**; Marc E. Engel[1]; T.M. Chandrasekhar[2]; Donald M. Axelrad[3]; *[1]FDACS, Tallahassee, FL; [2]FL Dept of Environmental Protection, Tallahassee, FL; [3]FAMU, Tallahassee, FL*

ThP 198 **A Confirmatory Multiresidue Method for the Determination of Polypeptide Antibiotic Residues by HPLC-MS/MS**; Pavel Metalnikov[1]; Ilya Batov[1]; Renat Selimov[1]; Irina Goncharova[1]; Alexander Komarov[1]; *[1]VGNKI, Moscow, Russian Federation*

ThP 199 **Discrimination of Bacillus Cereus and Bacillus Thuringiensis by Metabolomics Profile Differentiation Using UPLC-MS/MS**; Miyoung Ha[1]; Chi-Hu Park[2]; Bum Ho Yoo[2]; *[1]Nonghyup Food Research Institute, Suwon, South Korea; [2]HuGeX Co. Ltd.,, Incheon, South Korea*

ThP 200 **Using Pressurized Liquid Extraction (PLE) at Ambient Temperature for the Extraction and Analysis of Pesticides in Cannabis Samples**; Ruud Addink[1]; Matt Falkenstein[1]; *[1]Fluid Management Systems, Watertown, MA*

ThP 201 **Cannabis Pesticide Analysis: A Validated and Robust Analytical Method for Pesticides Measurement in Cannabis by Liquid Chromatography Tandem Mass Spectrometry**; Erasmus Cudjoe[1]; Avinash Dalmia[2]; Jacob Jalali[3]; Jingcun Wu[4]; Josh Ye[4]; Feng Qin[4]; *[1]PerkinElmer, Canada, Woodbridge, ON, Canada; [2]Perkinelmer, Shelton, CT; [3]Perkin Elmer, Los Angeles, CA; [4]PerkinElmer Inc., Woodbridge, ON, Canada*

ThP 202 **Development of A Fully Automated Multiclass Multiresidue Method For Analysis of Veterinary Drugs in Chicken Meat by SPME-LC-MS/MS**; Abir Khaled[1]; Emanuela Gionfriddo[1]; Varoon Singh[2]; Vinicius Acquaro[2]; Janusz Pawliszyn[2]; *[1]University of Waterloo, waterloo, Ontario; [2]University of Waterloo, Waterloo, ON, Canada*

ThP 203 **Detection and Quantitation of Trace Levels of Ethyl Carbamate in Alcoholic Beverages by GC-MS**; Louiza Mahrouche[1]; Alexandra Furtos[1]; *[1]Universite de Montreal, Montréal*

ThP 204 **Quick and Easy Determination of Aflatoxins in Food Matrices**; Hagen Schlicke[1]; Mareike Margraf[1]; Jan Wendrich[1]; *[1]Knauer Wissenschaftliche Geräte GmbH, Berlin, Germany*

ThP 205 **Determination of B-vitamins in Infant Formulas by Capillary Electrophoresis-Tandem Mass Spectrometry**; Daniela Daniel[1]; Claudimir Lucio do Lago[2]; Zuzana

Cieslarová[2]; *[1]AgilentTechnologies, Barueri, Brazil; [2]University of São Paulo, São Paulo, Brazil*

ThP 206 **Screening for More than 300 Pesticide Residues and Their Identification Using Polarity Swi**; Houssain El Aribi[1]; Ali Talmi[2]; Sami Darkaoui[2]; sanae Achour[3]; *[1]KariNor Scientific, Tangier, Morocco; [2]Office National de Sécurité Sanitaire des Produits Alimentaires ONSSA, Rabat, Morocco; [3]Université Sidi Mohamed Ben Abdellah Faculté de Médecine et de Pharmacie, Fes, Morocco*

ThP 207 **A Robust and Sensitive Method for the Direct Analysis of Polar Pesticides in Food and Environmental Samples**; Wim Broer[1]; Jianru Stahl-Zeng[2]; Ashley Sage[3]; Daniel McMillan[4]; *[1]Nofalab Laboratories, Schiedam, Netherlands; [2]Sciex, Darmstadt, Germany; [3]Sciex, Warrington, UK; [4]Sciex, Warrington, UK*

ThP 208 **Determination of Undesired Substances in Edible Oils by UHPLC-MS/MS**; Yufeng Gao[1, 2]; Zhenpeng Zhen[1, 2]; Mingli Zhu[3]; Minxing Huang[1, 2]; Lizhong Yang[4]; Xiangdong Zhou[4]; Chengyuan Cai[4]; Feng Qin[5]; Joshua Ye[5]; Yongming Xie[4]; *[1]GuangDong Provincial Bioengineering Institute, Guangzhou, China; [2]GuangZhou Sugarcane Industry Research Institute, Guangzhou, China; [3]Guangzhou Agricultural Products Quantity and Safety Supervisory Institute, Guangzhou, China; [4]Perkinelmer Management (Shanghai) Co., Ltd., Shanghai, China; [5]PerkinElmer Inc., Woodbridge, ON, Canada*

ThP 209 **Improved Detection of Pesticide Residues in Botanicals by LCMS**; Jeff Dahl[1]; Tairo Ogura[2]; *[1]Shimadzu, Columbia, MD; [2]Shimadzu Scientific Instrument, Columbia, MD*

ThP 210 **Analysis of Major Food Allergens in Different Food Matrices**; Tairo Ogura[1]; Robert Clliford[2]; *[1]Shimadzu Scientific Instruments, Inc., Columbia, MD; [2]Shimadzu Scientific Instruments, Inc, Columbia, MD*

ThP 211 **Improving Chromatographic Performance of Underivatised Anionic Polar Pesticides in Food to Overcome Renowned Analytical Challenges**; Benjamin Wuyts[1]; Euan Ross[1]; Dimple Shah[2]; Simon Hird[1]; Gareth Cleland[2]; Kenneth Rosnack[2]; *[1]Waters Corporation, Wilmslow, UK; [2]Waters Corporation, Milford, MA*

ThP 212 **Analysis of Pesticides in Edible Oil by Liquid Chromatography and Mass Spectrometry**; Subhra Bhattacharya[1]; Stephen C. Roemer[2]; *[1]Thermo Fisher Scientific, Fair Lawn, NJ; [2]Thermo Fisher Scientific, Fair Lawn, New Jersey*

ThP 213 **Estimation of Heavy Metals at Trace Level in Sugar Using Inductively-Coupled-Plasma-Mass Spectrometry**; Sampada Khopkar[1]; Amol Shinde[2]; Mangesh Pawar[2]; Ajit Datar[2]; Jitendra Kelkar[2]; Pratap Rasam[2]; *[1]Shimadzu Analytical (India) PVT LTD, Mumbai, India; [2]Shimadzu Analytical (India) PVT LTD, Mumbai, India*

ThP 214 **Retrospective, Multi-Evidence Veterinary Drug Screening Based on Drift Tube Ion Mobile Mass Spectrometry**; Xin Ma[1]; Jianzhong Li[1]; Tao Bo[1]; *[1]Agilent Technologies, Beijing, China*

ThP 215 **A Multi Class, Multi Residue Method for Analysis of Veterinary Drugs in Chicken by UHPLC-MS/MS**; Jingcun Wu[1]; Josh Ye[1]; Erasmus Cudjoe[1]; Feng Qin[1]; *[1]PerkinElmer Inc., Woodbridge, ON, Canada*

ThP 216 **Creating a Better Solution for Non-Targeted & Targeted Analysis: Fast and Flexible Analyte Finding for GC/MS and GCxGC/MS**; Gail A Harkey[1]; Todd Richards[1]; Joseph E Binkley[1]; Lorne Fell[1]; *[1]LECO Corporation, Saint Joseph, Michigan*

ThP 217 **Multi-Residue Analysis of 213 Pesticides in Rice Samples by Ultra High Performance Liquid Chromatography - Tandem Mass Spectrometry**; Jingcun Wu[1]; Josh Ye[1]; Erasmus Cudjoe[1]; Feng Qin[1]; *[1]PerkinElmer Inc., Woodbridge, ON, Canada*

ThP 218 **Quadrupole-Resolved All Ions MS/MS for Reliable Quantitation of Pesticides in Complex Matrices Using Untargeted Acquisition**; Christian Klein[1]; Tom Knotts[1]; Dorothy Yang[1]; Bill Frazer[1]; Laszlo Toelgyesi[2]; Tarun Anumol[3]; John Lee[4]; William E Barry[1]; *[1]Agilent Technologies, Inc., Santa Clara, CA; [2]Agilent Technologies Inc., Waldbronn, Germany; [3]Agilent Technologies, Wilmington, DE; [4]Agilent Technologies Inc., Brecknell, UK*

ThP 219 **Withdrawn**

ThP 220 **Accurate Quantitation of Pesticides and PCBs in Grape and Onion Extracts Using High-Resolution GC-Orbitrap Mass Spectrometry**; Dominic Roberts[1]; Jim Garvey[2]; Richard Law[3]; Paul Silcock[1]; *[1]Thermo Fisher Scientific, Runcorn, UK; [2]Department of Agriculture, Food and the Marine, County Kildare, Ireland; [3]Thermo Fisher Scientific, Runcorn, UK*

ThP 221 **Application of a TSQ MS with Acquisition Speed Improvements for Pesticide Analysis**; Harald Oser[1]; Michael Ugarov[1]; Qingyu Song[1]; Claudia Martins[1]; Neloni Wijeratne[1]; *[1]ThermoFisher, San Jose, CA*

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ThP 223 **Improvement for high sensitivity of the drug screening by thermal desorption and pyrolysis combined with DART-MS (TDP/DART-MS)**; Hiroko Abe[1]; Chikako Takei[2]; Motoshi Sakakura[3]; Teruhisa Shiota[3]; Kayako Suga[4]; Daisuke Yajima[5]; Hirotaro Iwase[5, 6]; *[1]University of Chiba, Chiba, Japan; [2]BioChromato, Inc., Fujisawa, Japan; [3]AMR Inc., Meguro-ku, Japan; [4]Sciex, Shinagawa-ku, Japan; [5]University of Chiba, Chiba-shi, Japan; [6]University of Tokyo, Bunkyo-ku, Japan*

ThP 224 **Effects of Physiological and Non-Physiological Factors on the Detection in Urine of Selective Androgen Receptor Modulators**; Monica Mazzarino[1]; Xavier de la Torre[1]; Annapia Dima[1]; Matteo Ricci[1]; Francesco Botrè[1]; *[1]Antidoping laboratory, Rome, Italy*

ThP 225 **Assessing the Financial Impact of Implementing Portable MS Systems for On-Site Processing of Drug Evidence**; Scott R. Cleary[1]; Chase M. Deberry[1]; Sara E. Bell[1]; Yasminda Ruiz[1]; Jamie R. Wieland[2]; Christopher C. Mulligan[1]; *[1]Department of Chemistry, Illinois State University, Normal, IL; [2]Department of Management and Quantitative Methods, Illinois State University, Normal, IL*

ThP 226 **Software Development for Screening Illegal Drugs and Analogues and Classification of Erectile Dysfunction Drugs Using Machine Learning Methods**; Inae Jang[1]; Han Bin Oh[1]; *[1]Sogang University, Seoul, South Korea*

ThP 227 **Mass Spectrometric Forensic Analysis of Botulinum Neurotoxins**; Suzanne R. Kalb[1]; Jakub Baudys[1]; John R. Barr[1]; *[1]CDC, Atlanta, GA*

ThP 228 **Quantitative and Qualitative Analysis of Dembrexine in Equine Plasma by LC-MS/MS**; Rachel M Proctor[1, 2]; Youwen You[1, 2]; Mary A Robinson[1, 2]; *[1]University of Pennsylvania, West Chester, PA; [2]PA Equine Toxicology and Research Laboratory, West Chester, PA*

ThP 229 **Hydrophobic Threads as Versatile Medium for Biofluid Sample Collection, Storage, and Direct Analysis by Ambient Mass Spectrometry**; Devin Swiner[1]; Sierra Jackson[1]; George R. Durisek[1]; Bridget K. Walsh[1]; Yaman Kouatli[1]; Abraham K. Badu-Tawiah[1]; *[1]The Ohio State University, Columbus*

ThP 230 **LC-MS/MS Detects Urobilinoids from Feces in Fly Guts**; Christine Skaggs[1]; Nick Manicke[1]; Charity Owings[1]; Christine Picard[1]; *[1]Indiana University, Purdue University-Indianapolis, Indianapolis, IN*

ThP 231 **Rapid Detection of Fentanyl and Fentanyl Analogues Using Hybrid ITMS-MS System**; Vladimir Romanov[1]; Marlen R. Menlyadiev[1]; Wilhelm Platow[2]; Eoin Lynch[1]; Stefan R. Lukow[1]; *[1]Rapiscan Systems, Andover, MA; [2]Axcelis Technologies, Beverly, MA*

ThP 232 **Detection, Quantification and Confirmation of Monophosphate AICAR (P-AIACR) in Equine Plasma, Urine and Red Blood Cell (RBC) by LC-MS/MS**; Xiaoqing Li[1]; Youwen You[1]; Fuyu Guan[1]; Mary A Robinson[1]; *[1]UPENN, West Chester, PA*

ThP 233 **Development of Low Blood Volume (15 µL) Collection Paper for THC Analysis and Quantification Using LDTD-MS/MS Technology**; Sylvain Letarte[1]; Pascal Belisle[1]; Serge Auger[1]; Pier-Luc Plante[2]; Jean Lacoursière[1]; Pierre Picard[1]; *[1]Phytronix Technologies, Quebec, QC, Canada; [2]Universite Laval, Quebec, QC, Canada*

ThP 234 **A Postmortem Application at the Miami-Dade Medical Examiner Department Based on an Automated Ion Trap LC-MSn Approach**; Elisa N Shoff[1]; Markus Meyer[2]; George W Hime[1]; Diane M Boland[1]; *[1]Miami-Dade Medical Examiner Department, Miami, FL; [2]Bruker Daltonik GmbH, Bremen, Germany*

ThP 235 **A Qualitative/Quantitative LC-QTOF-MS Assay for Forensic Drug Screening in Urine – Feasibility Study and Basic Method Validation**; Laura M. Huppertz[1]; Karin Wendt[2]; Michaela Schmidt[1]; Ronja Peter[1]; Franziska Ehrhardt[1]; Carsten Baessmann[2]; Volker Auwärter[1]; *[1]Institute of Forensic Medicine, Medical Center - University Freiburg, Freiburg, Germany; [2]Bruker Daltonik GmbH, Bremen, Germany*

ThP 236 **GC-MS and Product Ion MS-MS Studies on Isomeric Designer Drugs Related to 25I-N-BOMe**; Ahmad Almalki[1, 2]; Randall Clark[1]; Jack DeRuiter[1]; *[1]Auburn university, Auburn, AL; [2]King Abdulaziz University, Jeddah, Saudi Arabia*

ThP 237 **Toward Better Amino Acid Racemization Dating of Historical Objects by Understanding the Effect of Environmental Factors on Racemization**; Mehdi Moini; *George Washington University, Washington, DC*

ThP 238 **On-Site Screening of Volatile Accelerants Using a Portable Gas Chromatograph Ion Trap Mass Spectrometer**; Zachary E Lawton[1]; John D DeHaan[2]; David A Matthew[2]; *[1]PerkinElmer, New Haven, CT; [2]Fire-Ex Forensics Inc., Vallejo, California(CA)*

ThP 239 **Ultra-Rapid and Highly User-Friendly Drug Screening System by Direct Probe Ionization-Tandem Mass Spectrometry (DPiMS/MS)**; Tasuku Murata[1]; Koretsugu Ogata[2]; Tomomi Ohara[3]; Maiko Kusano[3]; Hitoshi Tsuchihashi[3]; Yumi Hayashi[4, 5]; Kei Zaitsu[3, 4]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]Shimadzu Corporation, MS Business Unit, Kyoto, Japan; [3]Department of Legal Medicine and Bioethics, Nagoya University Graduate School of Medicine, Nagoya, Japan; [4]in vivo Real-Time Omics Laboratory, Institute for Advanced Research, Nagoya University, Nagoya, Japan; [5]Pathophysiological Laboratory Sciences, Department of Radiological and Medical Laboratory Sciences, Nagoya University Graduate School of Medicine, Nagoya, Japan*

ThP 240 **Ultra-Fast Characterization of Novel Synthetic Opioids Using a Data-Independent Acquisition Analytical Workflow**; Alexandre Wang[1]; Oscar G. Cabrices[1]; Alex Krotulski[2]; Amol Kafle[1]; Xiang He[1]; Adrian Taylor[3]; *[1]Sciex, Redwood City,, CA; [2]3The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation, Willow Grove, PA; [3]Sciex, Concord, ON, Canada*

ThP 241 **Detecting Fluorinated Coatings on a Single Fiber Using Pyrolysis Gas Chromatography Plasma Assisted Reaction Chemical Ionization Mass Spectrometry**; Michael J Dolan Jr.[1]; Robert Blackledge[2]; Kaveh Jorabchi[1]; *[1]Georgetown University, Washington, DC; [2]Forensic Chemist Consultant, San Diego, CA*

ThP 242 **Application of Field-Portable Nano-Liquid Chromatography-Electron Ionization-Mass Spectrometry to the Analysis of Drugs and Explosives**; Jocelyn Abonamah[1]; Mehdi Moini[1]; *[1]George Washington University, Washington, DC*

ThP 243 **Potential Applications to New Psychoactive Substances Identification in Oral Fluid and Damiana leaf (Turnera diffusa) by DART-MS/MS and LC-MS/MS**; Heloa Santos[1, 2]; Tyler J. Davidson[1]; Joseph Cox[1]; Glen P. Jackson[1]; Wanderson Romao[2, 3]; Luis E. Arroyo[1]; *[1]West Virginia University, Morgantown, WV; [2]Federal University of Espírito Santo (UFES), Vitoria, Brazil; [3]Federal Institute of Espirito Santo, Vila Velha, Brazil*

ThP 244 **Identification of a Novel Fragmentation Pathway of Synthetic Cathinones**; J. Tyler Davidson[1]; Zachary J. Sasiene[2]; Younis Abiedalla[3]; C. Randall Clark[3]; Glen P. Jackson[1, 2]; *[1]Department of Forensic and Investigative Science, West Virginia University, Morgantown, WV; [2]C. Eugene Bennett Department of Chemistry, West Virginia University, Morgantown, WV; [3]Department of Drug Discovery and Development, Harrison School of Pharmacy, Auburn University, Auburn, AL*

ThP 245 **Biometrics from Isotope Ratio Analysis of Human Fingernails**; Halle M. Edwards[1]; Mayara P. V. Matos[2]; Glen P. Jackson[1, 3]; *[1]C. Eugene Bennett Department of Chemistry, West Virginia University, Morgantown, WV; [2]Department of Biology, West Virginia University, Morgantown, WV; [3]Department of Forensic and Investigative Science, West Virginia University, Morgantown, WV*

ThP 246 **Fast Screening of NPS blotters papers by DESI-IMS: A Prominent Approach to Traceability**; Géssica A Vasconcelos[1]; Andre Luiz Martini[2]; Renata Pereira Limberger[3]; Wanderson Romão[4]; Boniek Gontijo Vaz[1]; *[1]Universidade Federal de Goiás - UFG, Goiânia, Brazil; [2]Polícia Técnico-Científica do Estado de Goiás, Goiania, Brazil; [3]Universidade Federal do Rio Grande do Sul, Porto Alegre, Brazil; [4]UFES, Vitória, Brazil*

ThP 247 **On-Substrate Derivatization of Highly Volatile Chemical Warfare Agent for Capture and Analysis by Paper Spray Mass Spectrometry**; Phillip M. Mach[1]; Elizabeth S. Dhummakupt[2]; Daniel O. Carmany[1]; Michael W. Busch[1]; Trevor Glaros[3]; *[1]Excet, Inc., Gunpowder, MD; [2]National Research Council, APG-EA, MD; [3]US Army ECBC, Aberdeen Proving Ground, MD*

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ThP 248 **Mass Spectrometry's Role in Understanding and Evaluating the Clustering and Dissociation of Next-Generation Spacecraft Propellants**; Amanda Patrick[1]; Christopher Annesley[2]; *[1]NRC/AFRL, Albuquerque, NM; [2]Space Vehicles Directorate, Air Force Research Laboratory, Kirtland AFB, NM*

ThP 249 **Elucidation of Protonated Amino Acid Dissociation Mechanism Using Atmospheric Pressure Thermal Dissociation Mass Spectrometry (APTD-MS)**; Pengyi Zhao[1]; Travis White[1]; Graham Cooks[2]; Qinhao Chen[3]; Yong Liu[3]; Hao Chen[1]; *[1]Ohio University, Athens, OH; [2]Purdue University, West Lafayette, IN; [3]Merck Research Laboratories, Rahway, NJ*

ThP 250 **Rearrangement of β-phenyl-α, β-unsaturated Esters in EI Mass Spectra**; Quan-Long Pu[1]; Yufang Zheng[1]; Stephen E. Stein[1]; *[1]NIST, Gaithersburg, MD*

ThP 251 **Electron Ionization Dissociation of Proteins, Peptides, and Small Molecules using a Digital Ion Trap Mass Spectrometer**; Hidenori Takahashi[1]; Sadanori Sekiya[1]; Shosei Yamauchi[1]; Shinichi Iwamoto[1]; Koichi Tanaka[1]; *[1]Shimadzu corp., Kyoto, Japan*

ThP 252 **An EThcD-Based Method for Discrimination of Leucine and ISOLEUCINE Residues in Peptides**; Sergey V. Kovalev[1]; Miriam D. Tolpina[1]; Sergey S. Zhokhov[1]; Tatiana Yu Samguina[1]; Albert T Lebedev[1]; *[1]Moscow State University, Moscow, Russian Federation*

ThP 253 **Radical-Initiated Fragmentation of Complex Polysulfated Anions by Negative Polarity Helium Charge Transfer Dissociation Tandem MS**; David Ropartz[1]; Pengfei Li[2]; Glen P. Jackson[2, 3]; Helene Rogniaux[1]; *[1]INRA UR1268 BIA, Nantes, France; [2]C. Eugene Bennett Department of Chemistry, West Virginia University, Morgantown, WV; [3]Department of Forensic and Investigative Science, West Virginia University, Morgantown, WV*

ThP 254 **Gas-phase Structures and Fragmentation Chemistry of Anionic Glycans**; Jordan Rabus[1]; Joseph Frye[1]; Ashley Wagoner[1]; Maha Abutokaikah[1]; Philippe Maitre[2]; Benjamin Bythell[3]; *[1]University of Missouri-St. Louis, St Louis, MO; [2]University of Paris-South, Orsay, France; [3]Univ. of Missouri-St. Louis, St. Louis, MO*

ThP 255 **Utilizing Radical-Directed Dissociation to Unmask New Sites of Isomerization in α-Crystallins from Human Lenses**; Tyler R. Lambeth[1]; Yana A. Lyon[1]; Ryan R. Julian[1]; *[1]University of California-Riverside, Riverside, CA*

ThP 256 **Structural Design of Sequence-Defined Synthetic Polymers to Push the Boundaries of MS/MS Sequencing Efficiency**; Jean-Arthur Amalian[1]; Abdelaziz Al Ouahabi[2]; Gianni Cavallo[2]; Jean-François Lutz[2]; Laurence Charles[1]; *[1]Aix-Marseille University, Marseille Cedex 20, France; [2]Institut Charles Sadron, Strasbourg, France*

ThP 257 **Influence of Nucleobase and Sugar Modifications on the Proton Affinity of Cytidine and Base-Pairing Energies of Proton-Bound Dimers of Cytidines**; Mary T Rodgers[1]; Sahil S. Rafai[2]; Zachary J. Devereaux[2]; Harrison Roy[2]; Yakubu Seidu[2]; *[1]Wayne State University, Detroit, MI; [2]Wayne State University, Detroit , MI*

ThP 258 **Influence of Ion Activation Method on the Accuracy of *de-novo* Sequencing Using Peptides Converted to N-Terminal Imines**; Amanda Bubas[1]; Susan Kline[2]; Danielle E. Kirby[2]; Luke J. Metzler[2]; Arpad Somogyi[3]; Michael J. Van Stipdonk[2]; *[1]Duquesne University, Pittsburgh; [2]Duquesne University, Pittsburgh, PA; [3]Ohio State University, Columbus, OH*

ThP 259 **Mechanism studies of Free Radical Initiated Peptide Sequencing (FRIPS) Mass Spectrometry: A Model Gas-Phase Reaction of GGR tripeptide**; Jae-ung Lee; *Sogang university, Mapo-gu, Seoul, South Korea*

ThP 260 **Fundamentals of Charge Transfer Dissociation (CTD) of Oligosaccharides**; Praneeth M. Mendis[1]; Zachary J. Sasiene[1]; David Ropartz[2]; Helene Rogniaux[2]; Glen P. Jackson[1, 3]; *[1]C. Eugene Bennett Department of Chemistry, West Virginia University, Morgantown, WV; [2]INRA UR1268 BIA, Nantes, France; [3]Department of Forensic and Investigative Science, West Virginia University, Morgantown, WV*

ThP 261 **Direct Evidence for The Origin of Bis-Gold Intermediates: Probing Gold Catalysis with Mass Spectrometry**; Mei Lu[1]; Yijin Su[2]; Pengyi Zhao[1]; Xiaohan Ye[2]; Yi Cai[1]; Xiaodong Shi[2]; Eric Masson[1]; Fengyao Li[1]; J. Larry Campbell[3]; Hao Chen[1]; *[1]Ohio University, Athens, OH; [2]University of South Florida, Tampa, FL; [3]Sciex, Concord, ON, Canada*

FUNDAMENTALS: ION MOLECULE, ION/ION, ION/ELECTRON INTERACTIONS
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ThP 262 **Gas-Phase Crosslinking to Probe the Noncovalent Interactions in an Amyloid-Motif Peptide Dimer Complex**; Shu R. Huang[1]; Huong T.H. Nguyen[1]; Yang Liu[1]; Frantisek Turecek[1]; *[1]University of Washington, Seattle, WA*

ThP 263 **Ion/ion Reactions for Hyaluronic Mixture Analysis via Electrospray Ionization Mass Spectrometry**; Mack Shih[1]; Scott A McLuckey[1]; *[1]Purdue University, West Lafayette, IN*

ThP 264 **Disulfide Bond Formation in Relation to Relative Acidity in Cysteine Containing Peptides**; Michael Browne[1]; Brinnley Barthels[1]; Ekram Hossain[1]; Jianhua Ren[1]; *[1]University of the Pacific, Stockton*

ThP 265 **Impact of Resonant Excitation Parameters on the Intramolecular Gas Phase HDX within Small Non-Covalent Systems**; Ekaterina Dariy[1, 2, 3]; Yves Gimbert[4]; Sandra Alves[5]; Alain Perret[1, 2, 3]; Jean-Claude Tabet[5, 6]; *[1]CEA - Institut de biologie François Jacob, Genoscope, Evry, France; [2]CNRS, UMR 8030, Evry, France; [3]Université d'Evry, UMR 8030, Evry, France; [4]Université Grenoble Alpes (DCM), CNRS-UJF 5250, Grenoble, France; [5]Paris-Sorbonne, Faculté des Sciences, IPMC, Paris, France; [6]CEA, iBiTec-S, SPI, LEMM, Gif-sur-Yvette, France*

ThP 266 **Comparison of CID Versus ETD Based MS/MS Fragmentation for the Analysis of Aminoglycosides**; Chien-Chen Lai[1]; Han-Chih Ko[1]; *[1]Institute of Molecular Biology, National Chung Hsing University, Taichung, Taiwan*

ThP 267 **A Gas Phase Ion/ion Reaction Sensitive to the Presence of Zwitterions**; Anthony M Pitts-McCoy[1]; Christopher P Harrilal[1]; Scott A McLuckey[1]; *[1]Purdue University, West Lafayette*

ThP 268 **Ultrafast Synthesis of Peptides and Disulfides in Hypervelocity Nanoparticle Impacts**; Gabriel D. Shuffield[1]; Michael J. Eller[1]; Emile A. Schweikert[1]; *[1]Texas A&M University, College Station, TX*

ThP 269 **Study of the Effect of Charge State on H/D Scrambling in ECD by using Online HDX Mass Spectrometry**; Jing Yan[1]; Yining Huang[1]; Weidong Cui[1]; Don L. Rempel[1]; Michael L Gross[1]; *[1]Washington University in St. Louis, St. Louis, MO*

ThP 270 **Electron Induced Dissocation in Linear Ion Trap Using Hihg Energy Electrons**; Alexandre Giuliani[1, 2]; Milos Rankovic[3]; Aleksandar R. Milosavljevic[1]; *[1]Synchrotron Soleil, Gif-Sur-Yvette, France; [2]INRA, Nantes, France; [3]Instute of Physics, Belgrade, Serbia*

ThP 271 **An Interesting Ion-Molecule Formation Under the Collision Induced Dissociation (CID)**; Liang Zhu[1]; Julia Guo[1]; Michael Lyktey[1]; Laura Sears[1]; *[1]BASF, Research Triangle Park, NC*

FUNDAMENTALS: ION STRUCTURE/ENERGETICS
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ThP 272 **Determination of Gas-Phase Acidities of Di- and Tripeptides Containing Aspartic and Glutamic Acid Residues by Mass Spectrometry and Computational Methods**; Can Cui[1]; Michele Stover[1]; Ashley McNeill[1]; David A. Dixon[1]; Carolyn J. Cassady[1]; *[1]The University of Alabama, Tuscaloosa*

ThP 273 **Infrared Photodissociation Spectroscopy of Electrosprayed Water-Tagged Molecules to Determine the Effect of Solvation Energy on Conformer Populations**; Matthew R. Bell[1]; Vinicius W.D. Cruzeiro[1]; Adrian Roitberg[1]; Nicolas C Polfer[1]; *[1]University of Florida, Department of Chemistry, Gainesville, FL*

ThP 274 **An Interdisciplinary Investigation of Uranyl Benzoate or pentafluorobenzoate Species Using Density Functional Theory and High Accuracy Mass Measurements**; Cassandra Hanley[1, 2]; Wibe A de Jong[2]; Irena Tatosian[1]; Luke Metzler[1]; Michael Van Stipdionk[1]; *[1]Duquesne*

University, Pittsburgh, PA; [2]Ernest Orlando Lawrence Berkeley National Laboratory, Berkeley, CA

ThP 275 **Investigation on the Unimolecular and Collisional-Activated Fragmentation Mechanisms of Diethylaniline Derivatives with Isotopic Labelling Experiments**; Sarah Seulen[1]; Jurgen Grotemeyer[1]; *[1]Christian-Albrechts-Univ, Kiel, Germany*

ThP 276 **Hydrogen Bonding Network of Guanidinium Cation Water Clusters Observed via Cryogenic Ion Mobility-Mass Spectrometry**; Michael Hebert[1]; David H. Russell[1]; *[1]Texas A&M University, College Station, TX*

ThP 277 **The Effects of Peptide Structure on Enhanced Protonation Upon Addition of Chromium(III) During Electrospray Ionization**; Nnenna E Dieke[1]; Carolyn J. Cassady[1]; *[1]The University of Alabama, Tuscaloosa, AL*

ThP 278 **Unimolecular Dissociation Pathways of Alanylglycine Derivatized to Create N-terminal Imines**; Luke Metzler[1]; Mary Sherman[1]; Michael Van Stipdionk[1]; *[1]Duquesne University, Pittsburgh, PA*

ThP 279 **Chirality Induced Gas-Phase Acidity and Conformational Changes in Cysteine-Polyalanine Peptides**; Yuntao Zhang[1]; Jianhua Ren[1]; *[1]University of the Pacific, Stockton, CA*

ThP 280 **Investigation of the Gas Phase Structure of Polyproline Helix Through Acidity Measurement**; Yadwinder Mann[1]; Jianhua Ren[1]; *[1]University of the Pacific, Stockton, CA*

GC/MS: INSTRUMENTATION AND APPLICATIONS II
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ThP 281 **The Analysis of Thermally Labile and Low Volatility Large Compounds by GC-MS with Cold EI**; Aviv Amirav[1]; Alexander B. Fialkov[1]; Uri Keshet[1]; Tal Alon[1]; *[1]Tel-Aviv University, Tel-Aviv, Israel*

ThP 282 **Speeding up GC-MS Analysis – From Few Minutes Down to Real Time Analysis**; Alexander B. Fialkov[1]; Uri Keshet[1]; Tal Alon[1]; Aviv Amirav[1]; *[1]Tel-Aviv University, Tel-Aviv, Israel*

ThP 283 **Mass Spectrometry Study of Plasma Treated Polymer film**; Liepin Huang[1]; Wageesha Senaratne[1]; Li Liu[1]; Jiangwei Feng[2]; Ming Huang Huang[1]; *[1]Corning Research Center, Corning, NY 14831; [2]Corning Research Center, Chutung, Taiwan*

ThP 284 **Characterization of Amine Catalyst Emissions from Spray Polyurethane Foam by Thermal Desorption (TD) GC/MS for Monitoring Indoor Air Quality**; Dale A. Willcox[1]; Jenan M. Elias[1]; *[1]Intertek Allentown, Allentown, PA*

ThP 285 **Investigating Organic Ligands on Nanocrystals by Qualitative and Quantitative Mass Spectrometry**; Hyokeun Park[1]; In-Sun Jung[1]; Jin Hae Kim[1]; *[1]Samsung Advanced Institute of Technology, Suwon-si, South Korea*

ThP 286 **Analysis of Halogenated Polycyclic Aromatic Hydrocarbons in Atmosphere Around Metallurgical Plants by 7250 High-Resolution GC/Q-TOF**; Lili Yang[1]; Jiajia Wu[2]; Guorui Liu[1]; Minghui Zheng[1]; Zhe Cao[2]; *[1]Research Center for Eco-Environmental Science, Chinese Academy of Sciences, Beijing, China; [2]Agilent Technologies, Beijing, China*

ThP 287 **Detection of Cannabidiol and Terpenes in Hemp by Direct Thermal Extraction GC/MS**; Ron Shomo[1]; Christopher Baker[1]; *[1]Scientific Instrument Services, Ringoes, NJ*

ThP 288 **GC-MS/MS Pesticide Analysis in Green Tea using Targeted MRM and Full Scan Analysis in a Single Acquisition**; Jody Dunstan[1]; Adam Ladak[2]; Lauren Mullin[2]; Doug Stevens[2]; Kenneth Rosnack[2]; *[1]Waters Corporation, Wilmslow, UK; [2]Waters Corporation, Milford, MA*

ThP 289 **Quantitative Investigation of Volatile Organic Compounds using Thermal Desorption with a Portable Gas Chromatography Mass Spectrometry**; Joshua Wilhide[1]; Ian W Shaffer[1]; William R. LaCourse[1]; *[1]University of Maryland Baltimore County, Baltimore, MD*

ThP 290 **Peculiar Behavior of N-Alkoxycarbonyl Derivatives of Simplest Amino Acid Methyl Esters Under GC-MS Analysis**; Nino G. Todua[1]; Igor G Zenkevich[2]; Anzor I. Mikaia[3]; *[1]National Institute of Standards & Technology, NIST / Dakota Consulting Inc., Gaithersburg, MD; [2]St. Petersburg State University, Institute for Chemistry, St. Petersburg, Russia; [3]National Institute of Standards & Technology, NIST, Gaithersburg, MD*

ThP 291 **Stable Isotope Dilution Gas Chromatography–Mass Spectrometry Method for Determining Arbutin in Plants Extracts**; Yongsoo Choi[1]; Kyoung Bok Lee[2]; Jaehyuk Choi[2]; Soon Kil Ahn[2]; Jae Kwang Kim[2]; *[1]Systems Biotechnology Research Center, Korea Institute of Science and Technology, Gangneung, South Korea; [2]Incheon National University, Incheon, South Korea*

ThP 292 **Applications of the ThermoExactive™ GC Orbitrap™ GC-MS Systemin Agricultural Research**; Jeffrie Godbey[1]; Jeffrey Gilbert[1]; Chengli Zu[1]; Yelena Adelfinskaya[1]; JESSE L. Balcer[1]; Daniel Gachotte[1]; *[1]Dow AgroSciences, Indianapolis, IN*

ThP 293 **Rearrangement of 2-Chloroalkylphosphonates and its Related Compounds in EI Mass Spectra**; YUFANG ZHENG[1]; Weihua Ji[2]; Quanlong Pu[2]; Stephen Stein[2]; *[1]NIST / Dakota C., Gaithersburg, MD; [2]NIST, Gaithersburg, MD*

ThP 294 **Contemporary procedures for quality control in mass spectral databases**; Anzor Mikaia[1]; Vladimir G. Zaikin[2]; *[1]NIST, Gaithersburg, MD; [2]Topchiev Institute of Petrochemical Synthesis RAS, Moscow, Russia*

ThP 295 **Combination of chemical ionization (CI) and low electron energy ionization capabilities with high-resolution Time-of-Flight GC/MS**; Viorica Lopez-Avila[1]; Sofia Nieto[1]; Harry Prest[1]; Jeffrey Kernan[1]; George Yefchak[1]; Robert Clark[1]; Nathan Eno[1]; Jim Oppenheimer[1]; Bill Russ[1]; *[1]Agilent Technologies, Inc., Santa Clara, CA*

ThP 296 **Determination of 59 potential Allergens in Perfumesby twin-line fast GC-MS/MS**; Christopher Sowa[1]; Dr. Hans-Ulrich Baier[2]; Xaver Mönninghof[2]; *[1]Shimadzu Deutschland GmbH, Duisburg, Germany; [2]Shimadzu Europa GmbH, Duisburg, Germany*

ThP 297 **Evaluation of Agilent 7250 GC/Qtof-MS System for Identification of Impurities in Complex Organic Reaction mixtures**; Chengli Zu[1]; Jeffrey Gilbert[2]; Jeffrie A Godbey[2]; Daniel Gachotte[2]; Matthew Curtis[3]; Viorica Lopez-Avila[3]; Garrison Brich[4]; Bell Bruce[2]; *[1]Dow Chemical Company, Indianapolis, IN; [2]Dow AgroSciences, Indianapolis, IN; [3]Agilent Technologies, Inc., Santa Clara, CA; [4]Agilent Technologies, Santa Clara, California*

ThP 298 **Detection and Quantification of Organophosphorus Compounds by Formation of PO4- in a Microwave Plasma**; Peter Haferl[1]; Kaveh Jorabchi[1]; *[1]Georgetown University, Washington, DC*

ThP 299 **Fully Automated Online Trimmethylsilyl (TMS) Derivatization Protocol for Metabolite Profiling Using an Orbitrap GC-MS and High Resolution/Accurate Mass Metabolomics Library**; Xin Zheng[1]; Jason Cole[2]; Giulia Riccardino[3]; Paul Silcock[4]; *[1]Thermo Fisher Scientific, Austin, TX; [2]Thermo Fisher Scientific, Ausitn, TX; [3]Thermo Fisher Scientific, Milan, Italy; [4]Thermo Fisher Scientific, Runcorn, UK*

ThP 300 **Increasing Molecular Ion Production for unknown Formula Elucidation with Chemical Ionization and Low Energy-Electron Ionization on Orbitrap-GC/MS**; Brody Guckenberger[1]; Xin Zheng[2]; Dominic Roberts[3]; Jason Cole[1]; Paul Silcock[3]; *[1]Thermo Fisher Scientific, Ausitn, TX; [2]Thermo Fisher Scientific, Austin, TX; [3]Thermo Fisher Scientific, Runcorn, NA*

ThP 301 **Direct Analysis of Terpenes Using GC-MS/MS with a Plasma Source**; Reza Javahery[1]; Mehrnaz Sarrafzadeh[1]; Farshid Pashaee[1]; Heather Gamble[1]; Chuck Jolliffe[1]; *[1]PerkinElmer Inc., Woodbridge, ON, Canada*

ThP 302 **VOC Analysis Using GC-Dual Mode Electron Ionization-MS**; Lisa Cousins[1]; Anna Kornilova[1]; Dante Sanchez[1]; Reza Javahery[1]; *[1]PerkinElmer Inc., Woodbridge, ON, Canada*

H/D EXCHANGE: PROTEIN STRUCTURE/FUNCTION II
303-318

ThP 303 **Dynamics of L-Kynureninase Orthologs during Catalysis**; Kyle W Murray[1]; Christos S Karamitros[2]; Everett Stone[2]; George Georgiou[2]; Sheena D'Arcy[1]; *[1]University of Texas at Dallas, Richardson, TX; [2]University of Texas at Austin, Austin, TX*

ThP 304 **Interrogating a Multidrug Efflux Membrane Protein Transporter Involved in Bacterial Antibiotic Resistance Using Structural Mass Spectrometry**; Zainab Ahdash[1]; Eamonn Reading[1]; Argyris Politis[1]; *[1]King's College London, London, UK*

ThP 305 **Investigating Differences in ADCC Activity Between a mAb and mAb-scfv by Hydrogen Deuterium Exchange Mass Spectrometry**; Jon Fitchett[1]; Kai Zhang[1]; Bryan E. Jones[1]; *[1]Lilly Biotech Center-San Diego, San Diego, CA*

ThP 306 **Epitope Binning by Hydrogen Deuterium Exchange Mass Spectrometry: Understanding Epitope-Driven Effects**; Chris Morgan[1]; X. Kate Zhang[1]; *[1]Sanofi, Framingham, MA*

ThP 307 **Conformational Changes in Guanylate Kinase in the Presence of Nucleotides**; Roxana E. Iacob[1]; Andreas Zoephel[2]; Klaus Rumpel[2]; John R. Engen[1]; *[1]Northeastern University, Boston, MA; [2]Boehringer-Ingelheim Pharma GmbH & CO KG, Vienna, Austria*

ThP 308 **HDX and FPOP Footprinting Combine to Expose Changes in the Hydrogen Bonding Network in TEM β Lactamase Mutants**; Elizabeth Bergman[1]; Don L. Rempel[2]; Greg Bowman[3]; Michael L Gross[3, 4]; *[1]Washington University in St. Louis, Missouri; [2]Washington University in St Louis, MO; [3]Washington University School of Medicine, St Louis, MO; [4]Washington University, St. Louis, MO*

ThP 309 **Probing the Aggregation Properties of Aβ42 Disease Associated Mutants by Hydrogen Deuterium Exchange Mass Spectrometry**; Eva Illes-Toth[1]; Don L Rempel[2]; Michael L Gross[2]; *[1]Washington University in St Louis, St Louis, MO; [2]Washington University, St. Louis, St. Louis, MO*

ThP 310 **Structural Insights Into Fungal Cellulolytic System: Cellulose Dehydrogenase and Lytic Polysaccharide Monooxygenase Function and Interaction Studied by Mass Spectrometry**; František Filandr[1, 2]; Daniel Kracher[3]; Lukas Slavata[1, 2]; Roland Ludwig[3]; Petr Halada[1, 2]; Petr Man[1, 2]; *[1]Institute of Microbiology of the CAS, Prague 4, Czech Republic; [2]Faculty of Science, Charles University, Prague, Czech Republic; [3]University of Natural Resources and Life Sciences, Vienna, Austria*

ThP 311 **HDX MS as a Diagnostic Tool for Ligand-Induced Conformational Change**; Joel C. Bucci[1]; Thomas E. Wales[1]; John R. Engen[1]; *[1]Northeastern University, Boston, MA*

ThP 312 **Mass Spectrometry-Based Structural Analysis of MoFe and FeFe Nitrogenase to Elucidate the Role of Structure-Function in Nitrogen Reduction**; Luke Berry[1]; Monika Tokmina-Lukaszewska[1]; Derek F. Harris[2]; Oleg A. Zadvornyy[3]; John W. Peters[3]; Lance C. Seefeldt[2]; Brian Bothner[1]; *[1]Montana State University, Bozeman, MT; [2]Utah State University, Logan, UT; [3]Washington State University, Pullman, WA*

ThP 313 **Investigation of the "BASiC hypothesis" for Protein Folding Reactions with Hydrogen-Deuterium Exchange Mass Spectrometry, Circular Dichroism and Fluorescence Spectroscopy**; Rohit Jain[1]; Khaja Muneeruddin[1, 2]; Scott A Shaffer[1, 2]; C. Robert Matthews[1]; *[1]Department of Biochemistry and Molecular Pharmacology, University of Massachusetts Medical School, Worcester, Massachusetts; [2]Proteomics and Mass Spectrometry Facility, University of Massachusetts Medical School, Shrewsbury, Massachusetts*

ThP 314 **Tracking Structural Changes and Characterizing Allosteric Networks in IgM upon Antigen Recognition via Hydrogen/Deuterium Exchange with Mass Spectrometry**; Michael Watson[1]; Miklos Guttman[2]; *[1]University of Washington School of Pharmacy, Seattle, WA; [2]University of Washington, Seattle, WA*

ThP 315 **Studying the Transient Structure of IDPs Using Microfluidics-Enabled Millisecond HDX-MS**; Eleanor R. Dickinson[1]; Rasmus R. Svejdal[1]; Jörg P. Kutter[1]; Kasper D. Rand[1]; *[1]University of Copenhagen, Copenhagen, Denmark*

ThP 316 **Unravelling the Conformational Dynamics of α-Synuclein's Folding Pathway in the Presence of Phospholipid Nanodiscs by HDX MS**; Irina Oganesyan; *York University, Toronto, ON, Canada*

ThP 317 **Probing the Role of Conformational Dynamics of Beta Lactamases in the Modulation of Resistance in Bacteria by HDX-MS**; Rinat Abzalimov[1]; Eleftheria Mavridou[2]; Thomas J. Walsh[2]; Gyorgy Babnigg[3]; Dionysios Pantazatos[2]; *[1]CUNY Advanced Science Research Center, New York, NY; [2]Weill Cornell Medicine, New York City, New York; [3]Argonne National Laboratory, Lemont, IL*

ThP 318 **EX1 ETD to Decipher RIG-I intermediate Structure Involved in Autoimmunity**; Jie Zheng[1]; Mi Ra Chang[1]; Ruben Garcia-Ordonez[1]; Scott J Novick[1]; Patrick R. Griffin[1]; *[1]The Scripps Research Institute, Jupiter*

HIGH MASS ACCURACY/HIGH PERFORMANCE MS: APPLICATIONS AND INSTRUMENTATION
319-336

ThP 319 **High-Resolution Accurate Mass Fragmentation Analysis of Glycosylated Sensory-Active Volatile Phenols in Smoke-Exposed Grapes and Wine**; Matthew Noestheden[1, 2]; Eric G Dennis[1]; Wesley F Zandberg[1]; *[1]University of British Columbia Okanagan, Kelowna, BC, Canada; [2]Supra Research and Development, Kelowna, BC, Canada*

ThP 320 **A Rugged UHPLC/HRMS Method for the Quantitation of Pyrithione Glucuronides in Human Urine that could not be Analyzed by HPLC/QQQ**; Ann Zoller[1]; Kady L Krivos[1]; Kenneth R. Wehmeyer[1]; Jason M Price[1]; Peter J Stoffolano[1]; Michael J Karb[1]; Jay F Nash[1]; Guhan Balan[1]; Lynda Behymer[1]; Molly Seeck[1]; Jose Brum[1]; Yuanshu Zou[1]; *[1]Procter and Gamble, Mason, Ohio*

ThP 321 **High Energy Collisional Dissociation (HCD) Spectral Matching for the Global Identification of RNA Hydrolysates**; Robert L. Ross[1]; Ningxi Yu[1]; Manasses Jora[1]; Ralf Tautenhahn[2]; Patrick A. Limbach[1]; *[1]University of Cincinnati, Cincinnati, OH; [2]Thermo Fisher Scientific, San Jose, CA*

ThP 322 **timsTOF Pro and PASEF: Multiplying Sequencing Speed and Sensitivity in Proteomics**; Andreas-David Brunner[1]; Florian Meier[1]; Scarlet Koch[2]; Heiner Koch[2]; Markus Lubeck[2]; Niels Goedecke[2]; Nicole Drechsler[2]; Oliver Raether[2]; Jürgen Cox[1]; Matthias Mann[1]; *[1]Max Planck Institute of Biochemistry, Planegg, Germany; [2]Bruker Daltonik GmbH, Bremen, Germany*

ThP 323 **Multi linear Regression and GC Orbitrap analysis of Short Chain Chlorinated Alkanes in Biota and Consumer Products**; Helena Steer[1]; Maryl Dejong[1]; Daryl McGoldrick[1]; Pamela Martin[1]; Mike Knudsen[1]; Luke Cayley[2]; *[1]Environment and Climate Change Canada, Science and Technology Branch, Burlington, ON, Canada; [2]Environment and Climate Change Canada, Enforcement Branch, Toronto, ON, Canada*

ThP 324 **An Optimized Method for Achieving Maximal HLA-A*02:01 Immunopeptide Identifications from single Shot Analysis on an Orbitrap Lumos Mass Spectrometer**; Gregory K. Potts[1]; Damien B. Ready[1]; Stephanie M. Jensen[1]; Alayna M. George Thompson[1]; Jon D. Williams[1]; Melanie J. Patterson[1]; *[1]Abbvie Inc., North Chicago, IL*

ThP 325 **Development of UHPLC-HRMS Method for Simultaneous Determination of endogenous Anabolic Steroids and Their Metabolites for blood Doping Control in Sports**; Hatem Elmongy[1]; Michèle Masquelier[2]; Magnus Ericsson[2]; *[1]Department of Environmental Science and Analytical Chemistry, Stockholm University, Stockholm, Sweden; [2]Doping Control Laboratory, Karolinska University Hospital, Stockholm, Sweden*

ThP 326 **Origin Discrimination of Garlic Using UHPLC-Q-Orbitrap HRMS with Multivariate Analysis**; Dongjin Kang[1]; Eun-Hee Chang[1]; Da-Jeong Jeong[1]; Ji-Young Moon[1]; Seong-Hun Lee[1]; Hyeo-Kyeung Kim[1]; Byeung-Kon Shin[1]; *[1]National agricultural products quality management service, Gimcheon-Si, South Korea*

ThP 327 **Performance Comparison of Q Exactive Plus and Orbitrap Fusion Lumos Tribrid Mass Spectrometer for Shotgun Proteomics**; Chenqi Hu[1]; Liang Jin[1]; shichen Shen[2]; xue Wang[2]; Edit Tarcsa[1]; Jun Qu[2]; Yu Tian[1]; *[1]AbbVie, Worcester, MA; [2]SUNY at Buffalo, Buffalo, NY*

ThP 328 **Enhancements to NIST Mass Interpreter for Modeling High Mass Accuracy Tandem Mass Spectra**; Alexey Mayorov[1, 2]; Yuri A Mirokhin[1]; Dmitrii V. Tchekhovskoi[1]; Stephen E. Stein[1]; *[1]NIST, Gaithersburg, MD; [2]N.M.Emanuel Institute of Biochemical Physics RAS, Moscow, Russia*

ThP 329 **Operation and Development of Ion-Mobility Orbitrap Mass Spectrometer**; Jacob W. McCabe[1]; Michael L. Poltash[1]; Arthur Laganowsky[1]; David H. Russell[1]; *[1]Texas A&M University, College Station, TX*

ThP 330 **Absorption-Mode FT-ICR MS via In-Hardware Detection of Phased Transients**; Anton N. Kozhinov[1]; Konstantin O. Nagornov[1]; Christophe Masselon[2]; Edith Nicol[3]; Yury O. Tsybin[1]; *[1]Spectroswiss, Lausanne, Switzerland; [2]CEA, Grenoble, France; [3]Ecole Polytechnique, Palaiseau, France*

ThP 331 **Online Adjustment of Ion Transmission Conditions for Resolution-Dependent Operation of Orbitrap Mass Analyzers**; Jesse D. Canterbury[1]; Michael W. Senko[1]; Alexander Makarov[2]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Bremen, Germany*

ThP 332 **Computer-Assisted Structure Identification (CASI) for High-Throughput Identification of Small Molecules Using GC×GC-HRAM-TOFMS high Resolution Accurate Mass Spectrometry**; Arno Knorr[1]; Martin Almstetter[1]; Elyette Martin[1]; Antonio Castellon[1]; Pavel Pospisil[1]; Mark Bentley[1]; *[1]Philip Morris Products S.A., Neuchatel, Switzerland*

ThP 333 **Rapid Identification of Complex ConstituentsinGanoderma Lucidum Using High Resolution Mass Spectrometry with Targeted and Non-Targeted Processing Workflows**; Jing Xu[1]; Zhenghao Li[1]; Ting Liu[2]; Wenhai Jin[2]; Haijun Wu[2]; *[1]Shouxiangu Pharma Limited Corporation, Wuyi, China; [2]Sciex, Shanghai, China*

ThP 334 **Compositional Characterization of Complex Proto-Peptide Libraries via TENG Ionization and Million-Resolution Orbitrap Mass Spectrometry**; Marcos Bouza Areces[1]; Anyin Li[1]; Anton Petrov[1]; Zhong Lin Wang[1]; Facundo M. Fernandez[1]; *[1]Georgia Institute of Technology, Atlanta, GA*

ThP 335 **Screening of Risk Substances in Infant Formula Using High-Resolution Mass Spectrometry**; Wang Zhen[1]; Xiao gang chu[1]; *[1]Chinese Academy of Inspectionand Qarantine, Beijing, China*

ThP 336 **Transient-Centric FTMS: Performance and Applications**; Yury O. Tsybin[1]; Konstantin O. Nagornov[1]; Natalia Gasilova[2]; Laure Menin[2]; Anton N. Kozhinov[1]; *[1]Spectroswiss, Lausanne, Switzerland; [2]Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland*

IMAGING MS: METHOD DEVELOPMENT
337-370

ThP 337 **Towards Mass Spectrometry Imaging in the Metabolomics Scale using Multiple On-Tissue Chemical Modifications**; Maria Emilia Dueñas[1]; Young-Jin Lee[1]; *[1]Iowa State University, Ames, IA*

ThP 338 **Enhanced MALDI-Mass Spectrometry Imaging of Amino Acids in Maize Root Tissue Through Chemical Derivatization**; Kelly O'neill[1]; Jacqueline Sijore[1]; Adam Boey[1]; Young-Jin Lee[1]; *[1]Iowa State University, Ames, IA*

ThP 339 **Sonication after Sublimation/Hydration Improves Protein Signal in Matrix-assisted Laser Desorption Ionization Imaging**; Li-En Lin[1]; Pin-Rui Su[1]; HSIN-YI WU[1]; Cheng-Chih Hsu[1]; *[1]National Taiwan University, Taipei, Taiwan*

ThP 340 **Molecular Pathology of Surgically Resected Tissue Specimen Based on Lipids Characterization by Laser Microdissection and Liquid Vortex Capture Mass Spectrometry**; Tiffany Porta[1]; John F. Cahill[2]; Yves J.C. LeBlanc[3]; Vilmos Kertesz[2]; Gert B. Eijkel[1]; Pierre-Maxence Vaysse[1]; Heike Grabsch[4]; Steven W.M. Olde Damink[4]; Gary Van Berkel[2]; Ron M.A. Heeren[1]; *[1]M4I Institute, Maastricht, Netherlands; [2]Oak Ridge National Laboratory, Oak Ridge, TN; [3]Sciex, Concord, ON, Canada; [4]Maastricht University Medical Centre, Maastricht, Netherlands*

ThP 341 **Optically Guided High Throughput Single Cell Mass Spectrometry of Rat Dorsal Root Ganglia to Profile Lipids, Peptides and Proteins**; Thanh D Do[1, 2]; Joseph F Ellis[1, 2]; Elizabeth K Neumann[1, 2]; Troy J Comi[1, 2]; Emily G Tillmaand[1, 2]; Ashley E Lenhart[1]; Stanislav Rubakhin[1, 2]; Jonathan V Sweedler[1, 2]; *[1]University of Illinois at Urbana-Champaign, School of Chemical Sciences, Urbana, IL; [2]The Beckman Institute for Advanced Science and Technology, Urbana, IL*

ThP 342 **MALDI MSI Directed Laser Ablation Tissue Microsampling with DIA Mass Spectrometry**; Kelin Wang[1]; Fabrizio Donnarumma[1]; Carson W. Szot[1]; Michael E. Pettit[2]; Touradj Solouki[2]; Kermit K. Murray[1]; *[1]Louisiana State University, Baton Rouge, LA; [2]Baylor University, Waco, TX*

ThP 343 **3D Reconstruction of ToF-SIMS Tissue Depth Profiling: Digging Into the Details**; Daniel Graham[1]; Lara J Gamble[1]; Tina B Angerer[1]; *[1]UW NESAC/BIO, Seattle, WA*

ThP 344 **Imaging Shotgun Lipidomics: Addition of Parallel MS/MS Coverage to FTMS-MSI and Combined with Automated Lipid Annotations Using ALEX123**; Shane R. Ellis[1]; Martin R. L. Paine[1]; Gert B. Eijkel[1]; Josch K Pauling[2, 3]; Peter Husen[2]; Martin Hermansson[2]; Christer S. Ejsing[4, 5]; Ron M.A. Heeren[1]; *[1]M4I Institute, Maastricht, Netherlands; [2]Department of Physics, Chemistry and Pharmacy, University of Southern Denmark, Odense, Denmark; [3]Theoretical Biophysics, Institute of Biology, Humboldt-Universität zu Berlin, Berlin, Germany; [4]Department of Biochemistry and Molecular Biology, Villum Center for Bioanalytical Sciences, University of Southern Denmark, Odense, Denmark; [5]Cell Biology and Biophysics Unit, European Molecular Biology Laboratory, Heidelberg, Germany*

ThP 345 **Targeted Desorption Electrospray Ionization (DESI) for Higher Throughput Mass Spectrometry Imaging (MSI) Studies**; Andreas Dannhorn[1]; M Luisa Doria[1]; Paolo Inglese[1]; James McKenzie[1]; Gregory Hamm[2]; John G Swales[2]; Nicole Strittmatter[2]; Anna Mroz[1]; Richard Goodwin[2]; Zoltan Takats[1]; *[1]Department of Surgery and Cancer, Imperial College London, London, UK; [2]Pathology, Drug Safety and Metabolism, IMED Biotech Unit, AstraZeneca, Cambridge, UK*

ThP 346 **Combining Enzymes to Increase Glycan Profiling in Human Pancreatic Cancer Tissues Using Mass Spectrometry Imaging**; Meng Xu[1]; Jillian Johnson[2]; Yatao Shi[2]; Xudong Shi[3]; Adib Keikhosravi[2]; Kevin Eliceiri[2]; Melissa C Skala[2]; W. John Kao[4]; Lingjun Li[1, 5]; *[1]Department of Chemistry, University of Wisconsin, Madison, WI; [2]University of Wisconsin, Madison, WI; [3]Department of Surgery, School of Medicine and Public Health, University of Wisconsin, Madison, WI; [4]The University of Hong Kong, Pokfulam, Hong Kong; [5]School of Pharmacy, University of Wisconsin, Madison, WI*

ThP 347 **ToF-SIMS Characterization of Tumor Microenvironments**; Blake Bluestein[1]; Daniel Graham[1]; Fionnuala Morrish[2]; David Hockenbery[2]; Lara Gamble[1]; *[1]University of Washington, Seattle, WA; [2]Fred Hutchinson CRC, Seattle, WA*

ThP 348 **Complementary Bioimaging to Determine Nanoparticle and Phospholipid Distribution in Lung Tissue**; Ann-Christin Niehoff[1]; Dörthe Dietrich[2]; Michael Sperling[2]; Uwe Karst[2]; *[1]Shimadzu Europe, Duisburg, Germany; [2]Institute of Inorganic and Analytical Chemistry, Muenster, Germany*

ThP 349 **Monitoring the Distribution and Biochemical Effects of Nanoparticle Stabilized Capsules and Their Cargo using Mass Spectrometry Imaging**; Kristen N. Sikora[1]; Joseph M. Hardie[1]; Vincent M. Rotello[1]; Richard W. Vachet[1]; *[1]University of Massachusetts, Amherst, MA*

ThP 350 **MALDI Imaging MS of Proteins in the Negative Ion Mode**; Junhai Yang[1, 2]; Lisa Manier[3]; Richard M. Caprioli[1, 3, 4, 5]; *[1]Department of Biochemistry, Vanderbilt University, Nashville, TN; [2]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [3]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [4]Department of Chemistry, Vanderbilt University, Nashville, TN; [5]Department of Pharmacology and Medicine, Vanderbilt University, Nashville, TN*

ThP 351 **Imaging Cholesterol Metabolism in Brain Using Advanced on Tissue Derivatisation and LESA-NanoLC-MS**; Yuqin Wang[1]; Eylan Yutuc[1]; William James Griffiths[1]; *[1]Swansea University, Swansea, UK*

ThP 352 **Multivariate Analysis of MALDI Imaging Mass Spectrometry Data of Mixtures of Single Pollen Grains**; Franziska Lauer[1, 2]; Sabrina Diehn[1, 2]; Stephan Seifert[1, 2]; Janina Kneipp[1, 2]; Volker Sauerland[3]; Cesar Barahona[3]; Steffen Weidner[1]; *[1]Federal institute for Material Research and Testing, Berlin, Germany; [2]Humboldt-Universität zu Berlin, Department of Chemistry, Berlin, Germany; [3]Bruker Daltonik GmbH, Bremen, Germany*

ThP 353 **Improvements in Ambient MS Imaging of Intact Proteins: Combining Native LESA and DESI with Travelling-Wave Ion Mobility Spectrometry**; Rian L. Griffiths[1]; Emma K. Sisley[2]; Mark Towers[3]; James W. Hughes[2]; Emmanuelle Claude[3]; Iain B. Styles[2]; Helen J. Cooper[2]; *[1]The University of Birmingham, Birmingham, UK; [2]University of Birmingham, Birmingham, UK; [3]Waters Corporation, Wilmslow, UK*

ThP 354 **Mass Spectrometry–Ion Beam Analysis: A New Tool for Molecular and Elemental Speciation?**; Catia Costa[1]; Josephine Bunch[2]; Richard Goodwin[3]; Roger P Webb[1]; Vladimir Palitsin[1]; Guido Verbeck[4]; Janella de Jesus[1, 2]; Melanie J. Bailey[1]; *[1]University of Surrey, Guildford, UK; [2]National Physical Laboratory, Teddington, UK; [3]AstraZeneca, UK, Cambridge, UK; [4]University of North Texas, Denton, Texas*

ThP 355 **Temporospatial Changes in Lipid Composition in Infarcted Mouse Heart Tissue Elucidated by Multimodal Imaging MS**; Sanna Sämfors[1]; Ibrahim Kaya[2]; Marcus Ståhlman[3]; Martina Klevstig[3]; Jan Borén[3]; John S. Fletcher[4]; *[1]Chalmers University of Technology, Gothenburg, Sweden; [2]Department of Psychiatry and Neurochemistry, Sahlgrenska Academy at the University of Gothenburg, Mölndal, Sweden; [3]Institute of Medicine, Department of Molecular and Clinical Medicine at University of Gothenburg, and Sahlgrenska University Hospital, Gothenburg, Sweden; [4]Department of Chemistry and Molecular Biology, University of Gothenburg, Gothenburg, Sweden*

ThP 356 **Optimised Desorption Electrospray Ionisation Mass Spectrometry Imaging (DESI-MSI) Method for Ambient Analysis of Proteins/Peptides Directly from Tissue Sections**; Mark Towers[1]; James W Hughes[2]; Rian L. Griffiths[2]; Patricia F Lalor[2]; Helen J Cooper[2]; Emmanuelle Claude[1]; *[1]Waters Corporation, Wilmslow, UK; [2]University of Birmingham, Birmingham, UK*

ThP 357 **New Tools for Mass Spectrometry Imaging to Selectively Target Endogenous and Administered Aldehydes and Ketones by On-Tissue Derivatization**; Anna Nilsson[1]; Mohammadreza Shariatgorji[1]; Erica Bäckström[2]; Gregory Hamm[3]; Elva Fridjonsdottir[1]; Xiaoqun Zhang[4]; Markus Fridén[2]; Per Svenningsson[4]; Richard J.A. Goodwin[3]; Per E. Andren[1]; *[1]Uppsala University, Uppsala, Sweden; [2]AstraZeneca, Gothenburg, Sweden; [3]AstraZeneca, UK, Cambridge, UK; [4]Karolinska Institute, Stockholm, Sweden*

ThP 358 **A New Enzymatic Approach to Distinguish Fucosylation Isomers of N-linked Glycans in Tumor Tissues Using MALDI Imaging Mass Spectrometry**; Connor A West[1]; Hongyan Liang[1]; Anand S Mehta[1]; Richard R Drake[1]; *[1]Medical University of South Carolina, Charleston, SC*

ThP 359 **3,4-Dimethoxycinnamic Acid (DMCA) as a Novel Matrix for the in Situ Analysis of Small Metabolites in Biological Samples by MALDI-TOF-MS**; Xiaodong Wang[1]; Huixin He[1]; Liang Qin[1]; Yaqin Liu[1]; Yawen Zhang[1]; Manman Han[1]; *[1]Centre for Imaging & Systems Biology, College of Life and Environmental Sciences, Minzu University of China, Beijing, China*

ThP 360 **Next Generation Histology-Directed Imaging Mass Spectrometry for Rapid Molecular Characterization of 1000s of Human Kidney Glomeruli**; Heath Patterson[1]; Michael D. Tuck[1]; Haichun Yang[2]; Raf Van de Plas[1, 3]; Agnes B. Fogo[2]; Richard M. Caprioli[1]; *[1]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [2]Department of Pathology, Vanderbilt University, Nashville, TN; [3]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands*

ThP 361 **Complementary Features of Laser Desorption Ionization from Silicon Nanopost Arrays and MALDI for Mass Spectrometry Imaging**; Jacqueline E. Dyer[1]; Jarod A. Fincher[1]; Nicholas J. Morris[2]; Matthew J. Powell[3]; Derek Jones[4]; Victoria K. Shanmugam[5]; Sridevi Yadavilli[6]; Javad Nazarian[6]; Russell K. Pirlo[7]; Akos Vertes[1]; *[1]George Washington University, Washington, DC; [2]UES, Inc., Beavercreek, Ohio; [3]Protea Biosciences Inc., Morgantown, WV; [4]Division of Rheumatology, The George Washington University, School of Medicine and Health Sciences, Washington, DC; [5]Division of Rheaumatology, The George Washington University, School of Medicine and Health Sciences, Washington, DC; [6]Research Center for Genetic Medicine, Children's National Medical Center, Washington, DC; [7]Chemistry Division, U.S. Naval Research Laboratory, Washington, DC*

ThP 362 **On-Surface Chemical Modification of Vicinal Diols for Mass Spectrometry Imaging**; Trevor T Forsman[1]; Maria Emilia Dueñas[1]; Young-Jin Lee[1]; *[1]Iowa State University, Ames, IA*

ThP 363 **MSI-Compatible Optimized Lung Inflation Protocol as a Means to Investigate Pseudomonas aeruginosa Infection**; Courtney E. Chandler[1]; Alison J Scott[1]; Shane R. Ellis[2]; Ron M.A. Heeren[2]; Robert K. Ernst[1]; *[1]Department of Microbial Pathogenesis, School of Dentistry, University of Maryland, Baltimore, MD; [2]Maastricht MultiModal Molecular Imaging (M4I) insitute, Division of Imaging Mass Spectrometry (IMS), Maastricht, Netherlands*

ThP 364 **Optimization of DESI-MS Imaging of Proteins Directly from Biological Tissue Sections**; Kyana Y Garza[1]; Clara L Feider[2]; Jake A Rosenberg[2]; Jennifer S Brodbelt[2]; Livia S Eberlin[2]; *[1]University of Texas, Austin, TX; [2]University of Texas at Austin, Austin, TX*

ThP 365 **Identification Strategies for Proteins in Mass Spectrometry Imaging of Proteins After On-Tissue Digestion**; Katharina Huber[1]; Julia Kokesch-Himmelreich[2]; Alan M. Race[2]; Bastian Jahreis[2]; Bernhard Spengler[1];

Andreas Roempp[2]; [1]*Institute of Inorganic and Analytical Chemistry, Justus Liebig University Giessen, Giessen, Germany;* [2]*Chair of Bioanalytical Sciences and Food Analysis, University of Bayreuth, Bayreuth, Germany*

ThP 366 **Antibiotics from Predatory Bacteria: Probing Chemical Interactions of Microbial Colonies Using Imaging Desorption Electrospray- Ion Mobility – Mass Spectrometry**; Berkley Ellis[1]; Caleb N Fischer[2]; Brian O Bachmann[2]; John A McLean[2]; [1]*Vanderbilt University, Nashville, TN;* [2]*Vanderbilt University, Nashville*

ThP 367 **Establishing a Workflow for Co-Registering Matrix Assisted Laser Desorption Ionization Mass Spectrometry and Time-of-Flight Secondary Ion Mass Spectrometry Images**; Matthias Lorenz[1, 2]; Aleeza Leder Macek[2, 3]; Udaya C. Kalluri[2]; Anton V. Ievlev[2]; Olga S. Ovchinnikova[2]; [1]*University of Tennessee, Knoxville, TN;* [2]*Oak Ridge National Laboratory, Oak Ridge, TN;* [3]*University of Illinois at Urbana-Champaign, Urbana, Illinois*

ThP 368 **Nanoscale Characterization of Bottle-Brush Copolymers Using Combined Time-of-Flight Secondary Ion Mass Spectrometry and Atomic Force Microscopy Platform**; Anton Ievlev[1]; Matthias Lorenz[1]; Dongsook Chang[1]; Bobby Sumpter[1]; Olga S. Ovchinnikova[1]; [1]*Oak Ridge National Laboratory, TN*

ThP 369 **Optimizing Desorption Electrospray Ionization Mass Spectrometric Imaging for Detection of Water-Soluble Metabolites in Brain Tissue**; Kevin Y Cho[1]; Hong Jun Cho[2]; Joseph H. Kennedy[3]; Justin M. Wiseman[3]; Liviu Mirica[2]; Gary J Patti[1]; [1]*Washington University School of Medicine, St. Louis, MO;* [2]*Washington University, St. Louis, St. Louis, MO;* [3]*Prosolia, Inc., Indianapolis, IN*

ThP 370 **Fast Rastering Matrix-Assisted Laser Desorption Ionization for Mass Spectrometry Imaging of Lipids at High Lateral Resolution**; Florian Barré[1]; Beatriz Rocha[1]; Mark Towers[2]; Paul Murray[2]; Emmanuelle Claude[3]; Berta Cillero-Pastor[1]; Ron M.A. Heeren[4]; Tiffany Porta[1]; [1]*Maastricht MultiModal Molecular Imaging (M4I) insitute, Division of Imaging Mass Spectrometry (IMS), Maastricht, Netherlands;* [2]*Waters Corporation, Wilmslow, UK;* [3]*Waters Corporation, Wilmslow, UK;* [4]*Maastricht MultiModal Molecular Imaging (M4I) insitute, Division of Imaging Mass Spectrometry (IMS), Maastricht, Netherlands*

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ThP 371 **A Mass Spectrometry Imaging Method for Visualizing Synthetic Polymers by Using Average Molecular Weight and Polydispersity as Indices**; Takaya Satoh[1]; Susumu Fujimaki[1]; Kazuaki Murayama[1]; Yoshihisa Ueda[1]; Koji Okuda[2]; [1]*JEOL Ltd., Akishima, Tokyo, Japan;* [2]*JEOL USA, Inc., Peabody, MA*

ThP 372 **Computational Approaches for Localization and Quantification of Compounds, Toxicants and Their Metabolites**; Jan H. Kobarg[1]; Mélanie Lagarrigue[2]; *Régis Lavigne*[2]; Corinna Henkel[3]; Tobias Boskamp[1, 4]; Shannon Cornett[5]; Charles Pineau[2]; Dennis Trede[1]; [1]*SCiLS, Bremen, Germany;* [2]*IRSET - Institut de recherche en santé, environnement et travail, Rennes, France;* [3]*Bruker Daltonik GmbH, Bremen, Germany;* [4]*University of Bremen, Center for Industrial Mathematics, Bremen, Germany;* [5]*Bruker Daltonics, Billerica, MA*

ThP 373 **Error-Free Data Visualisation and Processing Through mzML and imzML Validation**; Alan M Race[1]; Andreas Römpp[1]; [1]*Chair of Bioanalytical Sciences and Food Analysis, University of Bayreuth, Universitätsstr.-30, Bayreuth, Germany*

INFORMATICS: ALGORITHMS AND STATISTICAL ADVANCES II
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ThP 374 **Predicting MS/MS Spectra of Modified Peptides with Transfer Learning**; Wen-Feng Zeng[1]; Xie-Xuan Zhou[1]; Si-Min He[1]; Jianfeng Zhan[1]; [1]*Institute of Computing Technology, Chinese Academy of Sciences, Beijing, China*

ThP 375 **Optimize your Method:rawDiagnostic An R Package to Support Method Development for Bottom-up Proteomics on Orbitrap Instruments**; Christian Trachsel[1]; Christian Panse[1]; Tobias Kockmann[1]; Jonas Grossmann[1]; Witold E. Wolski[1]; Laura Kunz[1]; Jay Tracy[1]; Claudia Fortes[1]; Paolo Nanni[1]; Ralph Schlapbach[1]; [1]*Functional Genomics Center Zurich, Zurich, Switzerland*

ThP 376 **A Quantitative Evaluation of Ion Chromatogram Extraction Algorithms**; Annika Tostengard[1]; Rob Smith[1]; [1]*University of Montana, Missoula, MT*

ThP 377 **Orthology-Directed Mapping Between Species for Comparative Proteomes in Sorghum Bicolor and Zea Mays**; Ali Elnaeim Elbasheir Ali[1]; Lizex H. H. Husselmann[1]; David Lee Tabb[2]; Ndomelele Ndiko Ludidi[1]; [1]*University of the Western Cape, Cape Town, South Africa;* [2]*Stellenbosch University, Durbanville, South Africa*

ThP 378 **Constrained *de novo* Sequencing of Neo-Epitope Peptides Using Tandem Mass Spectrometry**; Sujun Li[1]; Alex DeCourcy[1]; Haixu Tang[1]; [1]*Indiana University, Bloomington, IN*

ThP 379 **Fast and Efficient Mapping of Peptide Sequences and their Variants to Proteome Databases Using Full Inverted Indices**; Luis Mendoza[1]; Eric W Deutsch[1]; Robert L Moritz[1]; [1]*Institute For Systems Biology, Seattle, WA*

ThP 380 **Are Target and Decoy Competing Fair and Square?**; Mincheol Jeon[1]; Eunok Paek[2]; [1]*Department of Computer Science Hanyang University, Seoul, South Korea;* [2]*Hanyang University, Seoul, South Korea*

ThP 381 **Automated Deformulation of LCMS and GCMS Data Through Database Searching**; Anne Marie Smith[1]; Richard Lee[1]; Artsiom Piatrouski[2]; Andrey Paramonov[2]; Vitaly Lashin[2]; [1]*ACD/Labs, Toronto, ON, Canada;* [2]*ACD/Labs, Moscow, Russia*

ThP 382 **Philosopher: A Complete Pipeline for Both Conventional and Open Search-Based Shotgun Proteomics Data Analysis**; Felipe da Veiga Leprevost[1]; Avinash Kumar Shanmugam[1]; Dattatreya Mellacheruvu[1]; Hui-Yin Chang[1]; Dmitry M. Avtonomov[1]; Andy Kong[1]; Alexey I. Nesvizhskii[1]; [1]*University of Michigan Medical Center, Ann Arbor, MI*

ThP 383 **Machine Learning Improves Error Rates in Quality Control of Mass Spectrometry-Based Proteomics**; Eralp Dogu[1]; Roger Olivella[2]; Eduard Sabidó[2]; Olga Vitek[3]; [1]*Mugla University, Mugla, Turkey;* [2]*CRG, Barcelona, Spain;* [3]*Northeastern University, Boston, MA*

ThP 384 **Statistical and Bioinformatics Analysis of Proteome Dynamics in Mouse Model of NAFLD**; Rovshan Sadygov[1]; Ahma Borzou[1]; Kwangwon Lee[2]; Takhar Kasumov[2]; [1]*University of Texas, Galveston, TX;* [2]*Northeast Ohio Medical University, Rootstown, Ohio*

ThP 385 **Stratified FDR Results in Increased Identification Rates of Peptides and Proteins in Metaproteomics Data**; David Lyon[1, 2]; Christian von Mering[2]; Lars Juhl Jensen[1]; [1]*NNF CPR, University of Copenhagen, Copenhagen, Denmark;* [2]*Department of Molecular Life Sciences, and Swiss Institute of Bioinformatics, University of Zurich, Zurich, Switzerland*

ThP 386 **Kernel-Based Component Decomposition for Glycan Mixture Analysis Using Liquid Chromatography and Ion Mobility Spectrometry MS/MS**; Pengyu Hong[1]; Will Burnstein[1]; Juan Wei[2]; Cheng Lin[2]; [1]*Brandeis University, Waltham, MA;* [2]*Center for Biomedical Mass Spectrometry, Boston, Massachusetts*

ThP 387 **Tackle, A Data Analysis Toolbox For Routine Exploration of gpGrouper-Based Bottom-Up Proteomics Data**;

Alexander Saltzman[1]; Bhoomi Bhatt[1]; Anna Malovannaya[1]; *[1]Baylor College of Medicine, Houston, TX*

ThP 388 **In-Depth Proteomics Analysis Using a TIMS-QTOF with the PASEF Method and Deep Learning**; Zia Rahman[1]; Hieu Tran[2]; Clark Chen[1]; Gary Kruppa[3]; Baozhen Shan[1]; *[1]Bioinformatics Solutions Inc., Waterloo, ON, Canada; [2]University of Waterloo, Waterloo, ON, Canada; [3]Bruker Daltonics Inc., Billerica, MA*

ThP 389 **Internal Reference Scaling (IRS) is a Critical Component in Analyses of Biological Studies with Multiple TMT Experiments**; Phillip A. Wilmarth[1]; Ashok P. Reddy[1]; John E. Klimek[1]; Jennifer M. Cunliffe[1]; Larry L. David[1]; *[1]OHSU, Portland, OR*

ThP 390 **Confidence Assignment for Mass Spectrometry Based Peptide Identifications via the Extreme Value Distribution**; Gelio Alves[1]; Aleksey Y Ogurtsov[1]; Yi-Kuo Yu[1]; *[1]National Center for Biotechnology Information, NLM, NIH, Bethesda, MD*

ThP 391 **Building High-Quality Spectral Library from Massive Collections of Tandem Mass Spectra with Machine Learning**; Long WU[1]; Henry Lam[1]; *[1]HKUST, Hong Kong, China*

ThP 392 **High-Dynamic-Range Mass Spectrometry Through In Silico Integration of Isolation Windows: Rapid Class-wide Assessment of Molecular Changes in Cellular Response**; Raf Van de Plas[1, 2, 3]; Jamie L. Allen[2, 3]; Carrie E. Romer[2, 3]; Jeremy L. Norris[2, 3, 4]; Jeffrey M. Spraggins[2, 3, 4]; Richard M. Caprioli[2, 3, 4, 5, 6]; *[1]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [2]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [3]Department of Biochemistry, Vanderbilt University, Nashville, TN; [4]Department of Chemistry, Vanderbilt University, Nashville, TN; [5]Department of Pharmacology, Vanderbilt University, Nashville, TN; [6]Department of Medicine, Vanderbilt University, Nashville, TN*

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ThP 393 **The Evaluation of Genomic and Transcriptomic Data for Use as a Proxy Protein Database for Unsequenced Tree Nuts**; Cary Pirone-Davies[1]; Christine H. Parker[2]; Timothy Croley[2]; Melinda McFarland[2]; *[1]U.S. Food and Drug Administration, College Park, MD; [2]FDA-CFSAN, College Park, MD*

ThP 394 **Individualised Proteogenomics in Analysis of Single Amino Acid Variants in Malignant Melanoma**; Nicolas C Nalpas[1]; Marisa Schmitt[1]; Christoph Täumer[1]; Boris Maček[1]; *[1]Quantitative Proteomics, University of Tuebingen, Tuebingen, Germany*

ThP 395 **ProteomicsDB: An Interactive Multi-Omics Platform**; Patroklos Samaras[1]; Tobias Schmidt[1]; Martin Frejno[1]; Siegfried Gessulat[1, 2]; Maximilian Barnert[3, 4]; Harald Kienegger[3, 5]; Helmut Krcmar[3, 5]; Hans-Christian Ehrlich[2]; Stephan Aiche[2]; Bernhard Kuster[1, 6, 7]; Mathias Wilhelm[1]; *[1]Chair of Proteomics and Bioanalytics, Technical University of Munich (TUM), Freising, Germany; [2]SAP SE, Potsdam, Germany; [3]Chair for Information Systems, Technical University of Munich (TUM), Munich, Germany; [4]SAP University Competence Center, Technical University of Munich (TUM), Munich, Germany; [5]SAP University Competence Center, Technical University of Munich (TUM), Minuch, Germany; [6]Center for Integrated Protein Science (CIPSM), Munich, Germany; [7]Bavarian Center for Biomolecular Mass Spectrometry, Freising, Germany*

ThP 396 **Sorfs.org: A Public Repository of a Proteogenomics Endeavour to Identify Coding Micropeptides**; Volodimir Olexiouk[1]; Wim Van Criekinge[1, 2]; Gerben Menschaert[1, 2]; *[1]BioBix, Gent, Belgium; [2]Ghent University, Ghent, Belgium*

ThP 397 **Identification of Peptide Variants Without Customized Databases: Comparison of "Genome-Free" Approaches for Proteogenomics**; Anna A Lobas[1, 2]; Mark V Ivanov[1, 2]; Kira Vyatkina[3, 4, 5, 6]; Lev I Levitsky[1, 2]; Elizaveta M Solovyeva[1, 2]; Sergei A Moshkovskii[7, 8]; Mikhail V Gorshkov[1, 2]; *[1]Institute for Energy Problems of Chemical Physics of RAS, Moscow, Russia; [2]Moscow Institute of Physics and Technology, Moscow, Russia; [3]Center for Algorithmic Biotechnology, Institute of Translational Biomedicine, Saint Petersburg State University, St Petersburg, Russia; [4]Saint Petersburg Academic University, RAS, St Petersburg, Russia; [5]ITMO University, St Petersburg, Russia; [6]Saint Petersburg Electrotechnical University "LETI", St Petersburg, Russia; [7]Institute of Biomedical Chemistry, Moscow, Russia; [8]Pirogov Russian National Research Medical University, Moscow, Russia*

ThP 398 **Bioprocess Monitoring with an Automated Mass-Spectrometry–Based Multi-Omics Software Platform**; Chung Ping Chow[1]; Dominik Mertens[1]; Ying Swan Ho[2]; *[1]Genedata AG, Basel, Switzerland; [2]Bioprocessing technology Institute, Singapore, Singapore*

ThP 399 **A Customizable Pipeline for High-Throughput Integration and Analysis of Large-Scale Multi-Omics Datasets**; Danielle B. Gutierrez[1]; Tina Tsui[1]; James C. Pino[1]; Michael Ripperger[1]; Melissa A. Farrow[2]; Randi L. Gant-Branum[1]; Nicole D. Muszynski[1]; Stacy D. Sherrod[1]; John A. McLean[1]; D. Borden Lacy[2]; Eric P. Skaar[2]; John P. Wikswo[1]; Carlos F. Lopez[1]; Jeremy L. Norris[1]; Richard M. Caprioli[1]; *[1]Vanderbilt University, Nashville, TN; [2]Vanderbilt University Medical Center, Nashville, TN*

ThP 400 **Slice and Dice: An Accessible Galaxy-Based Metaproteomic Database Sectioning Approach Improves Taxonomic and Functional Microbiome Characterization**; Praveen Kumar[1]; James E Johnson[1]; Thomas McGowan[1]; Caleb W Easterly[1]; Subina Mehta[1]; Shane L Hubler[2]; Joel Rudney[1]; Jason Michael Gilmore[3]; Brook L Nunn[3]; Pratik D Jagtap[1]; Timothy J. Griffin[1]; *[1]University of Minnesota, Minneapolis, MN; [2]Rhapsody Data LLC, Madison, WI; [3]University of Washington Genome Sciences, Seattle, WA*

ThP 401 **Multiomic Approach to Characterize Sperm Maturation**; Miranda L. Gardner[1, 2]; So Maezawa[3, 4]; Michael A. Freitas[1, 2]; Satoshi H. Namekawa[3, 4]; *[1]Department of Cancer Biology and Genetics The Ohio State University, Columbus, Ohio; [2]Comprehensive Cancer Center The Ohio State University, Columbus, Ohio; [3]Division of Reproductive Sciences, Division of Developmental Biology, Perinatal Institute, Cincinnati Children's Hospital Medical Center, Cincinnati, Ohio; [4]Department of Pediatrics, University of Cincinnati College of Medicine,, Cincinnati, Ohio*

ThP 402 **Association Between Metabolomics and Metagenomics Features of Human Microbiome Revealed by Co-Occurrence Pattern Analysis**; Egor Shcherbin[1]; Liu Cao[2]; Alan K. Jarmusch[3]; Pieter C. Dorrestein[4]; Hosein Mohimani[5]; *[1]Saint Petersburg Academic University, Saint Petersburgh, Russia; [2]Carnegie Mellon University, Pittsburgh, PA; [3]University of California San Diego, San Diego, CA; [4]University of California, San Diego, San Diego, CA; [5]Carnegie Mellon University, Pittsburgh*

ThP 403 **The Encyclopedia of Proteome Dynamics – A Big Data Ecosystem for (Prote)Omics**; Alejandro Brenes[1]; Vackar Afzal[1]; *[1]University of Dundee, Dundee, UK*

ThP 404 **Quantifying Functional Microbiomes: An Integrated, Quantitative Metaproteomics Approach Reveals Connections Between Taxa, Function and Protein Expression in Complex Microbiomes**; Pratik Dilip Jagtap[1]; Caleb W Easterly[1]; Nadia Szeinbaum[2]; Bjoern Gruening[3]; Lee S Parsons[1]; Shane L Hubler[4]; Subina Mehta[1]; Bart Mesuere[5, 6]; James E Johnson[1]; Andrea

Argentini[6,7]; Alessando Tanca[8]; Carolin Kolmeder[9]; Praveen Kumar[1]; Lennart Martens[5,6]; Joel Rudney[1]; Brook L Nunn[10]; Timothy J. Griffin[1]; *[1]University of Minnesota, Minneapolis, MN; [2]Georgia Institute of Technology, Atlanta, GA; [3]University of Freiburg, Freiburg, Germany; [4]Rhapsody Data LLC, Madison, WI; [5]Ghent University, Ghent, Belgium; [6]VIB-UGent Center for Medical Biotechnology, VIB, Ghent, Belgium; [7]Ghent University, Ghent, Belgium; [8]Porto Conte Ricerche Science and Technology Park of Sardinia, Alghero, Italy; [9]University of Helsinki, Helsinki, Finland; [10]University of Washington Genome Sciences, Seattle, WA*

ThP 405 **Using Linear Modeling and Comprehensive Pathway Analysis to Integrate Metabolomics and Gene Expression: Application in Breast Tumor and Non-Tumor Tissue**; Bofei Zhang[1]; Jalal K. Siddiqui[1]; Andrew Patt[1,2]; Senyang Hu[1]; Elizabeth Baskin[1]; Kevin R. Coombes[1]; Joseph P. McElroy[1]; Ewy Mathe[1]; *[1]Ohio State University Medical Center, Columbus, OH; [2]Biomedical Sciences Graduate Program, The Ohio State University, Columbus, OH*

ThP 406 **From Raw Data to Results on Your Screen: A Suite of Accessible Software for Comprehensive Proteogenomic Informatics**; James Johnson[1]; Thomas G McGowan[1]; Matthew C Chambers[2]; Praveen Kumar[3]; Subina Mehta[2]; Pratik Jagtap[2]; Timothy J. Griffin[2]; *[1]Minnesota Supercomputing Institute, University of Minnesota, Minneapolis, Minneapolis, MN; [2]Biochemistry, Molecular Biology, and Biophysics, University of Minnesota, Minneapolis, Minneapolis, MN; [3]Bioinformatics and Computational Biology, University of Minnesota, Minneapolis, Minneapolis, MN*

ThP 407 **Data Analysis Strategies for Real-Time Processing and Statistical Classification for Rapid Evaporative Ionisation Mass Spectrometry Microbial Speciation**; Alvaro Perdones-Montero[1]; Simon Cameron[1]; Richard Schaffer[2]; JULIA BALOG[2]; Keith Richardson[3]; Steven D Pringle[3]; Zoltan Takats[1]; *[1]Imperial College London, London, UK; [2]Waters Research Center, Budapest, Hungary; [3]Waters Corporation, Wilmslow, UK*

ThP 408 **Computational Mathematics Assimilation of Large Multi-Omics Datasets**; Anna M. Nia[1]; Brooke L. Barnette[1]; Shinji K. Strain[1]; Cheryl F. Lichti[2]; Robert L. Ullrich[1]; Mark R. Emmett[1]; *[1]UTMB, Galveston, TX; [2]Washington University School of Medicine, St Louis, MO*

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ThP 409 **A Web-Based, User-Friendly Reporting Tool for Mass Spectrometry Proteomics**; Katherine Bishop[1]; Ryan Koning[1]; Rob Smith[1]; *[1]University of Montana, Missoula, MT*

ThP 410 **Reverse and Random Decoy Methods for False Discovery Rate Estimation in High Mass Accuracy Peptide Spectral Library Searches**; Zheng Zhang[1]; Meghan C. Burke[1]; Yuri A. Mirokhin[1]; Dmitrii V. Tchekhovskoi[1]; Sanford P. Markey[1]; Stephen E. Stein[1]; *[1]National Institute of Standards and Technology, Gaithersburg, MD*

ThP 411 **Benchmarking and Improving the NIST Peptide Library Search Program, MSPepSearch**; Sergey Sheetlin[1]; Dmitrii V. Tchekhovskoi[1]; Zheng Zhang[1]; Stephen E. Stein[1]; *[1]NIST, Gaithersburg, MD*

ThP 412 **Augmenting Protein Database Searching with Peptide Library Searching**; Robert J Chalkley[1]; Peter R Baker[1]; *[1]UCSF, San Francisco, CA*

ThP 413 **Improved HLA Peptide Sequencing Accuracy and Sensitivity Through Optimized Scoring and Correlation of Database Search Result with *de novo* Interpretation**; Karl R Clauser[1]; Susan E Klaeger[1]; Jennifer G Abelin[1]; Hasmik Keshishian[1]; Derin B Keskin[2]; Siranush Sarkizova[3]; Christina R Hartigan[1]; Nir Hacohen[1]; Catherine J Wu[2]; Steven A Carr[1]; *[1]Broad Institute of MIT and Harvard, Cambridge, MA; [2]Dana-Farber Cancer Institute, Boston, MA; [3]Harvard Medical School, Boston, MA*

ThP 414 **Quantitative MS3 Scans Triggered by Real-Time Database Search**; Trent Stohrer[1]; Dennis Goldfarb[1]; Wei Wang[2]; Ben Major[1]; *[1]University of North Carolina - Chapel Hill, Chapel Hill, NC; [2]University of California Los Angeles, Los Angeles, CA*

ThP 415 **Utilizing Peptide Sequence Tags for Controlling False Discovery Rates in Database Search**; Akiyasu C. Yoshizawa[1]; Tsuyoshi Tabata[1,2]; Mio Iwasaki[2]; Naoyuki Sugiyama[1]; Yasushi Ishihama[1]; *[1]Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, Japan; [2]Center for iPS Cell Research and Application (CiRA), Kyoto University, Kyoto, Japan*

ThP 416 **Mass++ ver.4: An Open-Source, Quick and Simple Data Viewer**; Satoshi Tanaka[1]; Masaki Murase[2]; Tsuyoshi Takahashi[1]; Masaki Kato[2,3]; Maiko Kusano[4]; Shin Kawano[5]; Akiyasu C. Yoshizawa[2]; Susumu Goto[5]; Yasushi Ishihama[2]; *[1]Trans-IT, Kaminokawa-machi, Tochigi Pref., Japan; [2]Grad. School of Pharma. Sci., Kyoto Univ., Kyoto, Japan; [3]NIBB, Okazaki, Japan; [4]Grad. School of Med., Nagoya Univ., Nagoya, Japan; [5]DBCLS, DS, ROIS, Kashiwa, Japan*

ThP 417 **Pulsar, the Swiss Army Knife of Search Engines: Using Libraries to Search TMT-Labeled Peptides Increases Quantifications in Single Cell Proteomics**; Lynn Verbeke[1]; Tejas Gandhi[1]; Oliver M. Bernhardt[1]; Nikolai Slavov[2]; Lukas Reiter[1]; *[1]Biognosys AG, Schlieren, Switzerland; [2]Northeastern University, Boston, MA*

ThP 418 **Database Matching of *de novo* Sequencing Candidates – A New Strategy for MHC Peptide Identification**; Jens T. Vanselow[1]; Bastian Schilling[2]; Andreas Schlosser[1]; *[1]Rudolf Virchow Center, Wuerzburg, Germany; [2]Dermatology, University of Wuerzburg, Wuerzburg, Germany*

ThP 419 **Quantitation of Misincorporations: Strategies and System Suitability**; Kathleen Cornelius[1]; Olga Friese[1]; Mary Denton[2]; Jason Rouse[2]; *[1]Pfizer, Inc, Chesterfield, MO; [2]Pfizer Inc., Andover, MA*

ThP 420 **Utility of EThcD and AI-ETD for the Differentiation of Leucine and Isoleucine Residues in Large-Scale Shotgun Proteomic Experiments**; Kevin L Schauer[1]; Nicholas M Riley[1,2]; Lei Xin[3]; Daniel T Maloney[3]; Baozhen Shan[3]; Michael S Westphall[1]; Joshua J Coon[1,2,4,5]; *[1]Genome Center of Wisconsin, Madison, WI; [2]Department of Chemistry, University of Wisconsin–Madison, Madison, WI; [3]Bioinformatics Solutions Inc., Waterloo, ON, Canada; [4]Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI; [5]Morgridge Institute for Research, Madison, WI*

ThP 421 **Evaluating the Possibility of Misinterpreting MS/MS Spectra Caused by Isobaric Substitutions: A Case Study on Human Missing Proteins**; Jen-Hung Wang[1]; Tung-Shing Mamie Lih[1]; Wai-Kok Choong[1]; Wen-Lian Hsu[1]; Ting-Yi Sung[1]; *[1]Institute of Information Science, Academia Sinica, Taipei, Taiwan*

ThP 422 **Improvement of NextSearch Using Indexed Exon Graph and Multi-Threading**; Seunghyuk Choi[1]; Eunok Paek[1]; *[1]Hanyang University, Seoul, South Korea*

ThP 423 **Evaluation of Label-Free Peptide Quantification Tools and Their Application to Multi-Omic Workflows Within the Galaxy-P Framework**; Subina Mehta[1]; Caleb W Easterly[1]; James E Johnson[1]; Bjoern Gruening[2]; Andrea Argentini[3]; Robert J. Millikin[4]; Michael R. Shortreed[4]; Thomas McGowan[1]; Praveen Kumar[1]; Lennart Martens[3]; Lloyd M Smith[4]; Timothy J. Griffin[1]; Pratik D Jagtap[1]; *[1]University of Minnesota, Minneapolis, MN; [2]University of Freiburg, Freiburg, Germany; [3]Ghent University, Ghent, Belgium; [4]University of Wisconsin–Madison, Madison, WI*

ThP 424 **Enhanced FlashLFQ for Ultrafast Label-Free Peptide Quantification with Match-between-Runs and Replicate**

Normalization; Robert J. Millikin[1]; Michael R. Shortreed[1]; Stefan K. Solntsev[1]; Lloyd M. Smith[1, 2]; *[1]University of Wisconsin–Madison, Madison, WI; [2]Genome Center of Wisconsin, Madison, WI*

ThP 425 **Using Sub-Ranked Database Matching Scores for Improving the Peptide and Protein Identification Performance**; Ying-Lan Chen[1]; Pao-Chi Laio[2]; Wei-Hung Chang[1]; Yet-Ran Chen[1]; *[1]Academia Sinica, Taipei, Taiwan; [2]National Cheng Kung University, Tainan, Taiwan*

ThP 426 **pNovo 3: Precise *de novo* Peptide Sequencing with Deep Learning and Learning-to-Rank**; Hao Yang[1]; Hao Chi[2]; Wen-Feng Zeng[2]; Wen-Jing Zhou[2]; Si-Min He[2]; *[1]Institute of Computing Technology, Chinese Academy of Sciences, Beijing, China; [2]Chinese Academy of Sciences, Beijing, China*

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ThP 427 **PANDA: A Comprehensive and Flexible Tool for Proteomics Data Quantitative Analysis**; Cheng Chang[1]; Kaikun Xu[1]; Fuchu He[1]; Yunping Zhu[1]; *[1]Beijing Proteome Research Center, Beijing, China*

ThP 428 **Method Development for the Extraction and Quantification of Brain Derived Neurotrophic Factor in Niemann-Pick Disease, Type C1**; Rathnayake A. Chathurika Rathnayake[1]; Stephanie M. Cologna[1]; *[1]University of Illinois, Chicago, IL*

ThP 429 **Characterization and Monitoring of Host Cell Proteins by ELISA and Orthogonal LC-MS/MS in Monoclonal Antibodies**; Jacquelynn Smith[1]; Olga V Friese[1]; Phoebe Baldus[1]; Thomas powers[1]; brown W. paul[1]; Ying Zhang[2]; Jason C Rouse[2]; *[1]Pfizer, Chesterfield, MO; [2]Pfizer, Andover, MA*

ThP 430 **MRMAssayDB: An Integrated Resource for Validated Targeted Proteomics Assays**; Pallab Bhowmick[1]; Yassene Mohammed[1, 2]; Christoph H. Borchers[1, 3, 4, 5]; *[1]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [2]Center for Proteomics and Metabolomics, Leiden University, Leiden, Netherlands; [3]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada; [4]Jewish General Hospital Proteomics Centre, McGill University, Montreal, QC, Canada; [5]Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC, Canada*

ThP 431 **Proteogenomics-Improved and -Guided Quantification Pipeline (PIGQpipe): Targeted Proteomics with Internal Proteotypic/Variant-typic Peptide Standards to Quantify Variants Identified by Proteogenomic Experiments**; Yassene Mohammed[1, 2]; Christoph H. Borchers[1, 3, 4, 5]; *[1]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [2]Center for Proteomics and Metabolomics, Leiden University, Leiden, Netherlands; [3]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada; [4]Jewish General Hospital Proteomics Centre, McGill University, Montreal, QC, Canada; [5]Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC, Canada*

ThP 432 **A Proteome Informatic Approach to Investigate the Role of Retroelement Proteins in Disease**; Nazrath Nawaz[1]; Dr. Paul J. Hurd[1]; Dr. Miguel R. Branco[1]; Prof. Conrad Bessant[1]; *[1]Queen Mary - University of London, London, UK*

ThP 433 **Integrating Protein Prospector Into the Trans-Proteomic Pipeline**; Peter R Baker[1]; Robert J Chalkley[2]; Giselle Knudsen[2]; Luis Mendoza[3]; Robert L Moritz[4]; *[1]UCSF, Rokietnica, Poland; [2]University of California San Francisco, San Francisco, CA; [3]Institute For Systems Biology, Seattle, WA; [4]Institute for Systems Biology, Seattle, WA*

ThP 434 **SWATH-Guidance: An Automated and Optimized Strategy for Accurate and Reproducible Protein Quantity Inference by SWATH/DIA-Mass Spectrometry**; Wenguang Shao[1]; Ludovic Gillet[1]; Shawn Tan[2]; Yansheng Liu[3]; Amon Sabine[1]; Ben Collins[1]; Ashok Venkitaraman[2]; Ruedi Aebersold[1, 4]; *[1]ETH Zürich, Zurich, Switzerland; [2]University of Cambridge, Cambridge, UK; [3]Yale Cancer Biology Institute, Yale School of Medicine, West Haven, CT; [4]University of Zurich, Zurich, Switzerland*

ThP 435 **Mixed Effects Linear Models for Correcting Biases in Isobaric Labeling Quantification**; Marina Gay[1]; Marta Vilaseca[1]; Camille Stephan Otto Attolini[1]; *[1]Institute for Research in Biomedicine (IRB Barcelona), The Barcelona Institute of Science and Technology, Barcelona, Spain*

ThP 436 **Streamlined Identification and Quantification of Host Cell Proteins (HCPs) in Human Plasma Derived Biotherapeutics**; Ilker Sen[1]; Rose D Lawler[1]; Laura Smoyer[2]; St John Skilton[1]; Marshall Bern[1]; Eric Carlson[1]; Kevin Van Cott[2]; *[1]Protein Metrics Inc., San Carlos, CA; [2]University of Nebraska - Lincoln, Lincoln, NE*

ThP 437 **A Distributed Spectral Index Method for Improved Relative Protein Quantification from Shotgun Mass Spectra**; Michael R. Hoopmann[1]; Jason M. Winget[2]; Luis Mendoza[1]; Robert L. Moritz[1]; *[1]Institute for Systems Biology, Seattle, WA; [2]Procter and Gamble, Mason, Ohio*

ThP 438 **Optimizing Data Processing Parameters for Samples Acquired on Different Instruments Using Advanced Peak Determination**; Bernard Delanghe[1]; Tabiwang N. Array[2]; Aaron Gajadhar[3]; David Horn[3]; Eugen N. Damoc[2]; Andreas Huhmer[3]; *[1]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [3]ThermoFisher, San Jose, CA*

ThP 439 **High Speed Analysis of Metaproteomic Data from Microbiomes**; Titus H Jung[1]; Robin S Park[2]; Ana Wang[2]; Peter Thuy-Boun[2]; Dennis Wolan[2]; John Yates[2]; *[1]The Scripps Research Institute, La Jolla, CA; [2]The Scripps Research Institute, La Jolla, California*

ThP 440 **Fast search engine using GPU**; Robin Park[1, 2]; Titus Jung[1, 2]; John Yates[1]; *[1]The Scripps Research Institute, La Jolla, CA; [2]Integrated Proteomics Applications, San Diego, CA*

ThP 441 **Bayesian Confidence Intervals for Multiplexed Proteomics Integrate Ion Statistics with Peptide Quantification Concordance**; Leonid Peshkin[1]; Lillia Ryazanova[2]; Martin Wühr[2]; *[1]Harvard Medical School, Boston, MA; [2]Princeton University, Princeton, NJ*

ThP 442 **MSFragger-Based Computational Framework for Conventional MS/MS Database Searching And Open Search-Based PTM Characterization**; Dmitry M. Avtonomov[1]; Andy Kong[1]; Felipe da Veiga Leprevost[1]; Hui-Yin Chang[1]; Alexey Nesvizhskii[1]; *[1]University of Michigan, Ann Arbor, MI*

ThP 443 **A Novel Computational Strategy for Top Down Proteomics, Based on All Ion Fragmentation and Capillary Electrophoresis**; Andrew Collins[1]; Andrew Dowsey[2]; Matthias Vonderach[1]; Claire E. Eyers[1]; Andrew R. Jones[1]; *[1]University of Liverpool, Liverpool, UK; [2]University of Bristol, Bristol, UK*

ThP 444 **The Protein Composition of Extracellular Polymeric Substances of *E. coli* Biofilms Grown on Various Mannoside Surfaces**; Yanxin Chen[1]; Guoting Qin[1]; Zhiling Zhu[2]; Jong Min Choi[3]; Sung Yun Jung[3]; Chengzhi Cai[1]; *[1]University of Houston, Houston, TX; [2]Qingdao University of Science and Technology, Qingdao, China; [3]Baylor College of Medicine, Houston, TX*

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ThP 445 **Extending Dynamic Range and Enhancing Compound Identification for Untargeted Ion Mobility-MS Workflows**; Aivett Bilbao[1]; Bryson C. Gibbons[1]; Joon Y. Lee[1]; Ed Darland[2]; Xueyun Zheng[1]; Kristin E. Burnum-Johnson[1]; Matthew E. Monroe[1]; Thomas O. Metz[1]; Richard D. Smith[1];

ERIN S. BAKER[1]; John Fjeldsted[2]; Samuel H. Payne[1]; *[1]Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA; [2]Agilent Technologies, Santa Clara, CA*

ThP 446 **Chemical Identification by Combined Use of GC Retention Indices, EI-MS Fingerprints, and VUV Spectroscopic Signatures**; Ian G. M. Anthony[1]; Matthew R. Brantley[1]; Adam R. Floyd[1]; Christina A Gaw[1]; Touradj Solouki[1]; *[1]Baylor University, Waco, TX*

ThP 447 **MassIVE: Empowering The Mass Spectrometry Community for Streamlined Reanalysis of Public Datasets**; Jeremy Carver[1]; Mingxun Wang[1]; Nuno Bandeira[1]; *[1]UCSD, La Jolla, CA*

ThP 448 **A Graphical User Interface for RAId, a Knowledge Integrated Proteomics Analysis Suite with Accurate Statistics**; Brendan Joyce[1]; Danny Lee[1]; Alex Rubio[1]; Aleksey Y Ogurtsov[1]; Gelio Alves[1]; Yi-Kuo Yu[1]; *[1]National Center for Biotechnology Information, NLM, NIH, Bethesda, MD*

ThP 449 **MASH Explorer, a Comprehensive and User-friendly Software Environment for Top-Down Proteomics**; Sean J Mcilwain[1, 2]; Zhijie Wu[3]; Sudharshanan Govindaraj Ramanathan[4, 5]; Yiwen Gu[5]; Xiaowen Liu[6, 7, 8]; Ruixiang Sun[9]; Irene M Ong[1, 2, 10]; Ying Ge[3, 5, 11]; *[1]Department of Biostatistics and Medical Informatics, University of Wisconsin, Madison, WI 53719; [2]Carbone Cancer Center, School of Medicine and Public Health, University of Wisconsin, Madison, WI; [3]Department of Chemistry, University of Wisconsin–Madison, Madison, WI; [4]Department of Computer Science, University of Wisconsin, Madison, WI; [5]Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI; [6]Department of BioHealth Informatics, Indianapolis, IN, 46202; [7]Center for Computational Biology and Bioinformatics, Indiana University, Indianapolis, IN, 46202; [8]Department of BioHealth Informatics, Indiana University, Indianapolis, IN, 46202; [9]Institute of Computing Technology, Chinese Academy of Sciences, Beijing, China; [10]Department of Obstetrics and Gynecology, University of Wisconsin, Madison, WI; [11]Human Proteomics Program, School of Medicine and Public Health, University of Wisconsin-Madison, Madsion, WI*

ThP 450 **Keep Improving Chemical Identification Using Tandem Mass Spectrometry Data in a Pharmaceutical Context**; Youzhong Liu[1, 2]; Thomas De Vijlder[3]; Aida Mrzic[1, 2]; Romijn Edwin P[3]; Wout Bittremieux[1, 2]; Dirk Valkenborg[4, 5, 6]; Laukens Kris[1, 2]; *[1]Department of Mathematics and Computer Science, Advanced Database Research and Modelling (ADReM), University of Antwerp, Antwerp, Belgium, Antwerpen, Belgium; [2]Biomedical Informatics Network Antwerp (Biomina), University of Antwerp, Antwerp, Belgium; [3]Pharmaceutical Development & Manufacturing Sciences (PDMS), Janssen Research & Development, Beerse, Belgium; [4]Interuniversity Institute for Biostatistics and Statistical Bioinformatics, Hasselt University, Diepenbeek, Belgium; [5]Center for Proteomics (CFP), University of Antwerp, Antwerpen, Belgium; [6]Flemish Institute for Technological Research (VITO), Mol, Belgium*

ThP 451 **Proposed Utility of an Optimized HDF5 File Architecture for Efficient Size and Speed LCMS Data Acquisition, Archival and Access**; Jeffrey J. Jones[1]; Ryan Benz[1]; *[1]SoCal Bioinformatics Inc., Montrose, CA*

ThP 452 **Proteomic Data Commons (PDC): A Node in NCI's Cancer Research Data Commons**; Paul A Rudnick[1]; Ratna R Thangudu[2]; Michael Holck[2]; Deepak Singhal[2]; Karen A Ketchum[2]; Nathan J Edwards[3]; Christopher Kinsinger[4]; Izumi Hinkson[5]; Anand Basu[2]; Michael J MacCoss[6]; *[1]Spectragen Informatics LLC, Bainbridge Island, WA; [2]ESAC, Inc., Rockville, MD; [3]Georgetown University Medical Center, Washington, DC; [4]National Cancer Institute, Bethesda, MD; [5]National Cancer Institute, Center for Biomedical Informatics and Information Technology, Rockville, MD; [6]University of Washington Genome Sciences, Seattle, WA*

ThP 453 **Assessment of Spectral Accuracy and Chemical Space Coverage in Small Molecule Tandem MS Libraries**; Lee Ferguson[1]; Jim Shofstahl[2]; Julie A Horner[2]; *[1]Duke University, Durham, NC; [2]ThermoFisher Scientific, San Jose, CA*

ThP 454 **High Throughput Purity Assessment Using Mass Spectrometry in Regulated Laboratories**; Hua Dong[1]; Leo Wang[2]; *[1]Agilent Technologies, Santa Clara, CA; [2]Agilent Technologies, Inc., Santa Clara, CA*

ThP 455 **PollyTM: A Novel Cloud-Based Platform for Metabolism Labs**; Abhishek Jha[1, 2]; Swetabh Pathak[1]; Sabu George[1]; Raghav Sehgal[1]; Shefali Lathwal[1]; Darren Dumlao[3]; Mary Piotrowski[3]; John Janiszewski[3]; *[1]Elucidata, New Delhi, India; [2]Elucidata, Cambridge, Massachusetts; [3]Pfizer, Groton*

ThP 456 **Best Practices for Data Sharing of Ocean Metaproteomic Data Workshop Results**; Matt McIlvin[1]; Erin M. Bertrand[2]; Megan Duffy[3]; David Gaylord[4]; Noelle Held[4]; W. Judson Hervey[5]; Robert L. Hettich[6]; Pratik D Jagtap[7]; Michael G. Janech[8]; Danie Kinkade[4]; Dasha Leary[5]; Eli Moore[9]; Robert Morris[3]; Benjamin Neely[10]; Brook Nunn[3]; Jaclyn K. Saunders[4]; Adam Shepherd[4]; Nick Symmonds[4]; David Walsh[11]; Mak Saito[4]; *[1]Woods Hole Oceanographic Inst., Woods Hole Ma 02543, MA; [2]Dalhousie University, Halifax, NS, Canada; [3]University of Washington, Seattle, WA; [4]Woods Hole Oceanographic Institution, Woods Hole, MA; [5]Naval Research Laboratory, Washington, DC; [6]Oak Ridge National Laboratory and University of Tennessee, Oak Ridge, TN; [7]University of Minnesota, Minneapolis, MN; [8]Medical University of South Carolina, Charleston, SC; [9]Rutgers University, New Brunswick, NJ; [10]National Institute of Standards and Technology, Charleston, SC; [11]Concordia University, Montreal, Qc*

ThP 457 **Proteomics Evaluation Tool, a R/Shiny Tool for Proteomics Method Comparisons**; Alex Campos[1]; Alicia Richards[1]; Ramon Diaz Peña[1]; Renuka Sabnis[1]; KM Shams Ud Doha[1]; *[1]Sanford Burham Prebys Medical Discovery Institute, San Diego, CA*

ThP 458 **Customization of LabKey Platform for Integration, In-Depth Analysis and Sharing of Isobarically-Labelled and Label-Free Based Quantitative Proteomics Data**; Wen Yu[1]; Jonathan Pryke[2]; Gina DAngelo[1]; Raghothama Chaerkady[1]; Xiaotao Qu[1]; Adolf Brown[2]; Sonja Hess[1]; David Fenstermacher[1]; *[1]MedImmune, Gaithersburg, MD; [2]AstraZeneca, UK, Cambridge, UK*

ThP 459 **WinProphet: A User-Friendly Pipeline Management System to Automatically Perform Protein and Peptide Identifications Based on Trans-Proteomic Pipeline**; Ching-Tai Chen[1]; Chu-Ling Ko[2]; Wai-Kok Choong[1]; Jen-Hung Wang[1]; Wen-Lian Hsu[1]; Ting-Yi Sung[1]; *[1]Institute of Information Science, Academia Sinica, Taipei, Taiwan; [2]National Chiao Tung University, Hsinchu, Taiwan*

ThP 460 **Using Machine Learning to Maintain Instrument Reliability**; David Cox[1]; Doina Nyman[1]; *[1]Sciex, Concord, ON, Canada*

ThP 461 **Towards Real-time Proteomics Data Analysis by a New Scalable Distributed Platform**; Lei Xin[1]; Lin he[1]; Shengying Pan[1]; Tom Andersen[1]; *[1]Bioinformatics Solutions Inc., Waterloo, ON, Canada*

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ThP 462 **Experimental Observation of the Effects of Translational and Rotational Electrode Misalignment on a Planar Linear Ion Trap Mass Spectrometer**; Yuan Tian[1]; Joshua S McClellan[1]; Trevor K Decker[1]; Qinghao Wu[1]; Abraham L De la Cruz Hernandez[1]; Aaron R Hawkins[1]; Daniel E Austin[1]; *[1]Brigham Young University, Provo, UT*

ThP 463 **Quantitation of Peptides by Miniature Mass Spectrometer**; Spencer Chiang[1, 2]; Wenpeng Zhang[1,

[2]; Kimberly Lee[3]; Zheng Ouyang[1, 2]; *[1]Weldon School of Biomedical Engineering, Purdue University, West Lafayette, IN; [2]State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instruments, Tsinghua University, Beijing, China; [3]Cell Signaling Technology, Danvers, MA*

ThP 464 **Comprehensive Scan Functions by Miniature Mass Spectrometer**; Xinwei Liu[1]; Jiexun Bu[2]; Xiaoyu Zhou[1]; Zheng Ouyang[1, 3]; *[1]State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instrument, Tsinghua University, Beijing, China; [2]PURSPEC Technologies Inc., Beijing, China; [3]Weldon School of Biomedical Engineering, Purdue University, West Lafayette, IN*

ThP 465 **Rapid Identification of Regulated Organic Chemical Compounds in Toys Using Ambient Ionization and a Miniature Mass Spectrometry System**; Xiangyu Guo[1]; Yueguang Lv[1, 2]; Zheng Ouyang[3, 4]; Qiang Ma[1]; *[1]Chinese Academy of Inspection and Quarantine, Beijing, China; [2]University of Chinese Academy of Sciences, Beijing, China; [3]Tsinghua University, Beijing, China; [4]Purdue University, West Lafayette, IN*

ThP 466 **Coupling Laser Desorption/Ionization with Miniature Mass Spectrometer for Direct and Rapid Analysis**; Wenbo Cao[1]; Jing Yang[1]; Xiaoxiao Ma[1]; Xiaoyu Zhou[1]; Zheng Ouyang[1, 2]; *[1]State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instrument, Tsinghua University, Beijing, China; [2]Weldon School of Biomedical Engineering and Department of Chemistry, Purdue University, West Lafayette, IN 47906*

ThP 467 **Comparison of Benchtop Quadrupole MS with Handheld Spectroscopic and Low-Cost Techniques for Detection of Falsified and Substandard Medicines**; Stephen Zambrzycki[1]; Celine Caillet[2, 3]; Serena Vickers[2, 3]; David V. Donndelinger[1]; Laura C. Winalski[1]; Marcos Bouza[1]; Nantasit Luangasanatip[4]; Yoel Lubell[4]; William R. Griggers[1]; Matthew C. Bernier[1]; Paul N. Newton[2, 3]; Facundo M. Fernandez[1]; *[1]School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA; [2]Lao-Oxford-Mahosot-Wellcome Trust Research Unit, Vientiane, Laos; [3]Infectious Diseases Data Observatory & Worldwide Antimalarial Resistance Network, Centre for Tropical Medicine & Global Health, University of Oxford, Oxford, UK; [4]The Mahidol Oxford Tropical Medicine Research Unit Faculty of Tropical Medicine, Mahidol University, Bangkok, Thailand*

ThP 468 **Development of a Low-Power Miniature GC-MS Instrument for Fieldable Applications**; Vladimir M. Doroshenko[1]; Victor Laiko[1]; Eugene Moskovets[1]; Konstantin Novoselov[1]; Tzu-Hsuan Chang[2]; Daniel Struk[2]; Jean-Marie D. Dimandja[2]; Milad Navaei[2]; Peter J. Hesketh[2]; *[1]MassTech, Inc., Columbia, MD; [2]Georgia Institute of Technology, Atlanta, GA*

ThP 469 **Monitoring of Nuclear Waste Hydrocarbons in Water Using Membrane Inlet Mass Spectrometry**; Boris Brkic[1]; Stamatios Giannoukos[2]; Stephen Taylor[2]; *[1]BioSense Institute, Dr Zorana Djindjica 1, Novi Sad, Serbia; [2]Department of Electrical Engineering and Electronics University of Liverpool, Liverpool, UK*

ThP 470 **3 Dimensional Monitoring of H2 Clouds as a Model of FCV Exhaust Gas**; Takashi Nohmi[1]; Toshio Mogi[2]; *[1]HysafeNohmi, Setagaya-Ku, Japan; [2]The University of Tokyo, Bunkyo, Japan*

ThP 471 **The Advanced Resolution Organic Molecular Analyzer (AROMA) – A Combined LIT-Orbirap for Planetary Exploration**; Adrian Southard[1]; Ricardo D Arevalo[2]; Emanuel Hernandez[3]; Ryan M. Danell[4]; Lars Hovmand[5]; Andrej Grubisic[2]; Steven Rogacki[6]; Christelle Briois[7]; Laurent Thirkell[7]; Fabrice Colin[7]; Cynthia Gundersen[8]; *[1]Universities Space Research Association, Greenbelt, MD; [2]University of Maryland, College Park, MD; [3]NASA Goddard Space Flight Center, Greenbelt, MD; [4]Danell Consulting, Inc., Winterville, NC; [5]Linear Labs, LLC, Washington, DC; [6]University of Michigan, Ann Arbor, MI; [7]LPC2E, UMR CNRS7328,Universitéd'Orléans, Orleans, France; [8]AMU engineering, Miami, Florida [FL]*

ThP 472 **Ozone-Induced Dissociation Implemented with a Dual-Trap Mass Spectrometer for Lipid Analysis**; Xinwei Liu[1]; Wenbo Cao[1]; Xiaoxiao Ma[1]; Xue Zhao[2]; Stephen J Blanksby[3]; Yu Xia[2]; Zheng Ouyang[1, 4]; *[1]State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instrument, Tsinghua University, Beijing, China; [2]Department of Chemistry, Tsinghua University, Beijing, China; [3]Central Analytical Research Facility, Queensland University of Technology, Brisbane, Australia; [4]Weldon School of Biomedical Engineering, Purdue University, West Lafayette, IN*

ThP 473 **An Automated, Sea-going Purge & Trap APCI-MS/MS for the Detection of Trace Dimethyl Sulfide in Ocean Waters**; Ross D McCulloch[1]; Alysia E Herr[1]; John H Dacey[2]; Phillipe D Tortell[1]; *[1]University of British Columbia, Vancouver, BC, Canada; [2]Woods Hole Oceanographic Institution, Woods Hole, MA*

ThP 474 **Instrumental Optimization and Applications of the Single-Particle Aerosol Mass Spectrometer LAMPAS 3**; Klaus-Peter Hinz[1]; Christof Barth[1]; Bernhard Spengler[1]; *[1]University of Giessen, Giessen, Germany*

ThP 475 **Simulation for High Resolution Condition in A Short High Quadrupole Mass Filter by Forming Band Stability Zones with Quadrupole Excitation**; Gong-Yu Jiang[1]; Hui Mu[1]; Chuanfan Ding[2]; Wenjian Sun[1]; *[1]Shimadzu Research Laboratory(Shanghai) Co.,Ltd., Shanghai, China; [2]Fudan Universiry, Shanghai, China*

ThP 476 **Radiofrequency Field Enhanced Chemical Ionization with Vacuum Ultraviolet Lamp for Miniature Time-of-Flight Mass Spectrometer**; Jichun Jiang[1]; Lijuan Zhou[1]; Ping cheng[1]; Jinxu Li[1]; Chengxin Wu[1]; Keyong Hou[1]; Haiyang Li[1]; *[1]Key Laboratory of Separation Science for Analytical Chemistry, Dalian Institute of Chemical Physics, Chinese Academy of Sciences., Dalian, China*

ThP 477 **Rapid Identification of Drug Seizures using a Prototype ASAP Source on a Low-Cost, Deployable, Single Quadrupole Mass Spectrometer**; Bryan McCullough[1]; Chris Hopley[1]; David Douce[2]; Nicola Lumley[2]; Kate Whyatt[2]; *[1]National Measurement Laboratory, LGC, Teddington, UK; [2]Waters Corporation, Wilmslow, UK*

ThP 478 **Improved ion transmission of a microchip CE benchtop HPMS platform for the analysis of amino acids and cell growth media**; Kenion H. Blakeman[1]; Drew Blouch[1]; Colin M. Gavin[2]; JOSHUA P. Guerrette[1]; J. Scott Mellors[1]; Christopher D. Brown[2]; Glenn A. Harris[1]; *[1]908 Devices Inc., Boston, MA; [2]908 Devices, Los Gatos, CA*

ThP 479 **A Simple 180-Degree Permanent Magnet Mass Analyzer with Arrayed Detection**; Noah Christian[1]; James S Ha[1]; Deborah Hunka[1]; Timothy K McPhail[1]; Sebastien Pradel[1]; Charlotte Wahl[1]; Gottfried Kibelka[2]; Luis Fernando Velasquez-Garcia[3]; Carol Livermore[4]; *[1]Leidos Inc., Reston, VA; [2]Xylem, Inc, Pelham, AL; [3]Massachusetts Institute of Technology, Cambridge, MA; [4]Northeastern University, Boston, MA*

ThP 480 **Development of a Portable MALDI-TOF-MS for Microbial Identification**; Ko-Keng Chang[1, 2]; Yi-Hong Cai[1]; Cheng-Chih Hsu[2]; Yi-Sheng Wang[1]; *[1]Genomics Research Center, Academia Sinica, Taiwan; [2]Chemistry Department, National Taiwan University, Taiwan*

ThP 481 **The Fine-Structure Ion Carpets for the Transport of Ions at Atmospheric Pressures**; Sergey Poteshin[1]; Anna Burykina[2]; *[1]National Research Nuclear University MEPHI, Moscow, Russian Federation; [2]National Research Nuclear University MEPHI, Moscow, Russia*

ThP 482 **Rapid, In Situ Detection of Synthetic Opioids**; Travis M. Falconer[1]; Sara E. Kern[1]; Sarah E. Voelker[1]; *[1]U.S. FDA Forensic Chemistry Center, Cincinnati, OH*

ThP 483 **Analysis of Fentanyl and Its Analogs with a Handheld API Mass Spectrometer and In-Source-CID**; Christopher D. Brown[1]; Gwen Bone[1]; Colin M. Gavin[1]; Michael P Goodwin[1]; *[1]908 Devices, Los Gatos, CA*

ThP 484 **Linear Ion Trap Mass Spectrometer for Exploration of Europa as part of the Europan Molecular Indicators of Life Investigation (EMILI)**; Andrej Grubisic[1]; Marco Castillo[2]; William B Brinckerhoff[3]; Stephanie Getty[3]; Ryan M. Danell[4]; Ricardo D Arevalo[2]; Xiang Li[5]; Friso H.w. Van Amerom[6]; Desmond A. Kaplan[7]; Jennifer L Eigenbrode[3]; Philip Chu[8]; Kris Zacny[8]; Justin Spring[8]; Megan Casey[3]; Erin Lalime[9]; Tori Hoehler[10]; *[1]NASA, Greenbelt, MD; [2]University of Maryland, College Park, MD; [3]NASA Goddard Space Flight Center, Greenbelt, MD; [4]Danell Consulting, Inc., Winterville, NC; [5]University of Maryland Baltimore County, Baltimore, MD; [6]Mini-Mass Consulting, Inc, Hyattsville, MD; [7]KapScience LLC, TEWKSBURY, MA; [8]Honeybee Robotics, Pasadena, CA; [9]Stinger Ghaffarian Technologies Inc., Greenbelt, MD; [10]NASA Ames Research Center, Moffett Field, CA*

ThP 485 **The Molecular Analyzer for Complex Refractory Organic-Rich Surfaces (MACROS)**; Xiang Li[1, 2]; Stephanie Getty[2]; Andrej Grubisic[2, 3]; Jamie Elsila[2]; Jerome Ferrance[4]; Timothy Cornish[5]; Manuel Balvin[2]; Adrian Southard[2, 6]; Jennifer Stern[2]; William B Brinckerhoff[2]; *[1]University of Maryland, Baltimore County, Greenbelt, MD; [2]NASA Goddard Space Flight Center, Greenbelt, MD; [3]University of Maryland, College Park, MD; [4]J2F Engineering, Charlottesville, VA; [5]Zeteo Tech Inc, Sykesville, MD; [6]Universities Space Research Association, Greenbelt, MD*

ThP 486 **Final Testing and Performance of the Flight Model Mars Organic Molecule Analyzer (MOMA) Mass Spectrometer**; Ryan M. Danell[1]; Andrej Grubisic[2]; Desmond A. Kaplan[3]; Veronica T. Pinnick[4]; Friso van Amerom[5]; Xiang Li[6]; Marco Castillo[2]; Stephanie Getty[4]; William B Brinckerhoff[4]; *[1]Danell Consulting, Inc., Winterville, NC; [2]University of Maryland, College Park, MD; [3]KapScience LLC, TEWKSBURY, MA; [4]NASA Goddard Space Flight Center, Greenbelt, MD; [5]Mini-Mass Consulting, Inc, Hyattsville, MD; [6]University of Maryland Baltimore County, Baltimore, MD*

ThP 487 **Laser Desorption Ionization for a Linear Ion Trap Mass Spectrometer (LITMS) for planetary measurements**; Friso H.w. Van Amerom[1]; Marco Castillo[2]; Ryan M. Danell[3]; Desmond A. Kaplan[4]; Stephanie Getty[5]; Andrej Grubisic[6]; Xiang Li[7]; Veronica T. Pinnick[5]; William B Brinckerhoff[5]; Paul R. Mahaffy[5]; *[1]Mini-Mass Consulting, Inc, Hyattsville, MD; [2]University of Maryland, Baltimore, Baltimore; [3]Danell Consulting, Inc., Winterville, NC; [4]KapScience LLC, TEWKSBURY, MA; [5]NASA Goddard Space Flight Center, Greenbelt, MD; [6]University of Maryland, College Park, MD; [7]University of Maryland Baltimore County, Baltimore, MD*

ThP 488 **Development and Performance Verification of a Robust MSMS Routine for the Mars Organic Molecule Analyzer (MOMA) Mass Spectrome**; Desmond A. Kaplan[1, 2]; Samuel Larson[2]; Ryan M. Danell[2, 3]; Friso van Amerom[2, 4]; Andrej Grubisic[2, 5]; Marco Castillo[2, 5]; Xiang Li[2, 5]; Stephanie Getty[2]; Veronica T. Pinnick[2]; William B Brinckerhoff[2]; Paul R. Mahaffy[2]; *[1]KapScience LLC, Tewksbury, MA; [2]NASA Goddard Space Flight Center, Greenbelt, MD; [3]Danell Consulting, Inc., Winterville, NC; [4]Mini-Mass Consulting, Inc, Hyattsville, MD; [5]University of Maryland, College Park, MD*

INSTRUMENTATION: NEW DEVELOPMENTS IN IONIZATION AND SAMPLING II
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ThP 489 **Condensed Phase Membrane Introduction Mass Spectrometry Utilizing Direct Liquid Electron Ionization (CP-MIMS-LEI)**; Gregory W. Vandergrift[1, 2]; Erik T. Krogh[1, 2]; Christopher G. Gill[1, 2, 3, 4]; *[1]Appl. Env. Res. Labs. (AERL), Nanaimo, BC, Canada; [2]Chemistry, University of Victoria, Victoria, BC, Canada; [3]Chemistry, Simon Fraser University, Burnaby, BC, Canada; [4]University of Washington, Seattle, WA*

ThP 490 **Mechanospray Ionization of Biomolecules and Synthetic Polymers**; Liam Dugan[1, 2]; Danica Duenas[2]; Mark E. Bier[2]; *[1]Allegheny College, Meadville, PA; [2]Carnegie Mellon University, Pittsburgh, PA*

ThP 491 **Adapting Photonics Fabrication Processes to the Development of Improved ESI-MS Emitter Tip Design**; Kyle J Bachus[1]; David Simon[2]; Richard D Oleschuk[2]; Mike Bailey[3]; Andrew Gooley[3]; Heike Ebendorff-Heidepriem[1]; *[1]University of Adelaide, Adelaide, Australia; [2]Queen's University, Kingston, ON, Canada; [3]Trajan Scientific and Medical, 7 Argent Place, Ringwood, Australia*

ThP 492 **Direct Mass Spectrometry Analysis of Perfluorinated Compounds Using In-Capillary Ionic Liquids-Based Dispersive Liquid-Liquid Microextraction and Sonic-Spray Ionization**; Yueguang Lv[1, 2]; Qiang Ma[1]; *[1]Chinese Academy of Inspection and Quarantine, Beijing, China; [2]University of Chinese Academy of Sciences, Beijing, China*

ThP 493 **Sensitivity Improvement for Bottom-up Proteomics using Silicon Microfluidic Chip-Based Multinozzle Emitter Arrays at Capillary Flow Rates**; Joshua A Silveira[1]; Pan Mao[2]; Eloy R Wouters[1]; Romain Huguet[1]; Jean-Jacques Dunyach[1]; Daojing Wang[2]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Newomics Inc., Emeryville, California*

ThP 494 **Development of a New Type of Electron Source for Electron Ionization**; Hirofumi Nagao[1]; Shinichi Miki[1]; Koichi Mori[2]; *[1]MSI Tokyo, Chofu, Japan; [2]Takeishi Electric Co., Ltd, Hadano, Japan*

ThP 495 **Development of mass spectrometry cartridge for sensitive detection of target protein using on-cartridge digestion**; Chengsen Zhang[1]; Nicholas E. Manicke*[1]; *[1]IUPUI, Indianapolis, IN*

ThP 496 **Piezoelectric-Driven Matrix Assisted Ionization**; Achala P Deenamulla Kankanamalage[1]; Bijay Banstola[1]; Carson W. Szot[1]; Fabrizio Donnarumma[1]; Kermit K Murray[1]; *[1]Louisiana State University, Baton Rouge, LA*

ThP 497 **Direct Ambient Analysis of Ultra-Small Complex Mixtures Using Transmission-Mode Liquid Desorption Electrospray Ionization (DESI)**; Taghi Sahraeian[1]; Dmytro S. Kulyk[1]; Abraham Kwame Badu-Tawiah[1]; *[1]The Ohio State University, Columbus, OH*

ThP 498 **Inline Capsular Extraction of Biological Tissue Samples for ESI for Lipidomic Analysis**; Vasily Eliferov[1]; Evgeny Zhvansky[1, 2]; Dina Berlina[1]; Nikita Levin[2]; Vsevolod Shurkhay[1, 3]; Igor Popov[1, 2]; Eugene (Evgeny) Nikolaev[4]; *[1]Moscow Institute of Physics and Technology, Moscow, Russia; [2]Institute for Energy Problems of Chemical Physics of RAS, Moscow, Russia; [3]N. N. Burdenko Scientific Research Neurosurgery Institute, Moscow, Russia; [4]Skolkovo institute of science and technology, Moscow Region, Russian Federation*

ThP 499 **Progress in the Development of a Kinetically Controlled Chemical Ionization Setup**; Kai Kroll[1]; Duygu Erdogdu[1]; Tobias Kutsch[1]; Walter Wissdorf[1]; Hendrik Kersten[1]; Thorsten Benter[1]; *[1]Bergische Universität Wuppertal, Wuppertal, Germany*

ThP 500 **Coanda Effect Sonic-Spray Ionization Mass Spectrometry (orthogonal-SSI-MS) for coupling conventional and microbore High Performance Liquid Chromatography to Mass Spectrometry**; Sofia Grafanaki[1]; Leonidas Mavroudakis[1]; Manos Christofakis[1]; Spiros Pergantis[1]; *[1]University of Crete, Heraklion, Greece*

ThP 501 **On-Line Discrimination of Thiophenes and Sulfides Based On Atmospheric Plasma Ionization**; Yehua Han[1]; Yanfen Zhang[1]; Zhaoyang Fan[1]; Yinghao Wang[1]; *[1]China University of Petroleum, Beijing, Beijing, China*

ThP 502 **ESI – APCI Fast Mode Switching for Single Method Analysis of Diverse or Difficult to Ionize Pesticides**; Heather Gamble[1]; Avinash Dalmia[2]; Tyrally Ordinario[3]; Feng Qin[3]; *[1]Perkin Elmer Health Sciences, Woodbridge, ON, Canada; [2]PerkinElmer, Shelton, CT; [3]PerkinElmer, Woodbridge, ON, Canada*

ThP 503 **The Production and CID Fragmentation of B-Chain Conformers of Bovine Insulin Using ESI/Impactor Ionization and Mobility-MS/MS**; Steve Bajic[1]; Jeff Brown[1]; *[1]Waters Corporation, Wilmslow, UK*

ThP 504 **Enhanced Triple Quadrupole Optics Robustness for Challenging Applications**; Byungchul Cha[1]; Harald Oser[1]; Michael Ugarov[1]; Terry Olney[1]; Mary Blackburn[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

ThP 505 **Matrix-Assisted-Ionization Coupled to High-Resolution Fourier Transform Mass Spectrometry (MAI-FTMS) for Characterizing Lipids in Cooking Oil and Bacteria**; Rohanna Liyanage[1]; Jennifer Gidden[1]; Jackson O. Lay, Jr.[1]; Charles L Wilkins[2]; *[1]University of Arkansas-Chemistry, Fayetteville, AR; [2]University of Arkansas-Chemistry, Fayetteville, Arkansas*

ThP 506 **Online Investigation of Coffee Roast Gases Using Photoionization Mass Spectrometry (PIMS)**; Courtney A. Benson[1]; Sven Ehlert[2]; Hendryk Czech[3]; Ralf Zimmermann[3]; Jessalin Howell[1]; *[1]The J.M. Smucker Company, Orrville, OH; [2]Photonion GmbH, Schwerin, Germany; [3]Joint Mass Spectrometry Centre (University of Rostock and Helmholtz Zentrum Munich), Rostock, Germany*

ThP 507 **A Multi-Ionization Automated Platform for Sample Analysis with ESI, SAI, and MAI**; Milan Pophristic[1]; Santosh Karki[1]; Anil Kumar Meher[1]; Wenzhe Jiao[2]; Charles N McEwen[1,3]; *[1]MSTM, LLC, Newark, DE; [2]Wayne State University, Detroit , MI; [3]Univ. of the Sciences, Philadelphia, PA*

ThP 508 **The Spectroscopic Emission from dissolved Metal Ions During an Arc Event in Electrospray Ionization**; Michael Jones[1]; D. Alex Thiel[1]; Eric Davis[1]; *[1]Department of Biology and Chemistry, Azusa Pacific University, Azusa, CA*

ThP 509 **ECD and EID Fragmentation of Peptides and Intact Proteins Using a Quadrupole Time-of-Flight Mass Spectrometer on a Chromatographic Time Scale**; Valery G. Voinov[1,2]; Yury V. Vasil'ev[1,2]; Nathan I. Lopez[1,2]; Joseph S. Beckman[1]; Christian Klein[3]; Kenneth Newton[3]; Ruwan T. Kurulugama[4]; George Stafford[3]; John C. Fjeldsted[5]; *[1]Oregon State University, Corvallis, OR; [2]e-MSion, Inc., Corvallis, OR; [3]Agilent Technologies, Santa Clara, CA; [4]Agilent Technologies, Santa Clara, California; [5]Agilent Technologies, Inc., Santa Clara, CA*

ThP 510 **New Plate Coatings for LDTD-MS/MS Analysis**; Annick Dion-Fortier[1]; Fanny Chevillot[1]; Serge Auger[2]; Pierre Picard[2]; Pedro A. Segura[1]; *[1]Université de Sherbrooke, Sherbrooke, QC, Canada; [2]Phytronix Technologies Inc., Québec, QC, Canada*

INSTRUMENTATION: NEW DEVELOPMENTS IN MASS ANALYZERS
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ThP 511 **Leveraging Ultra-High Resolution and UVPD on an Orbitrap Platform for Structural Elucidation in Pharmaceutical Settings**; G. Charles Cheng[1]; Ning Yang[1]; Kate Comstock[2]; Tawnya Flick[3]; Seema Sharma[2]; Romain Huguet[2]; *[1]Amgen, Cambridge, MA; [2]Thermo Fisher Scientific, San Jose, CA; [3]Amgen, Inc., Thousand Oaks, CA*

ThP 512 **MultiCRAFTI: Overcoming Kinetic Energy Dependence and Limits of Fourier Transform Based Single Collision Cross Section Measurements**; Brigham Pope[1]; Jacob Hickey[1]; Daniel Joaquin[1]; David V Dearden[1]; *[1]Brigham Young University, Provo, UT*

ThP 513 **Charge Detection Mass Spectrometry of Microparticles Using Printed Circuit Board Electrode Arrays**; Elaura L. Gustafson[1]; Halle V. Murray[1]; Daniel E. Austin[1]; *[1]Brigham Young University, Provo, UT*

ThP 514 **Insight Into Semiconductor Processes by a Novel Fourier-Transform Ion Trap**; Valerie Derpmann[1]; Ruediger Reuter[1]; Lukas Nattermann[2]; Yessica Brachthaeuser[3]; Alexander Laue[1]; Hin Yiu Chung[1]; Michel Aliman[1]; *[1]Carl Zeiss SMT GmbH, Oberkochen, Germany; [2]University of Marburg, Marburg, Germany; [3]University of Wuppertal, Wuppertal, Germany*

ThP 515 **Improved Performance of Linear Ion Trap Mass Spectrometer with Added Octopole and Dodecapole Fields**; Junichi Taniguchi[1]; Osamu Furuhashi[1]; *[1]Shimadzu Corporation, Kyoto, Japan*

ThP 516 **Operation of a Commercial Linear Ion Trap with Digital Waveforms**; Ashley Marie Moon[1]; Margaret Elizabeth Reece[1]; Adam Paul Huntley[1]; Bojana Opacic[1]; Zachary Philip Gotlib[1]; Nathan Michael Hoffman[1]; Peter T. A. Reilly[1]; *[1]Washington State University, Pullman, WA*

ThP 517 **Production and Evaluation of Micron-Sized Fine Grating Having High Aspect Ratio Suitable for Time-of-Flight Mass Spectrometer**; Osamu Furuhashi[1]; Tomoya Kudo[1]; Junichi Taniguchi[1]; Hideaki Izumi[1]; Hiromu Yamasaki[1]; Daisuke Okumura[1]; *[1]Shimadzu Corporation, Kyoto, Japan*

ThP 518 **Protein Identification of Synthesized Bovine Serum Albumin-Gold Nanoclusters Using inTrap MALDI Mass Spectrometry Combined with Pulse Type Resonance Ejection**; Shih-Chieh Yang[1]; Szu-Wei Chou[1]; Pin-Duo Lee[1]; Yao-Hsin Tseng[1]; Chun-Yen Cheng[1]; *[1]AcroMass, hsinchu, Taiwan*

ThP 519 **Enhanced Resolution via Miniaturization of a Fourier Transform Electrostatic Linear Ion Trap Mass Spectrometer**; Joshua T. Johnson[1]; Kenneth W. Lee[1]; Jay S. Bhanot[1]; Scott A McLuckey[1]; *[1]Purdue University, West Lafayette, IN*

ThP 520 **Evaluation of Space Charge Effects in Scanning- vs Fourier Transform (FT)-Quadrupole Ion Traps (QITs)**; Walter Wissdorf[1]; Yessica Brachthaeuser[1]; Hendrik Kersten[1]; Thorsten Benter[1]; *[1]Bergische Universität Wuppertal, Wuppertal, Germany*

ThP 521 **Simulation of Collisional Interactions of Background Gas Mixtures with Trapped Ions**; Thorsten Benter[1]; Walter Wissdorf[1]; Marco Thinius[1]; Hendrik Kersten[1]; *[1]Bergische Universität Wuppertal, Wuppertal, Germany*

ThP 522 **Beat Frequency Resonance Ejection as a Tool for Discriminating Ion Ejection Methods**; Dalton T. Snyder[1]; Lucas J. Szalwinski[1]; Mitch Wells[2]; R. Graham Cooks[1]; *[1]Purdue University, West Lafayette, IN; [2]FLIR Systems, Inc., West Lafayette, IN*

ThP 523 **Fundamentals of Cyclotron-Frequency FT-ICR MS**; Konstantin O. Nagornov[1]; Anton N. Kozhinov[1]; Edith Nicol[2]; Yury O. Tsybin[1]; *[1]Spectroswiss, Lausanne, Switzerland; [2]Ecole Polytechnique, Palaiseau, France*

ThP 524 **Improving the Sensitivity for Linear Ion Trap Tandem Mass Spectrometry with Novel Automatic Gain Control (AGC)**; Linfan Li[1]; Jae C. Schwartz[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

ThP 525 **Software Simulation of a Quadrupole Mass Filter Employing a Novel Digital Waveform (EC waveform) and Discontinuous Ion Introduction**; Benjamin Jeffrey[1]; Robert Appleby[1]; David Langridge[2]; Martin Green[2]; Keith Richardson[2]; *[1]University of Manchester, Manchester, UK; [2]Waters Corporation, Wilmslow, UK*

ThP 526 **Nonlinear Ion Trap Stability Diagram Mapping by Trajectory Harmonic Content**; Robert H Jackson[1]; Stephen A Lammert[2]; *[1]Instrumental Design Physics, LLC, Littleton, MA; [2]PerkinElmer Inc., American Fork, UT*

ThP 527 **Enhancement of Ion Activation and CID by Simultaneous Dual Dipolar Excitation in Digital Linear Ion Trap**; Fuxing Xu[1]; Mingfei Zhou[1]; Chuanfan Ding[1]; *[1]Fudan University, Shanghai, China*

ThP 528 **Orbitrap Detection Limit Measurement**; Wenzhu Zhang[1]; Brian T. Chait[1]; *[1]The Rockefeller University, New York, NY*

ThP 529 **Digital Operation of a Linear Quadrupole Mass Filter**; Bojana Opacic[1]; Adam Paul Huntley[1]; Zachary Philip Gotlib[1]; Nathan Michael Hoffman[1]; Peter T. A. Reilly[1]; *[1]Washington State University, Pullman, WA*

ThP 530 **Electron Capture Dissociation Device in a Branched RF Ion Trap on a QqToF Platform with Enhanced Duty Cycle**; Pavel Ryumin[1]; Takashi Baba[1]; Igor Chernushevich[1]; Bill Loyd[1]; *[1]Sciex, Concord, ON, Canada*

ThP 531 **Selectivity Enhancement by sequential Mass Window Acquisition by Hybrid Quadrupole Time of Flight Mass Spectrometry**; Ana Lozano[1]; Amadeo R. Fernández-Alba[1]; *[1]University of Almería, European Union Reference Laboratory for Pesticide Residue Analysis in Fruits and Vegetables, Almería, Spain*

ThP 532 **Digital Ion Trap Mass Analysis Utilizing β=2/3 Resonance Ejection and Pulsed He Buffer Gas**; Timothy Vazquez[1]; Colette Taylor[1]; Theresa Evans-Nguyen[1]; *[1]University of South Florida, Tampa, FL*

LIPIDS: PROFILE ANALYSIS II
533-549

ThP 533 **Mapping Desaturase Enzyme Activity in complex Lipids by Ozone-Induced Dissociation**; Stephen J Blanksby[1]; David L. Marshall[1]; Berwyck Poad[1]; Angela Criscuolo[2, 3, 4]; Martin Zeller[2]; Jan-Peter Hauschild[2]; Eva Duchoslav[5]; J. Larry Campbell[5]; James Broadbent[6]; Mengxuan Fang[7]; Gavin E Reid[7]; Todd W Mitchell[8]; *[1]Queensland University of Technology, Brisbane, Australia; [2]Thermo Fisher Scientific, Bremen, Germany; [3]Center for Biotechnology and Biomedicine, Leipzig, Germany; [4]Institute for Bioanalytical Chemistry, University of Leipzig, Leipzig, Germany; [5]Sciex, Concord, ON, Canada; [6]Sciex, Brisbane, Brisbane, Australia; [7]University of Melbourne, Parkville, Australia; [8]School of Medicine, Illawarra Health and Medical Research Institute, University of Wollongong, Wollongong, Australia*

ThP 534 **Application of Segmented Scan Spectral Stitching to Lipid Profile Analysis in Stable Isotope Resolved Metabolomics (SIRM)**; Woo-Young Kang[1]; Patrick T. Thompson[1]; Teresa W.M. Fan[1]; Andrew N. Lane[1]; Richard M. Higashi[1]; *[1]Center for Environmental and Systems Biochemistry (CESB), Markey Cancer Center, and Department of Toxicology and Cancer Biology, University of Kentucky, Lexington, KY*

ThP 535 **Lipidomic Signatures of Nonhuman Primates with Radiation-Induced Hematopoietic Syndrome**; Evan Pannkuk[1]; Evagelia C Laiakis[1]; Vijay K Singh[2, 3]; Albert J Fornace[1]; *[1]Georgetown University, Washington Dc, DC; [2]Armed Forces Radiobiology Research Institute, Bethesda, MD; [3]Uniformed Services University of the Health Sciences, Bethesda, MD*

ThP 536 **Chemical Imaging of Aggressive Basal Cell Carcinoma Using Time-of-Flight Secondary Ion Mass Spectrometry**; Marwa Munem; *Gothenburg university, gothenburg, Sweden*

ThP 537 **Analysis of Lipopolysaccharide (LPS) From Cell and Protein Samples**; Qingling Li[1]; Thomas Clairfeuille[1]; Kerry Buchholz[1]; Aedan Liu[1]; Peter Smith[1]; Steven Rutherford[1]; Jian Payandeh[1]; Wendy Sandoval[1]; *[1]Genentech, SSF*

ThP 538 **Effect of Green Tea on Hepatic Lipid Metabolism in Mice Fed a High-Fat Diet**; Miso Nam[1]; Geum-Sook Hwang[1]; *[1]Korea Basic Science Institute, Seoul, South Korea*

ThP 539 **Dual nESI–DIMS-MS/MS for Measurement of Differential Lipid Expression**; James E. Keating[1]; Gary L. Glish[1]; *[1]University of North Carolina at Chapel Hill, Chapel Hill, NC*

ThP 540 **Development of an MRM based Profiling method of major lipids in blood**; Masaki Yamada[1]; Tsuyoshi Nakanishi[2]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]Shimadzu corp., Kyoto, Japan*

ThP 541 **Metabolic Effects of a Ketogenic Diet in Epilepsy: A UPLC-MS Investigation**; Elizabeth J Want[1]; Tsz Law[1]; Holger Volk[2]; Brian Zanghi[3]; Yuanlong Pang[3]; *[1]Imperial College, London, UK; [2]Royal Veterinary College, London, UK; [3]Nestle, St Louis, MS*

ThP 542 **A ToF-SIMS Study of Lipid Changes in E coli Mutants with Impaired Plasmid Transfer Capability**; Kelly Dimovska Nilsson[1]; Martin Palm[1, 2]; Anne Farewell[1, 2]; John S Fletcher[1]; *[1]Department of Chemistry and Molecular Biology, University of Gothenburg, Gothenburg, Sweden; [2]Centre for Antibiotic Resistance Research (CARe), University of Gothenburg, Gothenburg, Sweden*

ThP 543 **Brain Lipid Changes in High Fat Diet Mice**; Ludovic Muller[1]; Shelley N Jackson[1]; Amina S. Woods[1]; *[1]NIH/NIDA-IRP, Baltimore, MD*

ThP 544 **Increased Depth and Confidence of Lipidome Analysis from Insect Tissues using Chromatography Based Methods with High-resolution Orbitrap MSn**; Daniel Gachotte[1]; Yelena Adelfinskaya[1]; Jeffrey Gilbert[1]; Reiko Kiyonami[2]; David Peake[2]; Yasuto Yokoi[3]; *[1]Dow AgroSciences, Indianapolis, IN; [2]Thermo Fisher Scientific, San Jose, CA; [3]Mitsui Knowledge Industry, Tokyo, Japan*

ThP 545 **Lipidomics Reveals the Effects of Xanthohumol and its Derivatives on Dysfunctional Lipid Metabolism**; Jaewoo Choi[1]; Cristobal L. Miranda[1, 2]; Johana S. Revel[1, 3]; Jan Frederik Stevens[1, 2]; *[1]Linus Pauling Institute, Oregon State University, Corvallis, Oregon; [2]College of Pharmacy, Oregon State University, Corvallis, Oregon; [3]Department of Chemistry, Oregon State University, Corvallis, Oregon*

ThP 546 **Human Plasma Lipidomics / Oxylipidomics as a Tool for Biomonitoring of Environmental Burden on Mothers and Newborns**; Vit Kosek[1]; Radim Sram[2]; Jana Pulkrabova[1]; Jana Hajslova[1]; *[1]University of Chemistry and Technology, Prague, Czech Republic; [2]Institute of Experimental Medicine AS CR, Prague, Czech Republic*

ThP 547 **LC-MSE Lipidomics for Establishing Plasma Small Molecule Signatures of Aging in Mouse Models**; Ashish Vaswani[1]; Dr Armando Alcazar Magana[1]; Dr Sanjiv Kaul[2]; Dr Nabil J. Alkayed[2]; Claudia S Maier[1]; *[1]Department of Chemistry, Oregon State University, Corvallis, Oregon; [2]Oregon Health & Science University, Portland, OR*

ThP 548 **Annatto Seed (Bixa orellana L.) Lipid Profile by GC-MS and EASI-MS**; Damila Rodrigues Morais; *University of Campinas, Campinas, Brazil*

ThP 549 **Lipidomics Approach to Understand the Mechanism of Brain Metastatic Breast Cancer**; Masoud Zabet Moghaddam[1]; Wenjing Peng[2]; susan San Francisco[2]; Yehia Mechref[2]; *[1]Texas Tech University, Box 43132 Lubbock, TX; [2]Texas Tech University, Lubbock*

METABOLOMICS: IDENTIFICATION OF UNKNOWN METABOLITES
550-572

ThP 550 **Differentiation of Deprotonated Acyl, N- and O-Glucuronide Drug Metabolites by Using Tandem Mass Spectrometry Based on Ion-Molecule Reactions**; Edouard Niyonsaba[1]; McKay W. Easton[1]; Zaikuan Yu[1]; Zhoupeng Zhang[2]; Huaming Sheng[3]; John Kong[1]; Leah F. Easterling[1]; Ravikiran Yerabolu[1]; Tiffany M. Jarrell[4]; Hilkka I. Kenttämaa[1]; *[1]Department of Chemistry, Purdue University, West Lafayette, IN, 47906; [2]Department of Pharmacokinetics, Pharmacodynamics, and Drug Metabolism, Merck & Co., Inc., West Point, PA, 19486; [3]Analytical Research & Development, Merck & Co., Inc., Rahway, NJ 07065; [4]Merck Animal Health, Merck & Co., Inc., Rahway, NJ 07065*

ThP 551 **Profiling and Annotation of Flavonoids Using a Product Ion-Dependent MSn Data Acquisition Method on a Tribrid Orbitrap Mass Spectrometer**; Reiko Kiyonami[1]; Iwao Sakane[2]; Seema Sharma[3]; Graeme Mcalister[1];

Caroline Ding[1]; Andreas Huhmer[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]ITO EN, LTD, Tokyo, Japan; [3]Thermo Fisher Scientific, Sunnyvale*

ThP 552 **Protein Metabolite Structure Identification: Automated Analysis of Atrial Natriuretic Peptide (ANP) Metabolites Using UPLC/ESI-Exact Mass-MSMS Data**; Marshall M. Siegel[1]; Gary Walker[1]; Serhiy Hnatyshyn[2]; Asoka Ranasinghe[2]; *[1]MS Mass Spec Consultants, Fair Lawn, NJ; [2]Bristol-Myers Squibb Company, Princeton, NJ*

ThP 553 **Evaluation of an Artificial Neural Network In-silico Retention Index Model for Chemical Structure Identification in Metabolomics**; Milinda A.K Samaraweera[1]; Mark L Hall[2]; Dennis W Hill[1]; David F Grant[1]; *[1]University of Connecticut, Storrs, CT; [2]Hall Associates Consulting, Quincy, Massachusetts*

ThP 554 **Elemental Formulas Determined Directly from Biological Samples by Ultra-High Mass Resolution LAESI-21T-FTICR-MS**; Sylwia A Stopka[1]; Christopher R Anderton[2]; Laith Z Samarah[1]; Dusan Velickovic[2]; Jared B Shaw[2]; Beverly J Agtuca[3]; Caroline Kukolj[3]; David W Koppenaal[2]; Gary Stacey[3]; Ljiljana Pasa-Tolic[2]; Akos Vertes[1]; *[1]George Washington University, Washington, DC; [2]Pacific Northwest National Laboratory, Richland, WA; [3]University of Missouri, Columbia, MO*

ThP 555 **Novel Strategies for Metabolite Identification Using Isotopic Ratio Outlier Analysis (IROA) with Ion Mobility-Mass Spectrometry**; Robin H.J. Kemperman[1]; Chris W.W. Beecher[2]; Timothy J. Garrett[3, 4]; Richard A. Yost[1, 3, 4]; *[1]University of Florida Department of Chemistry, Gainesville, FL; [2]IROA Technologies, Bolton, MA; [3]University of Florida, Department of Pathology, Immunology and Laboratory Medicine, Gainesville, FL; [4]Southeast Center for Integrated Metabolomics (SECIM), University of Florida, Gainesville, FL*

ThP 556 **Kendrick Mass Defect for Molecular Formula Assignment of Nonribosomal Peptides (NRPs)**; Mickaël Chevalier[1]; Emma Ricart[2]; Emeline Hanozin[3]; Frédérique Lisacek[2]; Sandra Matthijs[4]; Maude Pupin[5, 6]; Philippe Jacques[7]; Nicolas Smargiasso[3]; Edwin De Pauw[3]; Valérie Leclère[8]; Christophe Flahaut[8]; *[1]Charles VIOLLETTE institute, Lille & Lens, France; [2]Proteome informatics Group, Geneva, Switzerland; [3]Mass Spectrometry Platform, Department of Chemistry, Liège, Belgium; [4]Institut de Recherches Microbiologiques-Wiame, Campus du CERIA, Brussels, Belgium; [5]Univ Lille, CNRS, Centrale Lille, UMR 9189 – CRIStAL- Centre de Recherche en Informatique Signal et Automatique de Lille, Lille, France; [6]Inria-Lille Nord Europe, Bonsai team, Lille, France; [7]TERRA Research Centre, Microbial Processes and Interactions (MiPI), Gembloux Agro-Bio Tech, University of Liege, Gembloux, Belgium; [8]Charles VIOLLETTE institute, Lille, France*

ThP 557 **Enhancing the Performance of QUAL/QUANT LC-MS Metabolomics Using a Chimeric Collision Cell Including Electron-Based and Collision-induced Dissociation**; Anita O Hidasi[1]; Takashi Baba[2]; Gérard Hopfgartner[1]; *[1]Life Sciences Mass Spectrometry, University of Geneva, Geneva, Switzerland; [2]Sciex, Concord, ON, Canada*

ThP 558 **Biomarkers for Fatal Yellowing using Untargeted Metabolomics and Chemometric Validation Analysis**; Jorge Candido Rodrigues Neto[1, 2]; Mauro Vicentini Correia[1]; José Antônio de Aquino Ribeiro[1]; Manoel Teixeira Souza Junior[1]; Clenilson Martins Rodrigues[1]; Patrícia Verardi Abdelnur[1, 2]; *[1]Embrapa Agroenergy, Brasilia, Brazil; [2]Federal University of Goias, Goiania, Brazil*

ThP 559 **Untargeted LC-MS reveals the complexity of bile acid conjugation in urines from patients with cholestasis**; Stephen Barnes[1]; Landon S. Wilson[1]; Ashwani K Singal[1]; *[1]University of Alabama at Birmingham, Birmingham, AL*

ThP 560 **Combining Chemical Biology Tools with Metabolomics and Proteomics to Reveal the Mode of Action for Peroxide Antimalarials**; Darren J Creek[1]; Carlo Giannangelo[1]; Ghizal Siddiqui[1]; Susan Charman[1]; *[1]Monash Institute of Pharmaceutical Sciences, Monash University, Melbourne, Australia, Melbourne, Australia*

ThP 561 **HPLC/MS Retention Indexing for Improved Annotation, Identification and Dereplication of Metabolite Discovery**; Steven M. Hurney[1]; A. Daniel Jones[1]; *[1]Michigan State University, East Lansing, MI*

ThP 562 **Segmented Flow Strategies for Interfacing NMR with LC-MS for Identifying Unknown Metabolites**; Jiajun Lei[1]; Ram Khattri[1]; Timothy J. Garrett[1]; Matthew E. Merritt[1]; Richard A. Yost[1]; *[1]University of Florida, Gainesville, FL*

ThP 563 **Novel strategies for the Identification of Small Molecule-Protein Binding Partners**; Rebecca E Rose[1]; Jennifer Marden[2]; David Sauer[2]; Da-Neng Wang[2]; Drew R Jones[1]; *[1]NYU Langone Health, New York, NY; [2]NYU School of Medicine, New York, NY*

ThP 564 **Improved Metabolome Coverage and Increased Confidence in Unknown Identification Through Novel Automated Acquisition Strategy Combining Sequential Injections and MSn**; Ioanna Ntai[1]; Iman Mohtashemi[1]; Jenny Berryhill[1]; Ralf Tautenhahn[1]; Graeme C McAlister[1]; Derek J Bailey[1]; Linda Lin[1]; Ryo Komatsuzaki[1]; Caroline Ding[1]; Seema Sharma[1]; Tim Stratton[1]; Vlad Zabrouskov[1]; Amanda L. Souza[1]; Andreas FR Huhmer[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

ThP 565 **LC-MS/MS Metabolite Identification and Characterization of a Novel (2-Phenylcyclopropyl) methylamine Serotonin 2C Agonist Using Human and Mouse Liver Microsomes**; Daniel G Nosal[1]; Luying Chen[1]; Guiping Zhang[2]; Sida Shen[2]; Alan P Kozikowski[2]; Richard B van Breemen[1]; *[1]Oregon State University - Linus Pauling Institute, Corvallis, OR; [2]University of Illinois at Chicago, Chicago, IL*

ThP 566 ***In vitro* Metabolite Identification Studies of New Synthetic Opioids Cyclopropylfentanyl, Cyclopentylfentanyl, and Cyclohexylfentanyl with Confirmation in Authentic Human Specimens**; Kyle S Dobson[1]; Sean Yu[2]; Heather McKiernan[1]; Alex Krotulski[1]; *[1]The Center for Forensic Science Research and Education, Willow Grove, PA; [2]RMI Laboratories, North Wales, 19545*

ThP 567 **Using IROA Labeling and Variable Window SWATH Acquisition to Determine the Relationships and Identity of Coeluting Compounds**; Alexander Raskind[1]; Vanessa Rubio[2]; Baljit K Uhbi[3]; Timothy Garrett[2]; Felice de Jong[4]; Chris Beecher[4]; *[1]University of Michigan, Ann Arbor, MI; [2]University of Florida, Gainesville, FL; [3]Sciex, Redwood City, California; [4]IROA Technologies LLC, Bolton, MA*

ThP 568 **Increasing Confidence for Compound Identification by Fragmentation Database and In-Silicofragmentation Comparison with LC-HRAM-MS-Based Non-Targeted Screening of Complex Matrices**; Christoph Buchholz[1]; Daniel Arndt[1]; Christian Wachsmuth[1]; Mark Bentley[1]; *[1]Philip Morris International R&D, Neuchatel, Switzerland*

ThP 569 **Curator: A Full Feature Data Curation Solution for Comprehensive and High Quality HRAM MS/MS and MSn Library Building**; Tim Stratton[1]; Juraj Lutisan[2]; Samuel Benkovic[2]; Caroline Ding[3]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]HighChem, Bratislava, Slovakia; [3]Thermo Scientific, San Jose, CA*

ThP 570 **Adduct Ions in Electrospray Ionization: What Are They and Why Should We Care?**; Ron Bonner[1]; Thomas Stricker[2]; Gerard Hopfgartner[3]; *[1]Ron Bonner Consulting, Newmarket, ON, Canada; [2]Life Sciences Mass Spectrometry, University of Geneva, Geneva, Switzerland; [3]University of Geneva, Geneva, Switzerland*

ThP 571 **Advanced Biomarker Discovery Through Investigation of Gut Microbiota and human Host Co-Metabolism - Combining Metabolomics with Chemical Biology Methodologies**; Mario S. P. Correia[1]; Neeraj Garg[1]; Caroline Ballet[1]; Louis P. Conway[1]; Daniel Globisch[1, 2];

[1]Uppsala University, Uppsala, Sweden; [2]Science for Life Laboratories, Uppsala, Sweden

ThP 572 **New Targeted Metabolomics Methods for Biomarker Discovery**; Caroline Ballet[1]; Mario S. P. Correia[1]; Louis P. Conway[1]; Neeraj Garg[1]; Daniel Globisch[1, 2]; [1]Uppsala University, Uppsala, Sweden; [2]Science for Life Laboratories, Uppsala, Sweden

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573-579

ThP 573 **A Method of MHC-Associated Peptide Proteomics (MAPPs) with High Detection Performance to Effectively Identify Significant Immunogenic Sequences of Therapeutic Antibodies**; Nobuo Sekiguchi[1]; Chiyomi Kubo[1]; Ayako Takahashi[1]; Kumiko Muraoka[1]; Shunsuke Ito[1]; Mariko Yano[1]; Futa Mimoto[1]; Atsuhiko Maeda[2]; Yuki Iwayanagi[3]; Tetsuya Wakabayashi[1]; Shotaro Takata[1]; Naoaki Murao[1]; Masaki Ishigai[1]; [1]Chugai Pharmaceutical Co., Ltd., Gotemba, Japan; [2]Chugai Pharmaceutical Co., Ltd., Tokyo, Japan; [3]Chugai Pharmaceutical Co., Ltd., Kamakura, Japan

ThP 574 **Structure Elucidation of Siderophores Produced by Pseudomonas taiwanensisVLB120 Bacteria by Means of LC-HR-MS/MS**; Karen Scholz[1]; Heiko Hayen[1]; [1]Institute of Inorganic and Analytical Chemistry, Muenster, Germany

ThP 575 **The Effect of Signal Enhancement of Polypeptide Ladders Using Guanidination**; Dabin Lee[1]; Yeoseon Kim[1]; Jeongkwon Kim[1]; [1]Chungnam National University, Daejeon, South Korea

ThP 576 **Sex Estimation in Skeletal Remains by LC-MS/MS Using Sexually Dimorphic Amelogenin Protein Fragments in Human Enamel**; Michelle R Salemi[1]; Julia M Yip[2]; Jane Buikstra[3]; Laura Regan[4]; Brett S Phinney[1]; Jelmer W Eerkens[5]; Glendon J Parker[5]; [1]UC Davis Genome Center, Davis, California; [2]UC Davis, Davis; [3]Arizona State University, Tempe, AZ; [4]United States Air Force Academy, Department of Biology, Colorado Springs, CO; [5]UC Davis, Davis, CA

ThP 577 **Towards a Complete Non-linear Peptide MS/MS Characterization**; Eva Duchoslav[1]; Xu Guo[1]; Tanmaykumar Desai[1]; [1]Sciex, Concord, ON, Canada

ThP 578 **Electron Induced Dissociation of Class I HLA Peptides Provides Increased Sequence Coverage Compared to Collision-Induced Dissociation**; Emmanuel Raptakis[1]; Dimitris Papanastasiou[1]; Susan Klaeger[2]; Karl Clauser[2]; Hasmik Keshishian[2]; Steven A Carr[2]; [1]Fasmatech, Athens, Greece; [2]Broad Institute of MIT and Harvard, Cambridge, MA

ThP 579 **UHPLC-MS and Tandem MS Characterization of Peptides Modified by Chemoselective Photoredox Catalysis**; Li-Kang Zhang[1]; Younong Yu[1]; Alexei V. Buevich[1]; Guoqing Li[1]; Haiqun Tang[1]; Petr Vachal[1]; Steven L. Colletti[1]; R. Thomas Williamson[2]; Zhi-Cai Shi[1]; [1]Merck Research Laboratories, Kenilworth, NJ; [2]Merck Research Laboratories, Rahway, NJ

PEPTIDES: TARGETED AND QUANTITATIVE ANALYSIS
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ThP 580 **Targeted Proteomics Approach for Sensitive LC/MS/MS Detection of Bovine and Porcine Gelatins in Food, Pharmaceutical Capsules and Personal Care Products**; Udi Jumhawan[1]; Jie Xing[1]; Zhaoqi Zhan[1]; [1]Shimadzu Asia Pacific, Singapore, Singapore

ThP 581 **Internal Calibration Curves for Accurate Quantitation in Clinical Proteomics**; Cristina Chiva[1]; Eduard Sabidó[1]; [1]CRG, Barcelona, Spain

ThP 582 **Integrating Protein Precipitation Into an Immunoaffinity Purification-LC/MS/MS Workflow for Highly Sensitive Peptide Analysis in Human Plasma**; Li Sun[1]; Yang Xu[1]; Sheila Breidinger[1]; Melanie Anderson[1]; Dina Goykhman[1]; Eric Woolf[1]; [1]Merck & Co., Inc., Rahway, NJ

ThP 583 **Bridging the Analytical Workflows for Characterizing and Monitoring Product Quality Attributes (PQAs) of Biotherapeutics by a Common Data Acquisition Mode**; Jing Fang[1]; Ying Qing Yu[1]; Weibin Chen[1]; [1]Waters Corporation, Milford, MA

ThP 584 **Development of an LC-MS/MS Method to Quantitate Oxytocin in Human and Nonhuman Primate Plasma**; Amy V. Kaucher[1]; Tatiana A. Shnitko[1]; Steven W. Blue[1]; Mary R. Lee[2, 3]; Kathleen A. Grant[1]; David W. Erikson[1]; [1]Oregon National Primate Research Center, Beaverton, OR; [2]National Institutes of Health, Bethesda, MD; [3]National Institute on Alcohol Abuse and Alcoholism, Bethesda, MD

ThP 585 **A Standard Multiplexed Targeted Proteomic Assay Utilizing Isobaric Labels for Evaluation of TOMAHAQ**; Christopher Rose[1]; ROSA VINER[2]; Jae Choi[3]; John C. Rogers[3]; Devin K. Schweppe[4]; Brian K. Erickson[4]; Steven P. Gygi[4]; Donald S Kirkpatrick[1]; [1]Genentech Inc., South San Francisco, CA; [2]Thermo Fisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific, Rockford, IL; [4]Harvard Medical School, Boston, MA

ThP 586 **Does Methionine Oxidation Influence the Progression of Classical or Atypical Scrapie?**; Melissa Erickson-Beltran[1]; Christopher J Silva[2]; Inmaculada Martín-Burriel[3, 4]; Juan José Badiola[3]; Rosa Bolea[3]; Requena R Jesus[5]; [1]USDA-ARS, Albany, CA; [2]USDA/ ARS, Albany, CA; [3]Veterinary Faculty, Centro de Investigación en Encefalopatías y Enfermedades Transmisibles Emergentes (CIEETE), Universidad, Zaragoza, Spain; [4]LAGENBIO, Laboratorio de Genética Bioquímica, Facultad de Veterinaria, IA2 Universidad de Zaragoza, Zaragoza, Spain; [5]CIMUS Biomedical Research Institute & Department of Medical Sciences, University of Santiago de Compostela-IDIS, Santiago de Compostela, Spain

ThP 587 **Quality of Isotopically Labelled Internal Standards for Peptide Quantification**; Nathan Debunne[1]; Frederick Verbeke[1]; Yorick Janssens[1]; Liesa Tack[1]; Evelien Wynendaele[1]; Bart De Spiegeleer[1]; [1]DruQuaR, Gent, Belgium

ThP 588 **LC-MS/MS for *in vitro* Evaluation of Permeation Enhancers on Oral Delivery Peptides**; Xianyin Lai[1]; Arnold Huang[1]; Scott Lawrence[1]; Hongchang Qu[1]; Robert Brown[1]; Mohamed ElSayed[1]; Jason Tang[1]; [1]Eli Lilly and Company, Indianapolis, IN

ThP 589 **Absolute Quantification of Lipidated GLP-1 Analog Peptides in Plasma of Various Species with High Resolution Mass Spectrometer**; Yue Huang[1]; Anton I Rosenbaum[1]; [1]Medimmune, South San Francisco,, CA

ThP 590 **Quantification of Microcystins in Urine using LC-ESI-MS and MS/MS with Efficient Solid-Phase Extraction**; Dilrukshika S. W. Palagama[1]; David Baliu-Rodriguez[1]; Apurva Chandrakant Lad[1]; Bruce S Levison[1]; David J Kennedy[1]; Steven T Haller[1]; Judy Westrick[2]; Kenneth Hensley[3]; Dragan Isailovic[1]; [1]University of Toledo, Toledo, OH; [2]Wayne State University, Detroit , MI; [3]Arkansas College of Osteopathic Medicine, Fort Smith, Arkansas

ThP 591 **Quantitative Measurements of the Active KRAS Level in Cells with Different KRAS Mutations**; Xiaoying Ye[1]; Que N. Van[2]; Andrew G. Stephen[2]; [1]Frederick National Laboratory for Cancer Research, Frederick, Maryland; [2]Fredrick National Laboratory for Cancer reserach, Frederick, Maryland

ThP 592 **Blood Brain Barrier Penetration of Glycosylated Peptides by 'Shotgun Microdialysis' Coupled with LC-MS3**; Chenxi Liu[1]; Mitchell J. Bartlett[2]; Catherine L. Smith[1]; Dillon Hanrahan[1]; Lajos Szabo[1]; Torsten Falk[2]; Robin Polt[1]; Michael L. Heien[1]; [1]Department of Chemistry and Biochemistry, The University of Arizona, Tucson, AZ; [2]Department of Neurology, The University of Arizona, Tucson, AZ, Tucson, AZ

ThP 593 **Improving the Sensitivity and Selectivity During the Quantitative Analysis of Targeted Peptides Using**

a 4-Column Multidimensional Micro-UHPLCMS/MS System; Farid Jahouh[1]; Ronald De Vries[1]; Filip Cuyckens[1]; Rob J. Vreeken[1,2]; *[1]Discovery Sciences, Janssen Pharmaceutica, Beerse, Belgium; [2]M4i Maastricht Multimodal Molecular Imaging Institute, Maastricht, Netherlands*

ThP 594 **LC-HRMS/MS of Endogenous and Synthetic Neurohormone Peptides in Biological Fluids and Tissues**; Claudio Medana[1]; Federica Dal Bello[1]; Valentina Santoro[1]; Michael Zorzi[1]; Andrea Pellegrino[1]; Paolo Giacobini[2]; *[1]University of Turin, Torino, Italy; [2]INSERM Jean-Pierre Aubert Research Center, Lille, France*

ThP 595 **Speed for Sensitivity: Operating MRM in 'Packets' for Enhancement of Peptide Detection**; Atsuhiko Toyama[1]; Ichiro Hirano[2]; *[1]Shimadzu Corporation, Marketing Innovation Centre, Singapore; [2]Shimadzu Corporation, Kyoto, Japan*

ThP 596 **Absolute Quantification of Dystrophin in Muscle Biopsies of Becker and Duchenne Muscular Dystrophy Patients using Parallel Reaction Monitoring (PRM)**; Emily Canessa[1]; Mansi V Goswami[1]; Tchilabalo Alayi[1]; Eric P Hoffman[1]; Luca Bello[2]; Elena Pegoraro[2]; Yetrib Hathout[1]; *[1]Binghamton University State University of New York, Binghamton, NY; [2]University of Padova, Padova, Italy*

ThP 597 **Antibody-Independent Targeted Quantification of Cancer-Related Mutant Proteins by Parallel Reaction Monitoring Mass Spectrometry in breast and pancreatic cancer cell lines**; Carmen Gonzalez-Tejedo[1]; Evangelia K Papachristou[1]; Valar Nila R Franklin[1]; Jiaxuan Chen[1]; Verena Thewes[1]; Martin L Miller[1]; Jason S Carroll[1]; Clive S D'Santos[1]; *[1]Cancer Research UK Cambridge Institute, University of cambridge, Cambridge, UK*

ThP 598 **Detection of 32 Bioactive Peptides in Horse Urine by Ultra-High Performance Liquid Chromatography – High Resolution Mass Spectrometry**; Elvis Ming Kit Leung; *Racing Laobratory, The Hong Kong Jockey Club (HKJC), New Territories, Hong Kong*

PEPTIDOMICS
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ThP 599 **Improving Coverage and Quantification of the Crustacean Neuropeptidome via Custom 4-plex Dimethylated Leucine (DiLeu) Isobaric Tags**; Chris Sauer[1]; Amanda Buchberger[1]; Lingjun Li[1]; *[1]University of Wisconsin-Madison, Madison, WI*

ThP 600 **Quantitative Top-Down Analysis of Crustacean Hyperglycemic Hormones (CHHs) and CHH Precursor-Related Peptides in Response to Low pH Stress**; Yang Liu[1]; Lingjun Li[1]; *[1]University of Wisconsin, Madison, WI*

ThP 601 **Mass Spectrometric Investigation of Neuropeptide Changes in Blue Crab Callinectes Sapidus in Exposure to Silver Nanoparticles**; Zihui Li[1]; Yang Liu[1]; Lingjun Li[1]; *[1]University of Wisconsin-Madison, Madison, Wisconsin*

ThP 602 **The HLA-A*02 Peptide Atlas: A Powerful Resource for Generating Novel Immunotherapies**; Geert Mommen[1]; Ricardo Carreira[1]; David Lowne[1]; Floriana Capuano[1]; Michael Cundell[1]; Alex Powlesland[1]; *[1]Immunocore Ltd, Abingdon, UK*

ThP 603 **Bioactive Peptidome as a Driver of Systemic Functional Deficits Evoked by Inhalation of Multi-Walled Carbon Nanotubes**; Ekaterina Mostovenko[1]; Tamara L. Young[2]; Pretal P. Muldoon[1]; Aleksandar Vucetic[1]; Matthew J. Campen[2]; Andrew K. Ottens[1]; *[1]Anatomy and Neurobiology, Virginia Commonwealth University, Richmond, VA; [2]Pharmaceutical Sciences, University of New Mexico, Albuquerque, NM*

ThP 604 **Identification and Characterization of HLA Class I Presented Glycopeptides Using Immunopeptidomics Methodology**; Wenjun Wang[1]; Arnoud H de Ru[1]; Manfred Wuhrer[1]; Paul J. Hensbergen[1]; Peter A. van veelen[1]; *[1]Leiden University Medical Centre, Leiden, Netherlands*

ThP 605 **Evaluation of MHC-Associated Peptide Proteomics Technology for De-risking Anti-Drug Antibody Responses**; Qui Phung[1]; Lynn Kamen[1]; Ben Ordonia[1]; Shan Chung[1]; Jane Ruppel[1]; Jennie R. Lill[1]; *[1]Genentech, Inc., South San Francisco, CA*

ThP 606 **Characterization of Crustacean Neuropeptide Dynamics under Hypoxia Stress Using Mass Spectrometry**; Amanda Buchberger[1]; Kellen DeLaney[1]; Chris Sauer[1]; Kylie Helfenbein[1]; Yang Liu[1]; Nhu Quynh Vu[1]; Lingjun Li[1]; *[1]University of Wisconsin–Madison, Madison, WI*

ThP 607 **Characterization of Endoproteolytic Processing of Neuropeptide K using Rat Spinal Cord Cellular Fractions and High-Resolution Mass Spectrometry**; Jennifer Ben Salem[1]; Bruno Nkambeu[1]; Francis Beaudry[1]; *[1]Université de Montréal, St-Hyacinthe, QC, Canada*

ThP 608 **Deciphering the Role of Neuropeptides in C.elegans Heat Avoidance Behavior**; Bruno Nkambeu[1]; Jennifer Ben Salem[1]; Francis Beaudry[1]; *[1]Université de Montréal, St-Hyacinthe, QC, Canada*

ThP 609 **Development of a Novel Mass Spectrometry Approach for Comprehensive Neuropeptidome Characterization and its Application to Analysis of Human Pituitary Tumor**; Pingli Wei[1]; Qing Yu[2]; Haidan Sun[3]; Fengfei Ma[4]; Vaishali P Bakshi[5]; Wei Sun[3]; Zhi Zheng[3]; Chun Zeng[6,7]; Lingjun Li[1,4]; *[1]Chemistry department, University of Wisconsin Madison, Madison, WI; [2]Department of Cell Biology, Harvard Medical School, Boston, MA; [3]Institute of Basic Medical Sciences Chinese Academy of Medical Sciences, School of Basic Medicine Peking Union Medical College, Beijing, China; [4]School of Pharmacy, University of Wisconsin-Madison, Madison, WI; [5]Department of Psychiatry, University of Wisconsin-Madison, Madison, WI; [6]Department of Neurosurgery, Beijing Tiantan Hospital, Capital Medical University, Beijing, China; [7]China National Clinical Research Center for Neurological Diseases, Beijing, China*

ThP 610 **The Forgotten Proteome – Proteomics Approaches for the Identification of Short Open Reading Frame Encoded Peptides**; Andreas Tholey[1]; Liam Cassidy[1]; *[1]University Kiel, Proteomics & Bioanalytics (IEM), Kiel, Germany*

ThP 611 **Peptidomic Discovery and Identification of Polypeptides Encoded by lncRNA**; Qing Zhang[1,2]; Tanxi Cai[1,2]; Jifeng Wang[1]; Lili Niu[1]; Jianjun Luo[1]; Runsheng Chen[1,2]; Fuquan Yang[1,2]; *[1]Institute of Biophysics, Chinese Academy of Sciences, Beijing, China; [2]University of Chinese Academy of Sciences, Beijing, China*

ThP 612 **The Most Ancient Proteome Yet (~2 Ma old) Enables Molecular Phylogeny Beyond the Limits of Ancient DNA Preservation**; Enrico Cappellini[1]; Victor J. Moreno Mayar[2]; Jesper V. Olsen[3]; Eske Willerslev[2]; *[1]University of Copenhagen, Copenhagen, Denmark; [2]University of Copenhagen, Copenhagen, Denmark; [3]Novo Nordisk Foundation Center for Protein Research, University of Copenhagen, Copenhagen, Denmark*

ThP 613 **Data-Independent Acquisition Allows for a Sensitive and Extensive Characterization of Membranal and Blood-Soluble HLA Peptidomes**; Tim Fugmann[1]; Danilo Ritz[1]; Dario Neri[2]; *[1]Philochem AG, Otelfingen, Switzerland; [2]ETH Zurich, Zurich, Switzerland*

ThP 614 **Peptidogenomic Capture and Functional Characterization of a Conserved Microprotein in Community Associated MRSA**; Jacob Wozniak[1]; Julieta Aguilar[1]; John Lapek[2]; Dominic McGrosso[1]; Eri Nakatani-Webster[3]; Michael Dores[4]; Katrin Schilcher[5]; Anvesh Marchela[1]; JoAnn Trejo[1]; Brian J. Werth[3]; Abhinav Nath[3]; Ross Corriden[1]; Alexander Horswill[5]; David Gonzalez[1]; *[1]UCSD, San Diego, CA; [2]Pfizer Inc., San Diego, CA; [3]University of Washington, Seattle, WA; [4]Hofstra University, Long Island, NY; [5]University of Colorado - Denver | Anschutz Medical Campus, Aurora, CO*

ThP 615 **Peptidomic Analysis of Mouse Brain Striatum Identifies Novel sORF-Encoded Polypeptides**; Harshavardhan Budamgunta[1]; Volodimir Olexiouk[2]; Gerben Menschaert[2]; Kurt Boonen[1, 3]; Geert Baggerman[1, 4]; *[1]UAntwerp, Antwerpen, Belgium; [2]UGent, Gent, Belgium; [3]VITO, Mol, Belgium; [4]Vito, Mol, Belgium*

ThP 616 **Metabolomic and Peptidomic Characterization of Potentially Toxic Substances Extracted from the Disco Clam Ctenoides ales**; Kitty J. Brown[1]; Lindsey F. Dougherty[2]; Kevin L Schauer[3]; Jingchun Li[2]; Corey D. Broeckling[1]; *[1]Proteomics and Metabolomics Facility, Colorado State University, Fort Collins, CO; [2]Department of Ecology and Evolutionary Biology, University of Colorado Boulder, Boulder, CO; [3]Genome Center of Wisconsin, Madison, WI*

ThP 617 **Disclosing the Substrate Diversity of Angiotensin-Converting Enzyme with Mass Spectrometry**; Margarita Semis[1]; Gabriel B. Gugiu[2]; Kenneth E. Bernstein[3]; Markus Kalkum[1, 2]; *[1]Department of Molecular Imaging and Therapy, Diabetes and Metabolism Research Institute, City of Hope, Duarte, CA; [2]Mass Spectrometry & Proteomics Core Facility, Beckman Research Institute of the City of Hope, Duarte, CA; [3] Departments of Biomedical Sciences, Pathology and Laboratory Medicine, Cedars-Sinai Medical Center, Los Angeles, CA*

ThP 618 **Development of 3rdGeneration Free Radical Initiated Peptide Sequencing (FRIPS) Reagent forPeptide Characterization**; Kaylee Gaspar[1]; Kimberly Fabijanczuk[1]; Jinshan Gao[1]; *[1]Montclair State University, Montclair, NJ*

ThP 619 **Interferon Gamma Reshapes MHC-I and MHC-II Antigen Presentation: A Proteogenomic Investigation**; Niclas Olsson[1]; Lichao Zhang[1]; Suchit Jhunjhunwala[2]; Qui T Phung[2]; Veronica G Anania[2]; Sarah Y Lin[1]; Keith Rawson[1, 3]; Jennie R Lill[2]; Joshua E Elias[1]; *[1]Stanford University, School of Medicine, Dep. of Chemical and Systems Biology, Stanford, CA; [2]Genentech, South San Francisco, CA; [3]Juno Therapeutics, Seattle, WA, WA*

ThP 620 **Phosphopeptidomics Identifies Novel High-Occupancy Phosphosites on Endogenous Peptides with the Fam20C "SxE" Motif in Dense Core Secretory Vesicles**; Christopher B. Lietz[1]; Thomas Toneff[1]; Charles Mosier[1]; Sonia Podvin[1]; Anthony J O'Donoghue[1]; Vivian Hook[1, 2]; *[1]Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California, San Diego, La Jolla, California; [2]Department of Neurosciences, School of Medicine, University of California, San Diego, La Jolla, CA*

ThP 621 **Distinguishing MHC Peptides and Epitopes from Other Polypeptides with Trapped Ion Mobility Spectrometry(tims)-TOF**; Teesha C. Luehr[1]; Queenie W. T. Chan[1]; Thomas Clark[1]; Leonard J. Foster[1]; *[1]University of British Columbia, Vancouver, BC, Canada*

ThP 622 **Comparison of Plasma Peptides High-Effective Extraction Methods for Biomarker Discovery by High Resolution Mass Spectrometry**; Natalia V. Zakharova[1, 2]; Anna Bugrova[1]; Maria Indeykina[1, 2]; Alexey Kononikhin[1, 2, 3]; Evgeny Kukaev[2, 3]; Igor Popov[2, 3]; Eugene (Evgeny) Nikolaev[2, 3, 4]; *[1]Emanuel Institute of Biochemical Physics, Moscow, Russia; [2]Moscow Institute of Physics and Technology, Moscow, Russia; [3]Institute for Energy Problems of Chemical Physics of RAS, Moscow, Russia; [4]Skolkovo institute of science and technology, Moscow Region, Russian Federation*

ThP 623 **Discovery of Oncolytic Virus-Induced Tumor MHC Ligands for Cancer Immunotherapy**; Youra Kim[1]; J. Patrick Murphy[1]; Prathyusha Konda[1]; Derek R Clements[1]; Heiko Schuster[2, 3]; Daniel J Kowalewski[2, 3]; Joao A. Paulo[4]; Stefan Stevanovic[2]; Steven P Gygi[4]; Shashi Gujar[1, 5]; *[1]Dalhousie University, Halifax, NS, Canada; [2]University of Tübingen, Tübingen, Germany; [3]Immatics Biotechnologies, Tübingen, Germany; [4]Harvard Medical School, Boston, MA; [5]IWK Health Centre, Halifax, NS, Canada*

ThP 624 **Approaches to Discovery of Stress-Induced Non-Annotated Microproteins and Splice Variants**; Alexandra Khitun[1]; Nadia G D'Lima[1]; Aaron Rosenbloom[1]; Peijia Yuan[1]; Karl Barber[1]; Brandon Gassaway[1]; Jesse Rinehart[1]; Sarah Slavoff[1]; *[1]Yale University, West Haven, CT*

ThP 625 **The Characterization of Antimicrobial Peptides in Hemolymph from the Lobster, Homarus americanus: Heat-Treatment to Minimize Peptide Alterations**; Elizabeth A. Stemmler[1]; Daniel Do[1]; Giap H. Vu[1]; Patsy S. Dickinson[1]; Andrew E. Christie[2]; *[1]Bowdoin College, Brunswick, ME; [2]University of Hawaii at Manoa, Honolulu, HI*

ThP 626 **Neuropeptide Identification Outcomes from Transcriptome Informed Protein Databases and Empirical MS data**; Elena V. Romanova[1]; Bruce R. Southey[1]; Colin Lee[1]; Jonathan V Sweedler[1]; *[1]University of Illinois at Urbana-Champaign, Urbana, IL*

ThP 627 **The Facile Fabrication of Caliber Controllable Electrospray Emitter and its Effectiveness Evaluation**; Quanqing Zhang[1]; Yuanyu Huang[1]; Pengyuan Yang[1]; *[1]Fudan Universiry, Shanghai, China*

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ThP 628 **TiO2 Nanocages for Selective Enrichment and Identification of Phosphopeptides by Mass Spectrometry**; Chen Fang Xsiao[1]; Chih Che Wu[1]; *[1]National Chi Nan University, Nantou, Taiwan*

ThP 629 **Identification of Phosphorylation Sites of Imperata Cylindrica Microsomal Proteins with PolyMAC-Ti Nanoparticle Bead Enrichment and Mass Spectrometry Analyses**; Ing-Feng Chang[1]; Yun-Jhih Shih[1]; Man-Hsuan Lee[1]; Pei-Yuan Chen[1]; *[1]National Taiwan University, Taipei, Taiwan*

ThP 630 **Expanding the Landscape of Human Phosphorylation-Mediated Signalling**; Gemma Hardman[1]; Simon Perkins[1]; Philip Brownridge[1]; Dominic P. Byrne[1]; Patrick A. Eyers[1]; Andrew R. Jones[1]; Claire E. Eyers[1]; *[1]University Of Liverpool, Liverpool, UK*

ThP 631 **Evaluation of SMOAC Enrichment for Phosphopeptide Analysis from Small Sample Sizes Using ETD, HCD, and EThCD**; Deepali Rathore[1]; Rachel A. Jones Lipinski[1]; Matthew Waas[1]; Rebekah L. Gundry[1]; *[1]Medical College of Wisconsin, Milwaukee, WI*

ThP 632 **Adaption and Optimization of a Column Based Phospho-Peptide Enrichment Strategy**; Sascha Knecht[1]; Per Haberkant[1]; Mandy Rettel[1]; Frank Stein[1]; Mikhail Savitski[1, 2]; Dominic Helm[1]; *[1]Proteomics Core Facility, EMBL, Heidelberg, Germany; [2]EMBL, Heidelberg, Heidelberg, Germany*

ThP 633 **Enrichment and Separation of Phosphopeptides and Mannose-6-phosphate Glycopeptides by Ti(IV)-IMAC in a Typical HILIC-mode Elution**; Junfeng Huang[1]; Jing Dong[2]; Xudong Shi[3]; Zhengwei Chen[4]; Yusi Cui[4]; Xiaoyan Liu[2]; Mingliang Ye[2]; Lingjun Li[1, 4]; *[1]School of Pharmacy, University of Wisconsin-Madison, Madison, WI; [2]Key Laboratory of Separation Sciences for Analytical Chemistry, National Chromatographic R&A Center, Dalian Institute of Chemical Physics, Chinese Academy of Sciences (CAS), Dalian, China; [3]Department of Surgery, University of Wisconsin-Madison, Madison, WI; [4]Department of Chemistry, University of Wisconsin-Madison, Madison, WI*

ThP 634 **A Streamlined StageTip-Based Workflow for Deep and Sensitive Phosphoproteomic Profiling**; Yun-Chien Chang[1, 2]; Reta Birhanu Kitata[2]; Pei-Yi Lin[2]; Chia-Feng Tsai[3]; Yu-Ju Chen[1, 2]; *[1]National Taiwan University, Taipei, Taiwan; [2]Institute of Chemistry, Academia Sinica, Taipei, Taiwan; [3]Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, Japan*

ThP 635 **Specific Salts Confer a 10x Increase in Selectivity for Phosphopeptides in HILIC or ERLIC**; Andrew J Alpert; *PolyLC Inc., Columbia, MD*

ThP 636 **An Automated, High-Throughput Multi-Omics Platform for Maximizing Phosphopeptide Quantification from Small Volume Samples**; Carrie Romer[1]; Danielle B. Gutierrez[1]; Jamie L. Allen[1]; Melissa A. Farrow[2]; Jeremy L. Norris[1]; Eric P. Skaar[2]; D. Borden Lacy[2]; Richard M. Caprioli[1]; *[1]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [2]Department of Pathology, Microbiology, and Immunology, Vanderbilt University Medical Center, Nashville, TN*

ThP 637 **Development of an Automated Platform for Targeted Phosphoproteomics Analysis**; Renuka Sabnis[1]; Ramon Diaz Pena[1]; Alicia Richards[1]; Alexandre Rosa Campos[1]; Km Shams Ud Doha[1]; *[1]Sanford Burham Prebys Medical Discovery Institute, San Diego, CA*

ThP 638 **Comparison of Different IMAC Resins for High-Throughput Phosphopeptide Enrichments for Deep-Profiling of HCT 116 Cell Line**; Brian T Mullis[1]; Sunil Hwang[2]; Matthew Manter[2]; Michael Walla[1]; Jingyun Lee[3]; Christina M Furdui[3]; Andrew Lee[1, 2]; Qian Wang[1]; *[1]University of South Carolina, Columbia, SC; [2]Integrated Micro-Chromatography Systems, LLC, Irmo, SC; [3]Wake Forest School of Medicine, Winston-Salem, NC*

ThP 639 **Streamlined and Sensitive Sample Preparation for Phosphoproteomics Using the EasyPhos Workflow**; Sean J Humphrey[1, 2]; Ozge Karayel[2]; Jeff Liu[2]; Pengyi Yang[1]; Raja Jothi[3]; David E James[1]; Matthias Mann[2]; *[1]The University of Sydney, Sydney, Australia; [2]Department of Proteomics and Signal Transduction, Max Planck Institute of Biochemistry, Martinsried, Germany; [3]Systems Biology Section, Laboratory of Molecular Carcinogenesis, National Institute of Environmental Health Sciences, Research Triangle Park, NC*

ThP 640 **Development of FMS-like Tyrosine Kinase 3 (FLT3) Artificial Substrates (FAStides) Using Kinase Assay Linked with Phosphoproteomics (KALIP)**; Minervo Perez[1, 2]; John Blankenhorn[1]; Andy W. Tao[2]; Laurie L. Parker[1]; *[1]University of Minnesota, Minneapolis, MN; [2]Purdue University, West lafayette, Indiana*

ThP 641 **Automated High-Throughput Immunoaffinity Enrichment for phosphotyrosine Peptides Using Protein A and Streptavidin IMCStips**; Sunil Hwang[1]; Todd Mullis[2]; Michael Walla[2]; Matthew Manter[1]; Jingyun Lee[3]; Christina M Furdui[3]; Andrew Lee[1]; *[1]IMCS, Irmo, SC; [2]University of South Carolina, Columbia, SC; [3]Wake Forest School of Medicine, Winston-Salem, NC*

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ThP 642 **Absolute Quantification of Grapevine Red Blotch Virus in Grapevine Leaf Petioles by Proteomics**; Natasha Buchs[1]; Sophie Braga-Lagache[1]; Anne-Christine Uldry[1]; Justine Brodard[2]; Christophe Debonneville[3]; Jean-Sébastien Reynard[2]; Manfred Heller[1]; *[1]University of Bern, Bern, Switzerland; [2]Agroscope, Institute for Plant Production Science, Nyon, Switzerland; [3]Bioreba AG, Reinach, Switzerland*

ThP 643 **The Phosphorylated Redox Proteome of Chlamydomonas Reinhardtii: Revealing Novel Means for Enzymatic Regulation.**; Evan W Mc Connell[1]; Emily G Werth[1]; Leslie M Hicks[1]; *[1]University of North Carolina at Chapel Hill, Chapel Hill, NC*

ThP 644 **Mapping Proteome-Wide Targets of Protein Kinases in Response to Stresses**; Pengcheng Wang[1]; Chuan-Chih Hsu[2]; Yanyan Du[1]; Andy W. Tao[2]; Jian-Kang Zhu[1]; *[1]Shanghai Center for Plant Stress Biology, Chinese Academy of Sciences, Shanghai, China; [2]Department of Biochemistry, Purdue University, West Lafayette, IN*

ThP 645 **Investigating the Effect of Target of Rapamycin Kinase Inhibition on the Chlamydomonas Reinhardtiiphosphoproteome: From Known Homologs to New Targets**; Leslie M. Hicks[1]; Emily G Werth[1]; Evan W Mc Connell[1]; Inmaculada Couso Lianez[2]; James Umen[2]; *[1]University of North Carolina, Chapel Hill, NC; [2]Danforth Center, St. Louis, MO*

ThP 646 **Cuticle Removed Leaf Spray for Soybean Metabolomics**; Kevin J. Zemaitis[1]; Troy D. Wood[1]; Philip H. Lindhorst[1]; *[1]University at Buffalo, Buffalo, NY*

ThP 647 **A Combined Omics Approach Reveals 2,4-Diacetylphloroglucinol as a Key Stimulator of Jasmonic Acid-Dependent Defense Response in Arabidopsis**; Young-Sang Kwon[1]; Hee-Jung Sim[1]; Jong-Hwan Kim[1]; Jong-Su Seo[1]; *[1]Korea Institute of Toxicology, Jinju, South Korea*

ThP 648 **Application of a Rapid Microbore Metabolic Profiling HILIC Approach for Analysis of Anthocyanins in Red Wine with Ion Mobility HRMS**; Lauren Mullin[1]; Adam King[2]; Hernando Olivos[3]; Robert Plumb[1]; Kenneth Rosnack[1]; *[1]Waters Corporation, Milford, MA; [2]Waters Corporation, Wilmslow, UK; [3]Waters Corporation, Beverly, MA*

ThP 649 **Ubiquitin Signaling in the Nitrogen-Fixing Symbiosis Between Medicago Truncatula and Sinorhizobium Meliloti**; Erin Weisenhorn[1]; Junko Maeda[2]; Dhileepkumar Jayaraman[2]; Jean-Michel Ané[2]; Joshua J Coon[2]; *[1]University of Wisconsin, Madison, Madison, WI; [2]University of Wisconsin-Madison, Madison, Wisconsin*

ThP 650 **Applying Clustering and Protein Interaction Network Analysis to Define Plant Acclimation to High Light Stress**; Débora Vieira Parrine Sant'Ana[1]; Bo-Sen Wu[1]; Keith Rivera[2]; Darryl Pappin[2]; Mark Lefsrud[1]; *[1]McGill University, Saint-Anne-De-Bellevue, QC, Canada; [2]Cold Spring Harbor laboratory, Cold Spring Harbor, NY*

ThP 651 **Quantitative Proteomic Studies in flax Seed Development: Seed Coat-Embryo Interaction**; Mehdi Cherkaoui[1, 2]; Fabien Miart[1, 2]; François Mesnard[1, 2]; Paulo Marcelo[1, 3]; Karine Pageau[1, 2]; *[1]University of Picardie Jules Verne, Amiens, France; [2]Laboratoire de Biologie des Plantes et Innovation, EA-3900, Amiens, France; [3]Plateforme d'Ingénierie Cellulaire & Analyses des Protéines, Amiens, France*

ThP 652 **Assessing Evolutionary Patterns of Specialized Metabolite Diversity in the cosmopolitan Plant Genus Euphorbia: Application of an enhanced Metabolomics Workflow**; Madeleine Ernst[1, 2, 3]; Louis-Félix Nothias[1, 4]; Justin J. J. van der Hooft[1, 2, 5]; Ricardo R. da Silva[1, 2]; C. Haris Saslis-Lagoudakis[6]; Olwen M. Grace[7]; Karen Martinez[6, 8]; Gustavo Hassemer[6]; Luis Adriano Funez[9]; Henrik Toft Simonsen[10]; Marnix H. Medema[11]; Dan Staerk[12]; Niclas Nilsson[13]; Paola Lovato[14]; Pieter C. Dorrestein[1, 2, 15]; Nina Rønsted[6]; *[1]Skaggs School of Pharmacy & Pharmaceutical Sciences, University of California San Diego, San Diego, CA; [2]Collaborative Mass Spectrometry Innovation Center, Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California, San Diego, California; [3]Natural History Museum of Denmark, Faculty of Science, University of Copenhagen, Copenhagen, Denmark; [4]Collaborative Mass Spectrometry Innovation Center, Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA; [5]Bioinformatics Group, Department of Plant Sciences, Wageningen University, Wageningen, Netherlands; [6]Natural History Museum of Denmark, Faculty of Science, University of Copenhagen, Copenhagen, Denmark; [7]Comparative Plant & Fungal Biology, Royal Botanic Gardens, Kew, Surrey, UK; [8]Department of Biotechnology and Biomedicine, Technical University of Denmark, Kongens Lyngby, Denmark; [9]Herbário Dr. Roberto Miguel Klein (FURB), Universidade Regional de*

Blumenau, Blumenau, Brazil; [10]Department of Biotechnology and Biomedicine, Technical University of Denmark, Kongens Lyngby, Denmark; [11]Bioinformatics Group, Department of Plant Sciences, Wageningen University, Wageningen, Netherlands; [12]Department of Drug Design and Pharmacology, Faculty of Health and Medical Sciences, University of Copenhagen, Copenhagen, Denmark; [13]Front End Innovation, LEO Pharma A/S, Ballerup, Denmark; [14]Front End Innovation, LEO Pharma A/S, Ballerup, Denmark; [15]Center for Microbiome Innovation, University of California San Diego, La Jolla, CA

ThP 653 **Characterization of Native Protein Complexes Using Protein Correlation Profiling-Based Quantitative Proteomics**; Julia Mergner[1]; Martin Frejno[1]; Claus Schwechheimer[2]; Bernhard Kuster[1, 3]; *[1]Chair of Proteomics and Bioanalytics, Technical University of Munich (TUM), Freising, Germany; [2]Chair of PLant Systems Biology, Technical University of Munich (TUM), Freising, Germany; [3]Bavarian Center for Biomolecular Mass Spectrometry, Freising, Germany*

ThP 654 **Peeling Back the Layers of Crassulacean Acid Metabolism: Functional Deviation of Epidermal and Mesophyll Cells Revealed by Comparative Proteomics**; Paul E. Abraham[1]; Natalia Hurtado[2]; Suresh Poudel[1]; Robert L. Hettich[1]; Anne Borland[2]; *[1]Oak Ridge National Laboratory, Oak Ridge, TN; [2]School of Natural and Environmental Sciences, University of Newcastle, Newcastle upon Tyne, UK*

ThP 655 **A LC-QqQ-MS-Based Method for Evaluation of Plant Disease Resistance Inducers**; Yuji Sawada[1]; Shigemi Seo[2]; Muneo Sato[1]; Mami Okamoto[1]; Yutaka Yamada[1]; Naomi Seo[3]; Takeru Itabashi[3]; Masaaki Osaka[3]; Masami Yokota Hirai[1]; *[1]RIKEN Center for Sustainable Resource Science, Yokohama, Japan; [2]Institute of Agrobiological Sciences, NARO, Tsukuba, Japan; [3]Miyagi Prefectural Institute of Agriculture and Horticulture, Natori, Japan*

ThP 656 **Comparison of Atmospheric Pressure and Vacuum MALDI Orbitrap Platforms for the Examination of Salt Stress in Medicago truncatulaRoot Nodules**; Caitlin Keller[1]; Junko Maeda[1]; Dhileepkumar Jayaraman[1]; Michael R Sussman[1]; Jeanne Harris[2]; Jean-Michel Ané[1]; Lingjun Li[1]; *[1]University of Wisconsin–Madison, Madison, WI; [2]University of Vermont, Burlington, VT*

ThP 657 **Study of Plant Systemic Signaling Proteins in Response to Nitrogen, Phosphate, and Potassium Deficiency Using Quantitative Proteomics Approach**; Kai-Ting Fan[1]; Byung-Kook Ham[2]; Szu-Yu Liu[1]; William J. Lucas[3]; Yet-Ran Chen[1]; *[1]Academia Sinica, Taipei, Taiwan; [2]University of Saskatchewan, Saskatoon, SK, Canada; [3]UC Davis, Davis, CA*

ThP 658 **Draft Proteome Map of Chickpea (Cicer arietinum)**; Lekha Padmaram[1]; Baojin Zhou[2]; Zhe Ren[2]; Yan Ren[2]; Anu Chitikineni[1]; Varshney Kumar Rajeev[1]; Siqi Liu[2]; Xun Xu[2]; *[1]International Crops Research Institute for the Semi-Arid Tropics (ICRISAT), Hyderabad, India; [2]BGI-Shenzhen, Shenzhen, China*

ThP 659 **Traceability of Soybean Crops Growing Area Based on Plant Metabolomics Analysis by FIA-ESI-MS**; Pai-Chi Syue[1]; Hung-Yu Pan[1]; Yu-Chia Hsu[1]; Ching-Yi Lien[1]; Mai-Su Lin[1]; Kuo-Lung Ku[1]; *[1]National Chiayi University, Chiayi City, Taiwan*

ThP 660 **Metabolite Patterns in Wood Forming Cells and Tissues in Populus**; Ilara G. F. Budzinski[1]; Ilka Abreu[1]; Thomas Moritz[2, 3]; *[1]Umeå Plant Science Centre, Swedish University of Agricultural Sciences, Umeå, Sweden; [2]Umeå Plant Science Centre, Umeå, Sweden; [3]Swedish Metabolomics Centre, Swedish University of Agricultural Sciences, Umeå, Sweden*

ThP 661 **Profiling Analysis Via Mass Spectrometry and Antimicrobial Efficacy of Bombax malabaricaPlant Extract**; Alexandra Tori[1]; Lindsey Bodnar[1]; Rachana Bhatt[1]; Anima Ghosal[1]; Dil Ramanathan[1]; *[1]Kean University, Union, NJ*

ThP 662 **Quantitative Proteomic Approaches to Characterize the Dynamic and Comprehensive Defence Responses of Wheat to Leaf Rust**; Mei Huang[1]; Ursla Fernando[1]; Slavica Djuric-Ciganovic[1]; Xiben Wang[1]; Guus Bakkeren[2]; Rob Linning[2]; Bykova Natalia[1]; Christof Rampitsch[1]; *[1]Agriculture and Agri-food Canada, Morden, MB, Canada; [2]Agriculture and Agri-food Canada, Summerland, BC, Canada*

ThP 663 **Improving LC-MSnsensitivity for Structural Characterization of Lignin Oligomers Using Acetic Acid as the Mobile Phase Additive**; Wooyoung Song[1]; Tae-Young Kim[1]; *[1]Gwangju Institute of Science and Technology, Buk-gu, South Korea*

ThP 664 **Proteomic Profiling of Canadian Malting Barley and Wort**; Katherine Cordova[1]; Ray Bacala[1]; Marta Izydorczyk[1]; Dave Hatcher[1]; *[1]Canadian Grain Commission, Winnipeg, MB, Canada*

ThP 665 **Effects of Chemical Inhibition on Rapamycin-Hypersensitive Chlamydomonas Reinhardtii Strain Using Quantitative Phosphoproteomics**; Emily Werth[1]; James G Umen[2]; Leslie M Hicks[1]; *[1]University of North Carolina at Chapel Hill, Chapel Hill; [2]Donald Danforth Plant Science Center, St. Louis`, Missouri*

ThP 666 **Metabolomic Analysis of Sweet Basil Acclimation to Growth Temperature**; Tudor Muntean[1]; Lyle E Craker[1]; *[1]University of Massachusetts-Amherst, Amherst, MA*

ThP 667 **Exploring the Molecular Physiology of a model Root System in Response to Environmental Perturbations Using Multimodal Mass Spectrometry Imaging**; Rosalie K Chu[1]; Dusan Velickovic[1]; Gabriel L Myers[1]; Ljiljana Pasa Tolic[1]; Christopher R Anderton[1]; Amir H Ahkami[1]; *[1]PNNL, Richland, WA*

ThP 668 **A LC-QqQ-MS-Based Method for Metabolic Marker Development of Soybean under Environmental Stress Condition**; Mami Okamoto[1]; Yuji Sawada[1]; Kai Uchida[1]; Muneo Sato[1]; Yutaka Yamada[1]; Masami Yokota Hirai[1]; *[1]RIKEN Center for Sustainable Resource Science, Yokohama, Japan*

ThP 669 **Development of an Ocean Protein Portal for Exploration of Marine Metaproteomic Datasets**; Mak Saito[1]; David Gaylord[1]; Adam Shepherd[1]; Jacyln Saunders[1]; Noelle Held[1]; Michael Chagnon[2]; Nick Symmonds[1]; Danie Kinkade[1]; Alex Dorsk[1]; Matthew McIlvin[1]; *[1]Woods Hole Oceanographic Inst., Woods Hole Ma 02543, MA; [2]RPS Ocean Science, South Kingstown, RI*

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ThP 670 **Development of a Sensitive and Selective LBA Alternative Hybrid Immune-Capture LC-MS/MS Method for Protein Quantification of NOV001**; Adam Bentley[1]; Harvey Chin[1]; Jim Glick[1]; Jimmy Flarakos[1]; *[1]Novartis, East Hanover, NJ*

ThP 671 **High-Throughput Multi-Attribute Method (MAM) Data Acquisition with Capillary Zone Electrophoresis – Mass Spectrometry (CZE-MS)**; Andrew Dykstra[1]; Tawnya Flick[1]; Laura Blue[1]; Nic Angell[1]; *[1]Amgen, Thousand Oaks, CA*

ThP 672 **Sub-ng/ml-Sensitivity for mAb Quantification Without Antibody-Enrichment and Application to Investigate Solid Tumor Penetration and Effector Cell Activation/ Retention By Bi-Specific Antibody(bs-Ab)**; Bo An[1]; Ming Zhang[1]; Jun Qu[1]; *[1]SUNY at Buffalo, Buffalo, NY*

ThP 673 **Quantitative Profiling of Host Cell Proteins and CHO Proteome in Biotherapeutic mAb Bioprocesses by SWATH MS Using 10,000-Proteins Spectral Library**; Chia-Yi L. Liu[1]; Kae Hwan Sim[1]; Stephen Tate[2]; Xuezhi Bi[1]; *[1]Bioprocessing technology Institute, Singapore, Singapore; [2]Sciex, Concord, ontario*

ThP 674 **Quantitative Bioanalysis of Antibody Drug Conjugates Using a Multiple LC-MS/MS Assay Approach: Development & Validation for MEDI4276 and Metabolites in Human Plasma**; Eric Ma[1]; Morse Faria[1]; Marlking Peay[1]; Moucun Yuan[1]; Michael Waldron[1]; William R. Mylott Jr. [1]; Anton I. Rosenbaum[2]; Meina Liang[3]; Brandon Lam[3]; *[1]PPD Laboratories, Richmond, VA; [2]MedImmune LLC, South San Francisco, California; [3]MedImmune, LLC, South San Francisco, CA*

ThP 675 **Development of a Liquid Chromatography Tandem Mass Spectrometry (LC-MS/MS) Method for the Quantification of Ranibizumab in Human Serum**; Eugene Miller[1]; Elizabeth Hyer[1]; Bob Xiong[1]; *[1]ICON, Whitesboro, NY*

ThP 676 **Enhanced Sensitivity of Protein Therapeutics Quantification Using a Newly-Developed ESI Interface Coupled with microLC System**; Fang Xie[1]; Xiaomeng Shen[1]; Jianxia Shi[1]; Dan Rock[1]; Ji Ma[1]; *[1]Amgen, South San Francisco*

ThP 677 ***In vivo* Assessment of Multiple Quality Attributes of Protein Therapeutics by High Resolution Liquid Chromatography Mass Spectrometry**; Haihong Zhou[1]; Yi Wang[2]; Richard S Rogers[3]; Douglas Richardson[2]; Bhumit Patel[2]; Daniela Tomazela[4]; Richard Wong[2]; Dong Hun Lee[2]; Sejal Patel[2]; Maribel Beaumont[4]; Yan-Hui Liu[2]; David Pollard[2]; Shuangping Shi[2]; Christine M. Fandozzi[5]; Lucinda R Hittle[6]; *[1]Merck Inc. & Co., Kenilworth, NJ; [2]Merck & Co., Inc., Kenilworth, NJ; [3]Just Biotherapeutics, Seattle, WA; [4]Merck & Co., Inc., Palo Alto, CA; [5]Merck Research Labs, West Point, PA; [6]Merck & Co., Inc., Rahway, NJ*

ThP 678 **Quantitation of the Monoclonal Antibody Rituximab Using Volumetric Absorptive Microsampling, Impact-Assisted Extraction, Trypsin Digestion and LC-MRM**; Jean-Nicholas Mess[1]; Kevork Mekhssian[1]; Anahita Keyhani[1]; *[1]Algorithme Pharma, Laval, QC, Canada*

ThP 679 **A Streamlined Workflow for Rapid Digestion and Quantitation of Therapeutic Proteins Utilizing H-SRM LCMSMS Analysis**; Keeley Murphy[1]; Jonathan Josephs[2]; Jon Bardsley[3]; David Brant[2]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Scientific, San Jose, CA; [3]Thermo Fisher Scientific, Runcorn, UK*

ThP 680 **A Novel Approach for Achieving High Extraction Recovery in LC-MS/MS Large Molecule Quantitation Assays**; Li Pan[1]; Sheng Wang[2]; Dawei Zhou[1]; *[1]WuXi AppTec, Plainsboro, NJ; [2]WuXi AppTec, Suzhou, China*

ThP 681 **Determination of Proteins Detected by Host Cell Protein ELISA Assays**; Martha Stapels[1]; Michelle Busch[1]; Joanne Cotton[1]; Helena Awad[1]; Jean Gamble[1]; *[1]Sanofi, Framingham, MA*

ThP 682 **Characterization of BiTE® by Cation Exchange Chromatography Coupled to Mass Spectrometry**; Yang Song[1]; Hao Zhang[1]; Aaron Kammer[1]; Alla Polozova[1]; Xin Zhang[2]; Zhe Huang[1]; *[1]Amgen, Cambridge, MA; [2]Amgen, Thousand Oaks, CA*

ThP 683 **Optimizing Data Processing Parameters for HRMS-Based Intact Level mAb Quantification**; Yun Wang Alelyunas[1]; Mark Wrona[1]; Jayne Kirk[2]; Ian Edwards[1]; Kelly B Doering[1]; *[1]Waters Corporation, Milford, MA; [2]Waters Corporation, Wilmslow, UK*

ThP 684 **Bioanalytical Strategies for the Quantification of Surrogate mAbs in Rodent Matrices using LC-MS/MS**; John T. Mehl[1]; France Landry[2]; Lorell N. Discenza[2]; Bogdan G. Sleczka[2]; Alexander T. Alexander Kozhich[2]; Huadong Sun[2]; Priyanka A. Madia[1]; Ruchira DasGupta[2]; Timothy V. Olah[1]; *[1]Bristol-Myers Squibb, Princeton, NJ; [2]Bristol Myers Squibb, Princeton, NJ*

ThP 685 **Application of the LC/MS-Based Multi-Attribute Method (MAM) for Early Stage Therapeutic Monoclonal Antibodies**; Leah(Hanliu) Wang[1]; Olga V Friese[1]; Jason C Rouse[2]; *[1]Pfizer Inc., Chesterfield, MO; [2]Pfizer Inc., Andover, MA*

ThP 686 **Automatic Detection of Clipped Monoclonal Antibodies from High-Resolution Native Mass Spectrometry**; Wilfred Tang[1]; Marshall W. Bern[1]; Andrew Nichols[1]; K. Ilker Sen[1]; Yong J. Kil[1]; Eric Carlson[1]; Tomislav Caval[2]; Vojtech Franc[2]; Albert J.R. Heck[2]; *[1]Protein Metrics, San Carlos, CA; [2]Utrecht University, Utrecht, Netherlands*

ThP 687 **A Promising Alternative to SRM: Very-High-Resolution Selected-Ion-Monitoring (vHR-SIM@500k) Enables Ultra-Sensitive and Selective Biotherapeutics Quantification in Biomatrics**; Shihan Huo[1]; Bo An[1]; Ming Zhang[1]; Yang Qu[1]; Jun Qu[1]; *[1]University at Buffalo, NY*

ThP 688 **Absolute Multiplex mAbs Quantification in Biological Fluids**; Xavier Homo-Prault[1]; Chloé Bardet[1]; Mathieu Trauchessec[1]; Christelle Jacquet[1]; Quentin Enjalbert[1]; Tanguy Fortin[1]; *[1]Anaquant, Villeurbanne, France*

ThP 689 **An Immunoaffinity-HRAMS Assay for the Pre-Clinical Quantification of Trastuzumab in Rat Plasma**; Jason Causon[1]; Neil Devenport[1]; *[1]Sciex, Warrington, UK*

ThP 690 **A Novel LC/MS-Based Pipeline Enabling Comprehensive Investigation of Tumor/Tissue Disposition of Antibody-Drug-Conjugate, *in vivo* DAR, Free Toxin and Antigen Turnover**; Yang Qu[1]; Bo An[1]; Jun Qu[1]; *[1]SUNY at Buffalo, NY*

ThP 691 **Improving the Dynamic Range of Host Cell Proteins Analysis Using a HRAM Orbitrap Mass Spectrometer**; Stephane Houel[1]; Romain Huguet[2]; Susan E. Abbatiello[1]; David Sarracino[1]; Jonathan Josephs[2]; *[1]Thermo Fisher Scientific, Cambridge, MA; [2]Thermo Fisher Scientific, San Jose, CA*

ThP 692 **Strategies for Monitoring Host Cell Proteins in Biopharmaceutical Development, Production, and Quality Control**; Joe Shambaugh[1]; Peter Haberl[2]; Albert van Wyck[3]; John N McCarter[1]; David Bush[4]; Dominik Mertens[5]; Cassandra Wigmore[5]; Chung Ping Chow[5]; Aude Tartiere[1]; Arnd Brandenburg[5]; *[1]Genedata, Inc., Lexington, MA; [2]Genedata GmbH, Munich, Germany; [3]Genedata Ltd, Duxford, UK; [4]Genedata Inc., Lexington, Massachusetts; [5]Genedata AG, Basel, Switzerland*

ThP 693 **An Automated Approach for Comprehensive Characterization and Quantification of low-Abundance Sequence Variants in a Standard Monoclonal Antibody**; Dominik Mertens[1]; Stefano Gotta[1]; Arnd Brandenburg[1]; David Bush[2]; Joe Shambaugh[2]; *[1]Genedata AG, Basel, Switzerland; [2]Genedata, Inc., Lexington, MA*

ThP 694 **Employing MS-Based Multi-Attribute Methods (MAMs) for Automated Quality Monitoring of Biotherapeutics**; Albert Van Wyk[1]; Peter Haberl[2]; Joe Shambaugh[3]; David Bush[3]; Dominik Mertens[4]; Cassandra Wigmore[4]; Chung Ping Chow[4]; John McCarter[3]; Aude Tartiere[3]; Arnd Brandenburg[4]; *[1]Genedata Ltd, Duxford, UK; [2]Genedata GmbH, Munich, Germany; [3]Genedata Inc., Lexington, Massachusetts; [4]Genedata AG, Basel, Switzerland*

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ThP 695 **Quantitative Proteomics Reveals Involvement of Cytoskeletal Proteins in Resistance to Kinase Inhibitors in Malignant Melanoma Cells**; Marisa Schmitt[1]; Tobias Sinnberg[2]; Annika Maaß[1]; Birgit Schittek[2]; Boris Macek[1]; *[1]Quantitative proteomics, University of Tuebingen, Tuebingen, Germany; [2]Division of Dermatooncology, University of Tuebingen, Tuebingen, Germany*

ThP 696 **Nano-Flow Liquid Chromatography with Triple-Quadrupole Mass Spectrometry to Quantify Oncology Biomarkers in FFPE Tissues: Achieving Sensitivity, Reproducibility and Throughput**; Chao Gong[1]; Wei-li Liao[1]; Jie Cheng[1]; Heather Jordan[1]; Robert Heaton[1]; Todd Hembrough[1]; *[1]NantOmics, Rockville, MD*

ThP 697 **MSGUIDE: A Mass-Spectrometry Driven Strategy for Clinical Assay Development**; Sandra Goetze[1]; Peter

Schüffler[2]; Annalisa Macagno[3]; Alcibiade Athanasiou[3]; Anja Wittig[3]; Ramy Huber[3]; Cedric Poyet[4]; Daniel Gygax[5]; Thomas Fuchs[2]; Peter Wild[4]; Ralph Schiess[3]; Bernd Wollscheid[1]; *[1]ETH Zurich, Zurich, Switzerland; [2]Memorial Sloan Kettering Cancer Center, New York, NY; [3]Proteomedix AG, Schlieren, Switzerland; [4]University Hospital Zurich, Zurich, Switzerland; [5]FHNW School of Life Sciences, Muttenz, Switzerland*

ThP 698 **Development of a Targeted Mass Spectrometry Serum Assay to Quantify M-Protein in the Presence of Therapeutic Monoclonal Antibodies**; Marina Zajec[1]; Joannes F.M. Jacobs[2]; Patricia Groenen[2]; Corrie de Kat Angelino[2]; Christoph Stingl[1]; Theo Luider[1]; Yolanda B. De Rijke[1]; Martijn M. Vanduijn[1]; *[1]Erasmus University Medical Center, Rotterdam, Netherlands; [2]Radboud University, Nijmegen, Netherlands*

ThP 699 **Single Cell Proteome Profiling and SAAVs Detection in a Panc-1 Cell Line**; Zhijing Tan[1]; Nicholas J. Carruthers[2]; Paul M. Stemmer[2]; David M. Lubman[3]; *[1]University of Michiagan, Ann Arbor, MI; [2]Wayne State University, Detroit , MI; [3]University of Michigan, Ann Arbor, MI*

ThP 700 **System-Wide Analysis of Protein Expression in Formalin-Fixed Paraffin-Embedded Rare Histological Types of Breast Cancer**; Hyeyeon Kim[1]; Min-Sun Jin[2]; Hyeyoon Kim[1, 3]; Han Suk Ryu[3]; Dohyun Han[1]; *[1]Proteomics Core Facility, Seoul National University Hospital, Seoul, South Korea; [2]Department of Pathology, Bucheon St. Mary's Hospital, College of Medicine, The Catholic University of Korea, Bucheon, South Korea; [3]Department of Pathology, Seoul National University Hospital, Seoul, South Korea*

ThP 701 **In-Depth Proteome Profiling of Formalin-Fixed Paraffin-Embedded Urothelial Carcinoma and Benign Disease Tissues**; Hyeyoon Kim[1, 2]; Hyeyeon Kim[1]; Han Suk Ryu[2]; Dohyun Han[1]; *[1]Proteomics Core Facility, Seoul National University Hospital, Seoul, South Korea; [2]Department of Pathology, Seoul National University Hospital, Seoul, South Korea*

ThP 702 **Proteomic Portraits of Localized Human Prostate Cancer**; Dorothea Rutishauser[1]; Qing Zhong[2]; Tiannan Guo[3]; Yi Zhu[3]; Niels Rupp[1]; Jan Henrik Rueschoff[1]; Laura de Varga Roditi[1]; Christian Fankhauser[1]; Thomas Hermanns[4]; Cedric Poyet[4]; Ailsa Christiansen[1]; Helena Fischer[1]; Holger Moch[1]; Andreas Beyer[5]; Ruedi Aebersold[6]; Peter Johannes Wild[1]; *[1]Department of Pathology and Molecular Pathology, University Hospital Zurich, Zurich, Switzerland; [2]Cancer Data Science Group, Children's Medical Research Institute, University of Sydney, Sydney, Australia; [3]Westlake Universtity, Hangzhou, Zhejiang, Zhejiang, China; [4]Department of Urology,University Hospital Zurich, Zurich, Switzerland; [5]Cellular Networks and Systems Biology, University of Cologne, CECAD, University of Cologne, Cologne, Germany; [6]Department of Biology, Institute of Molecular Systems Biology, ETH Zurich, Zürich, Switzerland*

ThP 703 **Discovery and Qualification of Candidate Urinary Biomarkers of Disease Activity in Lupus Nephritis**; Veronica Anania[1]; Kebing Yu[1]; Francesco Pingitore[1]; Qingling Li[1]; Christopher Rose[1]; Peter Liu[1]; Wendy Sandoval[1]; Ann E Herman[1]; Jennie R. Lill[1]; W. Rodney Mathews[1]; *[1]Genentech Inc., San Francisco, CA*

ThP 704 **Robust Quantification of FANCD2 Mono-Ubiquitination in Response to DNA Damage**; Jeffrey R. Whiteaker[1]; Lei Zhao[1]; Richard G Ivey[1]; Marilyn Sanchez-Bonilla[1, 2]; Heather D Moore[1]; Regine M Schoenherr[1]; ping Yan[1]; Chenwei Lin[1]; Akiko Shimamura[3]; Amanda G Paulovich[1]; *[1]1. Fred Hutchinson Cancer Research Center, Seattle, WA; [2]2. Seattle Children's Research Institute, Seattle, WA; [3]3. Dana-Farber/Boston Children's Cancer and Blood Disorders Center, Harvard Medical School, Boston, MA*

ThP 705 **Library Matching Enhances Proteome Coverage in Sample Limited FFPE Clinical Specimens**; Bin Fang[1]; Victoria Izumi[1]; John Koomen[1]; Joseph Markowitz[1]; *[1]H. Lee Moffitt Cancer Center, Tampa, FL*

ThP 706 **High Sensitivity Proteomics: 3,000 Proteins from 3,000 Cells in One Hour**; Dalia Elinger[1]; Silvia Carvalho[1]; Yishai Levin[1]; *[1]Weizmann Institute of Science, Rehovot, Israel*

ThP 707 **Differentiating Controls and Sarcoidosis Phenotypes in BAL-Fluid and Serum via SpotLight Proteomics**; Susanna Lundström[1]; Tina Heyder[1]; Emil Wiklundh[1]; Bo Zhang[1]; Anders Eklund[1]; Johan Grunewald[1]; Roman Zubarev[1]; *[1]Karolinska Institutet, Stockholm, Sweden*

ThP 708 **Deep Quantification of the Stem Cell Secretome Using Data-Independent Acquisition LC-MS/MS Analysis**; Jakob Vowinckel[1]; Jakub Smolar[2]; Daniel Eberli[2]; Claudia Escher[1]; *[1]Biognosys AG, Schlieren, Switzerland; [2]University Hospital Zurich, Department for Urology, Schlieren, Switzerland*

ThP 709 **Targeted Proteomic Quantitation of 4 Hormone Receptors in Formalin-Fixed Paraffin-Embedded (FFPE) Breast Cancer Tissues Using Parallel Reaction Monitoring-Mass Spectrometry (PRM-MS)**; Joonho Park[1]; Joseph I. Wang[1]; Youngsoo Kim[1]; *[1]Interdisciplinary Program for Bioengineering, Seoul National University College of Engineering, Seoul, South Korea*

ThP 710 **Rapid Classification and Identification with Accurate Statistical Significance for Microorganisms in Mixtures via High Resolution Tandem Mass Spectrometry**; Gelio Alves[1]; Guanghui Wang[2]; Aleksey Y. Ogurtsov[1]; Steven K. Drake[3]; Marjan Gucek[2]; David B. Sacks[4]; Yi-Kuo Yu[1]; *[1]National Center for Biotechnology Information, NLM, NIH, Bethesda, MD; [2]Proteomics Core, National Heart, Lung, and Blood Institute, Bethesda, MD; [3]Critical Care Medicine Department, Clinical Center, National Institutes of Health, Bethesda, MD; [4]Department of Laboratory Medicine, Clinical Center, National Institutes of Health, Bethesda, MD*

ThP 711 **Proteogenomic Analysis of Mucosa Samples from IBD Patients**; Liang Jin[1]; Chenqi Hu[1]; Yingtao Bi[1]; Li Li[1]; Ivan Mascanfroni[1]; Jesus Paez-Cortez[1]; Jing Wang[1]; Edit Tarcsa[1]; Yu Tian[1]; *[1]AbbVie, Worcester, MA*

ThP 712 **Absolute Quantitation of Apolipoprotein (a) Together with Apo A-I, B100, C-I, C-II, C-III and E Using a Multiplexed LC-MS Method**; Renee Ruhaak[1]; Yuri van der Burgt[1]; Nico P.M. Smit[1]; Fred P.H.T.M. Romijn[1]; Mervin M. Pieterse[1]; Arnoud van der Laarse[1]; Christa M. Cobbaert[1]; *[1]LUMC, Leiden, Netherlands*

ThP 713 **Global Quantitative Phosphoproteomics to Identify Mechanisms of Resistance to the third Generation EGFR TKIs in Human Lung Adenocarcinoma**; Xu Zhang[1]; Tapan Maity[1]; Karen Ross[2]; Shaojian Gao[1]; Khoa Dang Nguyen[1]; Fatos Kirkali[1]; Jacob Jaffe[3]; Michele Forlin[4]; Stephan Schürer[4]; Cathy Wu[5]; Udayan Guha[1]; *[1]Thoracic and GI Oncology Branch, CCR, NCI, NIH, Bethesda, MD; [2]Georgetown University Medical Center, Washington, D.C., Washington, D.C.; [3]Broad Institute of MIT and Harvard, Cambridge, MA; [4]University of Miami, Coral Gables, FL; [5]University of Delaware, Newark, DE*

ThP 714 **Collect Your Own Proteome: Demonstrating the Feasibility of Personal Proteome Data Collection and Analysis**; Ryan Benz[1]; Jeffrey J. Jones[1]; *[1]SoCal Bioinformatics Inc., Montrose, CA*

ThP 715 **A Novel Workflow for Label-free Quantification of Low Molecular Weight Urine Proteome**; Pamela S. Cantrell[1]; Andrea J. Detlefsen[1]; Richard T. Cattley[1]; Xuemei Zeng[1]; Nathan A. Yates[1, 2]; *[1]Biomedical Mass Spectrometry Center, University of Pittsburgh Schools of the Health Sciences, Pittsburgh, Pennsylvania; [2]Department of Cell Biology, University of Pittsburgh School of Medicine, Pittsburgh, Pennsylvania*

ThP 716 **Three's Company: Methodological Variance with Metrological Anchoring for Clinical Harmony**; WILLIAM SLADE[1]; Grace Van Der Gugten[2]; Jacqueline Luehmann[3]; Christopher M. Shuford[4]; Daniel T Holmes[2]; Ravinder Singh[3]; Stefan Grebe[3]; Russell P. Grant[4]; *[1]LabCorp, Burlington, NC; [2]St. Paul's Hospital, Vancouver, BC, Canada; [3]Mayo Clinic, Rochester, MN; [4]Laboratory Corporation of America, Burlington, NC*

ThP 717 **Quantitation of K-Ras Isoforms Using Liquid Chromatography-Tandem Mass Spectrometry (LC-MS/MS) with MRM and PRM Approaches**; Constance A. Sobsey[1, 2]; Vincent R. Richard[1, 3]; Adriana Aguilar-Mahecha[3]; Mark Basik[3]; Gerald Batist[3, 4]; Christoph H. Borchers[1, 4, 5, 6]; *[1]Jewish General Hospital Proteomics Centre, McGill University, Montreal, QC, Canada; [2]Department of Medicine, Division of Experimental Medicine, McGill University, Montreal, QC, Canada; [3]Jewish General Hospital, Segal Cancer Center, Lady Davis Institute, Montréal, QC, Canada; [4]Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC, Canada; [5]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [6]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada*

ThP 718 **Discovery and Verification of Breast Cancer Protein Biomarkers Related to Distant Metastasis**; Dongyoon Shin[1]; Joonho Park[2]; Joseph Injae Wang[2]; Youngsoo Kim[1, 2]; *[1]Biomedical science, Seoul National University, College of Medicine, Seoul, South Korea; [2]Interdisciplinary Program for Bioengineering, Seoul National University College of Engineering, Seoul, South Korea*

ThP 719 **A Rapid, Global Proteomic Screen for the Assessment of Cellular Response**; Jamie Allen[1]; Carrie E. Romer[1]; Danielle B. Gutierrez[1]; Melissa Farrow[2]; Brad Williams[3]; LeRoy Martin[4]; Jeremy L. Norris[1]; Richard M. Caprioli[1]; *[1]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [2]Department of Pathology, Microbiology, and Immunology, Vanderbilt University Medical Center, Nashville, TN; [3]Waters Corporation, Beverly, MA; [4]Waters Corporation, Milford, MA*

ThP 720 **Analysis of Limiting Protein Quantities from Formalin Fixed Paraffin Embedded (FFPE) Tumor Tissue Across Three Platforms**; Wei-Li Liao[1]; Yuan Tian[1]; Eunkyung An[1]; Kerry Hassell[2]; Eric Huang[3]; Claudia P.B. Martins[3]; Todd Hembrough[1]; *[1]NantOmics, Rockville, MD; [2]Thermo Fisher Scientific, Somerset, NJ; [3]Thermo Fisher Scientific, San Jose, CA*

ThP 721 **Targeted Data-independent Acquisition (DIA) for Mass Spectrometric Detection of RAS Mutations in Formalin-fixed, Paraffin-embedded Tumor Biopsies**; Yeoun Jin Kim[1]; Andrew G Chambers[1]; Fabiola Cecchi[1]; Todd Hembrough[1]; *[1]NantOmics, Rockville, MD*

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ThP 722 **Quantitative Affinity-Purification and Surface-Adsorption Data Independent Acquisition Mass Spectrometry (DIA-MS) in Host-Pathogen Interactions**; Lotta Happonen[1]; Simon Hauri[1]; Christofer Karlsson[1]; Magdalena Wisniewska[2, 3]; Mats Wikström[3, 4]; Lars Björck[1]; Lars Malmström[5]; Johan Malmström[1]; *[1]Lund University, Lund, Sweden; [2]Selvita, Kraków, Poland; [3]Novo Nordisk Foundation Center for Protein Research, Copenhagen, Denmark; [4]Amgen, Thousand Oaks, CA; [5]University of Zurich, Zurich, Switzerland*

ThP 723 **Deep-Proteome Coverage of Latently Infected Cells Reveals the Extent of Cellular Awareness of HIV and New Targets for Immunotherapy**; Sri H Ramarathinam[1]; Geroges Khoury[2]; Damian F.J Purcell[2]; Anthony W Purcell[1]; *[1]Department of Biochemistry and Molecular Biology, Biomedicine Discovery Institute, Monash University, Clayton, Australia; [2]Department of Microbiology and Immunology, University of Melbourne, Parkville, Australia*

ThP 724 **Phosphoproteome and Supernatant Analyses Reveal Novel Effectors of TNF Signaling**; Maria Tanzer[1]; Annika Frauenstein[1]; Felix Meissner[1]; Matthias Mann[1]; *[1]Max Planck Institute of Biochemistry, Munich, Germany*

ThP 725 **Deep Proteome Profiling of the Growth Forms of the Growth Forms of Chlamydia Trachomatis Causing Ocular Disease**; Ole Østergaard[1, 2]; Swathi Pranavi Kausika[3]; Anja Olsen[3]; Peter L. Andersen[3]; Jesper V. Olsen[1]; Frank Follmann[3]; Ida Rosenkrands[3]; *[1]NNF Center for Protein Research, Copenhagen, Denmark; [2]Department of Autoimmunology and Biomarkers, Statens Serum Institut, Copenhagen, Denmark; [3]Department of Infection Immunology, Statens Serum Insitut, Copenhagen, Denmark*

ThP 726 **Proteomic Profiling of Virulent Phase I and Avirulent Phase II of Coxiella Burnetii Employing Axenic and Cell Culture-Based Cultivation**; Jiri Dresler[1]; Katja Mertens[2]; Jana Klimentova[3]; Barbora Salovska[4]; Petr Pajer[4]; Alena Myslivcova Fucikova[3]; Martin Chmel[4]; Zuzana Krocova[3]; Libor Pisa[4]; *[1]Military Health Institute, Prague, Czech Republic; [2]Federal Research Institute for Animal Health, Jena, Germany; [3]Faculty of Military Heatlh Sciences, Hradec Kralove, Czech Republic; [4]Military Health Institute, Prague, Czech Republic*

ThP 727 **Development of a targeted peptide LC-MS method for detection of residual toxins from Bordetella pertussis**; Lisa R Szymkowicz[1, 2]; Derek J. Wilson[1]; Andrew James[1, 2]; *[1]York University, Toronto, ON, Canada; [2]Sanofi Pasteur, Toronto, ON, Canada*

ThP 728 **Metabolic Differences between Monoculture and Co-culture Pseudomonas aeruginosa and Staphylococcus aureus Compared by Label Free Quantitation Proteome Analyses**; Yeni P. Yung[1]; S. Lee McGill[2]; Stephanie M. Cologna[1]; Hui Chen[1]; Ross P. Carlson[2]; Luke Hanley[1]; *[1]University of Illinois at Chicago, Chicago, IL; [2]Montana State University, Bozeman, MT*

ThP 729 **An Integrated Proteomics and Functional Genomics Approach to Define Influenza A Viral Endonuclease Mechanisms for Host Shutoff**; Kelsey M. Haas[1, 2]; Michael J. McGregor[1, 2]; Judd F. Hultquist[1, 2]; Robyn M. Kaake[1, 2]; Danielle L. Swaney[1, 2]; Nevan J. Krogan[1, 2]; *[1]University of California San Francisco, San Francisco, CA; [2]J David Gladstone Institutes, San Francisco, California*

ThP 730 **Dissecting Nlrp3 Inflammasome Activation with Quantitative Spatial Proteomics**; Kshiti S Phulphagar[1, 2]; Daniel N. Itzhak[2]; Georg H. H. Borner[2]; Eicke Latz[1]; Felix Meissner[2]; *[1]Institute of Innate Immunity, University of Bonn, Bonn, Germany; [2]Max Planck Institute of Biochemistry, Martinsried, Germany*

ThP 731 **Mass Spectrometry-Based Affinity Proteomics Discovered Toll-Like Receptor 2 Protein Interaction Partners in TLR2 Over-Expressed HEK293 cells**; Abu Hena M Kamal[1]; Saiful M. Chowdhury[1]; *[1]University of Texas, Arlington*

ThP 732 **Discovery and Targeted Proteomics on Skin Biopsies for the Diagnosis of Tick-Borne Diseases**; Paola Cantero[1]; Antoine Grillon[2]; Benoit Westermann[1]; Ludivine Esteves-Gloria[1]; Benoit Jaulhac[2]; Nathalie Boulanger[2]; Laurence Sabatier[1]; *[1]Laboratoire de Spectrométrie de Masse BioOrganique, CNRS-IPHC UMR7178, Strasbourg, France; [2]EA7290, Virulence bactérienne précoce, groupe Borréliose de Lyme, Facultés de Médecine et de Pharmacie, Strasbourg, France*

ThP 733 **Proteomics Characterization of Chlamydia Trachomatis Virulence Plasmid Using Isobar (TMT) Labelling**; Christopher Grant[1]; Stuart McCorrister[1]; Michael Patton[2]; Harlan Caldwell[2]; Garrett Westmacott[1]; Chih-Yu Chen[1];

Grant McClarty[1]; [1]*Public Health Agency of Canada, Winnipeg, MB, Canada;* [2]*Laboratory of Clinical Microbiology and Immunology, NIAID, Bethesda, MD*

ThP 734 **Application of Multiplexed Ion Mobility-MS for Identification of Host Response Protein Signatures of Treatment of Pulmonary Tuberculosis**; Komal Kedia[1]; Jason Wendler[1]; Jon Jacobs[1]; Richard D. Smith[1]; ERIN S. BAKER[1]; Aaron T. Wright[1]; Paul D. Piehowski[1]; Marina A Gritsenko[1]; Kristin E. Burnum-Johnson[1]; Leah G. Jarsberg[2]; Mark H. Weiner[3]; Payam Nahid[2]; [1]*Pacific Northwest National Lab, Richland, WA;* [2]*UCSF, San Francisco, CA;* [3]*University of Texas Health Science Center, San Antonio, Texas*

ThP 735 **The Birth and Death of Neurons: a Proteotranscriptomic Investigation of Congenital Zika Syndrome**; Amanda J. Guise[1, 2]; Tojo Nakayama[1, 2]; Dylan Vaughan[1]; Hanno Steen[1, 2]; Ganeshwaran H. Mochida[1, 2, 3]; Judith A. Steen[1, 2]; [1]*Boston Children's Hospital, Boston;* [2]*Harvard Medical School, Boston, MA;* [3]*Massachusetts General Hospital, Boston, MA*

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ThP 736 **Improved Intact Protein Sequence Analysis by 21 Tesla FT-ICR MS/MS Drives Development of "Tuned" Mass Spectral Acquisition and Interpretation Strategies**; Lissa C. Anderson[1]; Jeffrey Shabanowitz[2]; Chad W. Weisbrod[1]; Greg T. Blakney[1]; Donald F. Hunt[2, 3]; Christopher L. Hendrickson[1, 4]; [1]*NHMFL-FSU, Tallahassee, FL;* [2]*Department of Chemistry, University of Virginia, Charlottesville, VA;* [3]*Department of Pathology, University of Virginia, Charlottesville, VA;* [4]*Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL*

ThP 737 **Constructing Human Proteoform Families in Proteoform Suite Using Intact-Mass and Top-Down Proteomics with a Multi-Protease Sample-Specific Database**; Yunxiang Dai[1]; Katherine E. Buxton[1]; Leah V. Schaffer[1]; Rachel M. Miller[1]; Stefan K. Solntsev[1]; Michael R. Shortreed[1]; Robert J. Millikin[1]; Mark Scalf[1]; Anthony J. Cesnik[1]; Brian L. Frey[1]; Lloyd M. Smith[1]; [1]*University of Wisconsin-Madison, Madison, Wisconsin*

ThP 738 **A Native Capillary Zone Electrophoresis-Mass Spectrometry Platform for Characterization of Protein Complexes and a Complex Proteome**; Xiaojing Shen[1]; Liangliang Sun[1]; [1]*Michigan State University, East Lansing, MI*

ThP 739 **Identification of Milk Proteins via Resonance Ejection Technique on inTrap MALDI Mass Spectrometry**; Shih-Chieh Yang[1]; Szu-Wei Chou[1]; Yao-Hsin Tseng[1]; Pin-Duo Lee[1]; Chun-Yen Cheng[1]; [1]*AcroMass, hsinchu, Taiwan*

ThP 740 **Innovative Mass Spectrometry to Assess the Clinical Value of Proinsulin as Early Biomarker for Diabetes**; Roel Tans[1]; Ryan Hannam[2]; Tarif Islam[2]; Bryon Ricketts[2]; Alex Davidson[2]; Stephan Bakker[3]; Jolein Gloerich[1]; Hans Wessels[1]; Alain van Gool[1]; [1]*Radboud university medical center, Nijmegen, Netherlands;* [2]*Avacta Life Sciences, Wetherby, UK;* [3]*University Medical Center Groningen, Groningen, Netherlands*

ThP 741 **Intact and Top Down Analysis of the Yeast Rpd3S Protein Complex Components on the Orbitrap Fusion Lumos Mass Spectrometer**; Michaella Levy[1]; Yan Hao[1]; Michael P. Washburn[1]; Laurence Florens[1]; [1]*Stowers Institute for Medical Research, Kansas City, MO*

ThP 742 **Microchip Capillary Electrophoresis-ESI-MS for Rapid, Multi-level Analysis of Complex Proteins**; Ashley Bell[1]; Erin Redman[2]; Aditya Kulkarni[1]; J. Scott Mellors[2]; [1]*908 Devices Inc., Boston, MA;* [2]*908 Devices, Inc., Carrboro, NC*

ThP 743 **Proteoform Profiling Workflow with Retention Time Alignment and Intensity Normalization Provides 50-fold Dynamic Range and Prediction of LOD/LOQ**; Ray Bacala[1, 2]; Katherine Cordova[1]; Helene Perreault[2]; Dave Hatcher[1]; [1]*Canadian Grain Commission, Winnipeg, MB, Canada;* [2]*Department of Chemistry, University of Manitoba, Winnipeg, Manitoba*

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ThP 744 **Investigation of Environmental *E. coli* from Marine Sediment in Their Interactions by Shotgun Proteomics**; Chun Ning Ng[1]; Long Wu[1]; Stanley Chun Kwan Lau[1]; Henry Hei Ning Lam[1]; [1]*Hong Kong University of Science and Technology, Hong Kong*

ThP 745 **Large-Scale IonStar-Based Quantification of Cortex and Hippocampus Proteomes Revealed Novel Neuroprotective Mechanisms of Two Drug Candidates Against Traumatic Brain Injury**; Shichen Shen[1]; Ming Zhang[1]; Jennifer Osei[1]; Sailee Rasam[1]; David J Poulsen[1]; Jun Qu[1]; [1]*University at Buffalo, Buffalo, NY*

ThP 746 **Importance of Analytical Replicate Analysis in Quantitative Proteomics Using Isobaric Tags**; David M. Smalley[1]; Ming Tong[1]; Fantashia Goolsby[1]; Shriprasad R. Deshpande[2, 3]; Kevin O. Maher[3, 4]; [1]*Georgia Institute of Technology, Atlanta, GA;* [2]*Children's Healthcare of Atlanta, Atlanta, GA;* [3]*Emory University School of Medicine, Atlanta, GA;* [4]*Children's Hospital of Atlanta, Atlanta, GA*

ThP 747 **The Usual Subsets: Proteomic Profiling of the Immune System**; Jens L. Hukelmann[1]; Andy Howden[1]; Laura Spinelli[1]; Alejandro Brenes[1]; Doreen A. Cantrell[1]; Angus I. Lamond[1]; [1]*University of Dundee, Dundee, UK*

ThP 748 **Tandem-Mass-Tag-Based (TMT) Quantification for Shotgun Proteomics on a Trapped-Ion-Mobility quadrupole-Time-Of-Flight Mass Spectrometer (TIMS-QTOF) powered by Parallel-Accumulation and SErial-Fragmentation (PASEF)**; Markus Lubeck[1]; Scarlet Koch[1]; Heiner Koch[1]; Florian Meier[2]; Andreas-David Brunner[2]; Niels Goedecke[1]; Matthias Mann[2]; Oliver Raether[1]; [1]*Bruker Daltonik GmbH, Bremen, Germany;* [2]*Max Planck Institute of Biochemistry, Martinsried, Germany*

ThP 749 **Quantification of Platelet Biomarkers by Targeted Mass Spectrometry**; Sebastian Malchow[1]; Christina Loosse[1]; Albert Sickmann[1, 2, 3]; Christin Lorenz[1]; [1]*Leibniz-Institut für Analytische Wissenschaften-ISAS-e.V., Dortmund, Germany;* [2]*Medizinisches Proteom-Center, Ruhr-Universität, Bochum, Germany;* [3]*Department of Chemistry, College of Physical Sciences, University of Aberdeen, Aberdeen, UK*

ThP 750 **Glycoproteomics Characterization of the Stable Isotope Labeled HepG2 Secretome**; Emmanuel Kenneth Cudjoe[1]; Adam M Hawkridge[1]; [1]*Virginia Commonwealth University School of Pharmacy, Richmond, VA*

ThP 751 **A Universal Standard Approach for Host Cell Protein Accurate Label-Free Quantification**; Mathieu Trauchessec[1]; Guillaume Cognet[1]; Christelle Jacquet[1]; Quentin Enjalbert[1]; Xavier Homo-Prault[1]; Chloé Bardet[1]; Tanguy Fortin[1]; [1]*ANAQUANT, Villeurbanne, France*

ThP 752 **Determining and Characterizing Substrates of Impaired Protein Degradation in Models of Alzheimer's Disease**; Timothy Hark[1]; Yi-Zhi Wang[1]; Samuel N. Smukowski[1]; Laith Ali[1]; Jeffrey N. Savas[1]; [1]*Northwestern University, Chicago, IL*

ThP 753 **Developing an Assay to Quantify Nuclear Receptors by Mass Spectrometry**; Michael Saikali[1]; Carolyn L Cummins[1]; [1]*Leslie Dan Faculty of Pharmacy, University of Toronto, Toronto, ON, Canada*

ThP 754 **Abundant Protein Depletion of Human Plasma Samples – Sample Preparation Approaches for Quantitative Comparison Studies**; Sergei Snovida[1]; Katherine Herting[1]; Ramesh Ganapathy[1]; Ryan Bomgarden[1]; Barbara Kaboord[1]; Chris Etienne[1]; John C. Rogers[1]; [1]*Thermo Fisher Scientific, Rockford, IL*

ThP 755 **Integrated Genetic and Proteomic Analysis Identifies PLK1 as a Candidate Therapeutic Target for SETD2-Deficient Clear Cell Renal Cell Carcinoma**; Lin LI[1]; Weili Miao[1]; Ming Huang[2]; Preston Williams[1]; Yinsheng Wang[1, 2]; *[1]Department of Chemistry, University of California, Riverside, Riverside, CA; [2]Environmental Toxicology Graduate Program, University of California, Riverside, Riverside, California*

ThP 756 **Proteome-wide Discovery of Isoprenoid Pyrophosphate-Binding Proteins**; Rong Cai[1]; Yinsheng Wang[1]; *[1]University of California, Riverside, Riverside, CA*

ThP 757 **Targeted Quantitative Proteomic Profiling of Small GTPase Regulators-Discovery of Drivers and Suppressors for Melanoma Metastasis**; Tianyu Qi[1]; Weili Miao[1]; Ming Huang[1]; Yinsheng Wang[1]; *[1]UC Riverside, Riverside, CA*

ThP 758 **Evaluation of a High-Flow LC-MRM Analysis for a Highly Multiplexed Targeted-Discovery Synaptosomal Proteomic Panel**; Greg M. Waitt[1]; Tyler W. Bradshaw[2]; Tricia C. Ho[1]; Scott Soderling[3]; M. Arthur Moseley[1]; Erik J. Soderblom[1]; *[1]Duke University School of Medicine, Proteomics and Metabolomics Shared Resource, Durham, NC; [2]Duke University School of Medicine, Deparment of Neurobiology, Durham, NC; [3]Duke University School of Medicine, Deparments of Cell Biology and Neurobiology, Durham, NC*

ThP 759 **Quantifying the Effects of 2'-Hydroxyflavanone Treatment in Breast Cancer Cells by TMT 10-plex Proteomics**; Lokesh Nagaprashanta[1]; Gabriel B Gugiu[2]; Helen Ge[2]; Roger Moore[2]; Shireen Chikara[1]; Sharad Singhal[1]; *[1]City of Hope, Medical Oncology, Monrovia, CA; [2]City of Hope, Shared Resources, Duarte, CA*

ThP 760 **Active Kinase Characterization in Cancer Cell Line using an Isobaric Labeling Activity-Correlated Protein Profiling Platform (TMT-ACPP)**; Hongyan Ma[1]; Morgan Mann[1]; Paul Sims[1]; Alethia Li[1]; Katie Thorisch[1]; Willow Arana[1]; Si Wu[1]; *[1]University of Oklahoma, Norman, OK*

ThP 761 **Isobaric Labeling-Based Quantitative Studies of Protein Expression and N-glycosylation of AT-1 sTg Mouse Model Reveal Molecular Basis of Aging**; Yusi Cui[1]; Inca Dieterich[1]; Timothy W. Rhoads[1]; Zhengwei Chen[1]; Rozalyn Anderson[1]; Luigi Puglielli[1]; Lingjun Li[1]; *[1]University of Wisconsin–Madison, Madison, WI*

ThP 762 **Super-SILAC Analysis Reveals Sex Differences in Alcohol-Induced Microglial Activation: Potential Link to Anxiety Development after Chronic Alcohol Exposure in Mice**; Jennifer Guergues[1]; Meera Rath[2]; Joao P. C. Pinho[1]; Truc G. Nguyen[2]; Ping Zhang[2]; Joanna P. Peris[2]; Jay P. McLaughlin[2]; Kaley MacFadyen[2]; Bin Liu[2]; Stanley M. Stevens[3]; *[1]University of South Florida, Tampa, FL; [2]University of Florida, Gainesville, FL; [3]Albany College of Pharmacy and Health Sciences, Colchester, VT*

ThP 763 **An Optimized Analytical Platform for Mapping Ligandable Binding Pockets Using Covalent Ligands**; Jason Murphy[1]; Scott Brittain[1]; Claude Shelton[1]; Jennifer Lipps[1]; Lynn Mcgregor[1]; Michael Jones[1]; Markus Schirle[1]; Jason Thomas[1]; *[1]Novartis Institutes for BioMedical Research, Inc., Cambridge, MA*

ThP 764 **Identification of Binding Proteins for Histone H3 Binary Modification K4me1K27ac in M Phase Through SILAC-Based Quantitative Proteomics**; Minghui Chen[1]; Congcong Lu[1]; Simone Sidoli[1]; Benjamin A. Garcia[1]; *[1]University of Pennsylvania, Philadelphia, PA*

ThP 765 **Advantages of Multiplexing MS Data Processing Tools on Protein Identification and Quantitation**; Ying Zhang[1]; Zhihui Wen[1]; Michael P. Washburn[1, 2]; Laurence Florens[1]; *[1]Stowers Institute for Medical Research, Kansas City, MO; [2]Department of Pathology and Laboratory Medicine, University of Kansas Medical Center, Kansas City, Missouri*

ThP 766 **Protein Abundance Inference for Shotgun Proteomics: Single vs. Mashed Measurement**; Mai Sun[1]; Xuemei Zeng[1]; Nathan A. Yates[1, 2]; *[1]Biomedical Mass Spectrometry Center, University of Pittsburgh Schools of the Health Sciences, Pittsburgh, Pennsylvania; [2]Department of Cell Biology, University of Pittsburgh School of Medicine, Pittsburgh, PA*

ThP 767 **A High-Multiplex PRM Assay for Global Kinase Quantification and Pan-cancer Analyses**; Robert Sprung[1]; Petra Erdmann-Gilmore[2]; Qiang Zhang[2]; Sherri R Davies[2]; John A Wrobel[3]; Rose Connors[2]; Yiling Mi[2]; Gary Johnson[3]; Katherine Fuh[2]; David Mutch[2]; R. Reid Townsend[2]; *[1]Washington University School of Medicine, St. Louis, MO; [2]Washington University School of Medicine, St Louis, MO; [3]University of North Carolina, Chapel Hill, NC*

ThP 768 **Assessing Donor Secretome Variability of Lung Spheroid Cells Using LC/MS/MS Analysis**; Dipti Paudel[1]; Phuong-Uyen Dinh[1]; Jhon Cores[1]; Kevin Blackburn[1]; Ke Cheng[1]; Michael Goshe[1]; *[1]NC State University, Raleigh, NC*

PROTEOMICS: TISSUE
769-792

ThP 769 **Proteomic Analysis of FFPE Tissue Using Laser Ablation Sampling**; Fabrizio Donnarumma[1]; Michael E Pettit[2]; Kelin Wang[1]; Touradj Solouki[2]; Kermit K. Murray[1]; *[1]Louisiana State University, Baton Rouge, LA; [2]Baylor University, Waco, TX*

ThP 770 **Influence of Intestinal Flora on the Hepatic Function of Drug, Glucose and Lipid Metabolism**; Takuya Kuno[1]; Shingo Ito[1]; Sumio Ohtsuki[1]; *[1]Kumamoto University, Kumamoto, Japan*

ThP 771 **Quantitative Microproteomics for the Characterization of Central and Peripheral Nervous System of the Twitcher mouse**; Davide Pellegrini[1, 2]; Ambra Del Grosso[1, 3]; Lucia Angella[3]; Nadia Giordano[4, 5]; Ilaria Tonazzini[3]; Matteo Caleo[4]; Marco Cecchini[1, 3]; Liam A. McDonnell[2, 6, 7]; *[1]NEST, Scuola Normale Superiore, Pisa, Italy; [2]Fondazione Pisana per la Scienza - ONLUS, Pisa, Italy; [3]NEST, Nanoscience Institute - CNR, Pisa, Italy; [4]Neuroscience Institute - CNR, Pisa, Italy; [5]Scuola Normale Superiore, Pisa, Italy; [6]Center for Proteomics and Metabolomics, Leiden University Medical Center, Leiden, Netherlands; [7]Department of Pathology, Leiden University Medical Center, Leiden, Netherlands*

ThP 772 **Liquid Extraction Surface Analysis Mass Spectrometry Imaging for Top-Down and Bottom-Up Investigation of Protein Biomarkers in Renal Fibrosis**; Emma K. Sisley[1, 2]; Tim Johnson[3]; Peter Hall[3]; Iain B. Styles[4]; Helen J. Cooper[2]; *[1]Physical Sciences for Health Centre for Doctoral Training, University of Birmingham, UK; [2]School of Biosciences, University of Birmingham, UK; [3]UCB Pharma Ltd, Slough, UK; [4]School of Computer Science, University of Birmingham, UK*

ThP 773 **The Key to Big Biobanks: Analyzing 24 Proteomes per Day by Micro-Flow SWATH® Acquisition and Spectronaut Analysis**; Jan Muntel[1]; Roland Bruderer[1]; Lukas Reiter[1]; *[1]Biognosys AG, Schlieren, Switzerland*

ThP 774 **Large Scale Tissue Immunopeptidomics; Challenges and Opportunities**; Ricardo Carreira[1]; Geert Mommen[1]; Michael Cundell[1]; David Lowne[1]; Floriana Capuano[1]; Alex Powlesland[1]; *[1]Immunocore Ltd, Abingdon, UK*

ThP 775 **A Mutation in PNPLA3 Alters the Lipid Droplet Proteome**; Jeffrey A. Culver[1]; Sharath P. Sasi[2]; Collin P. Crowley[2]; Trenton T. Ross[2]; Gregory J. Tesz[2]; Kendra K. Bence[2]; Thomas V. Magee[2]; Michelle F. Clasquin[2]; Mara Monetti[2]; *[1]Pfizer, Cambridge, MA; [2]Pfizer, Cambridge, MA*

ThP 776 **Proteomic Atlas of the Human Brain in Alzheimer's Disease**; Justin McKetney[1]; Rosie Runde[1, 2]; Subhojit Roy[2]; Joshua J Coon[1]; *[1]University of Wisconsin-Madison, Madison, WI; [2]Wisconsin Institute for Medical Research, Madison, WI*

ThP 777 **Quantitative Profiling of Neurofibrillary Tangles and Pathologic Tau Identifies Diagnostic Signatures Specific to Dementia Related Tauopathy Diseases**; Hendrik Wesseling[1]; Waltraud Mair[1]; Shaojun Tang[2]; Judith A. Steen[1]; Hanno Steen[1]; *[1]Boston Children's Hospital and Harvard Medical School, Boston, MA; [2]Georgetown University, Washington, DC*

ThP 778 **MS-Based Analysis Identifies that Skeletal Muscle-Specific Methyltransferase METTL21C Trimethylates p97 and Regulates Autophagy-Associated Protein Breakdown**; Janica L Wiederstein[1]; Hendrik Nolte[1]; Stefan Günther[2]; Tanja Piller[3]; Marco Sandri[4]; Bert Blaauw[4]; Thomas Braun[2]; Soraya Hölper[2, 5]; Marcus Krüger[1]; *[1]CECAD Research Center/ University of Cologne, Köln, Germany; [2]Max Planck Institute for Heart and Lung Research, Bad Nauheim, Germany; [3]Goethe University, Institute of Biochemistry, Frankfurt am Main, Germany; [4]Venetian Institute of Molecular Medicine, Padua, Italy; [5]Sanofi, Frankfurt, Germany*

ThP 779 **Getting to the Heart of the Matter: Multispecies Heart Tissue Proteome Characterization**; Joel D. Federspiel[1]; Caralynn M. Wilczewski[2]; Laura E. Herring[2]; Samvida Venkatesh[1]; Lauren Wasson[2]; Frank L. Conlon[2]; Ileana M. Cristea[1]; *[1]Princeton University, Princeton, NJ; [2]University of North Carolina at Chapel Hill, NC*

ThP 780 **Dynamics of Zebrafish Heart Regeneration Using an HPLC-ESI-MS/MS Approach**; Danjun Ma[1]; Baixuan Cheng[2]; Lingxiao Chen[2]; *[1]Dongguan University of Technology, Dongguan, China; [2]Dongguan University of Technology, China*

ThP 781 **The Role of MMP-28 in Autoimmune Neurodegenerative Diseases Revealed by Whole Proteome Profiling**; Dorota Tokmina-Roszyk[1]; Lillian Onwuha-Ekpete[1]; Mohammed Refai[2]; Monika Tokmina-Lukaszewska[2]; Brian Bothner[2]; Gregg Fields[1]; *[1]Florida Atlantic University, Jupiter, FL; [2]Montana State University, Bozeman, MT*

ThP 782 **Direct Molecular Dissection of Tumor Parenchyma from Tumor Stroma in Human-Mouse Tumor Xenografts Using MS-Based Glyco-Proteomics**; Xiaoying Ye[1]; Brian T Luke[1]; Bih-Rong Wei[1]; Jan A Kaczmarczyk[1]; Donald J Johann[2]; Richard G Saul[1]; Gordon R Whiteley[1]; Josip Blonder[3]; *[1]Fredrick National Laboratory for Cancer reserach, Frederick, Maryland; [2]Winthrop P. Rockefeller Cancer InstituteMyeloma Institute, University of Arkansas for Medical Sciences,, Little Rock, Arkansas; [3]Frederick Nat'l Lab for Cancer Research, Frederick, MD*

ThP 783 **Development of Synthetic RORγ Modulators to Enhance Protective Immunity**; Mi Ra Chang[1]; Patrick R. Griffin[1]; *[1]The Scripps Research Institute, Jupiter, Florida*

ThP 784 **Proteomic Analysis of the Lake Trout (Salvelinus Namaycush)**; Emmalyn Dupree[1]; Bernard Crimmins[2]; Thomas Holsen[2]; James Pagano[3]; Costel C. Darie[1]; *[1]Biochemistry and Proteomics Group, Department of Chemistry and Biomolecular Science, Clarkson University, Potsdam, NY; [2]Department of Civil and Environmental Engineering, Clarkson University, Potsdam, NY; [3]Environmental Research Center, Suny Oswego, NY*

ThP 785 **Deep Proteome Mining of FFPE Tissue Using HILIC Peptide Enrichment Followed by PASEF Technology**; Kratika Singhal[1]; Christopher M Adams[1]; Ryan D Leib[1]; Allis S Chien[1]; *[1]Stanford University Mass Spectrometry, Stanford, CA*

ThP 786 **Proteome-Wide Mapping of Phosphorylation Sites and Quantitative Analysis of Post-Natal Heart Development**; Clara Tuerk[1]; Sriram Aravamudhan[2]; Hendrik Nolte[3]; Marcus Krüger[3]; *[1]University of Cologne, CECAD, Cologne, Germany; [2]Cell Signaling Technology, Danvers, MA; [3]CECAD Research Center/ University of Cologne, Köln, Germany*

ThP 787 **Proteome Characterization of Neurofibrillary Tangles And Amyloid Plaques From Alzheimer's Disease post mortem FFPE tissue**; Shruti Nayak[1]; Eleanor Drummond[2]; Manor Askenazi[3]; Thomas Wisniewski[2]; Beatrix M. Ueberheide[4]; *[1]NYULMC, New York, NY; [2]NYU Langone Health, New York, NY; [3]Biomedical Hosting LLC, Arlington, MA; [4]NYU Langone Health, Proteomics Laboratory, New York, NY*

ThP 788 **Quantitative Proteomics to Elucidate the Role of Sirt2 in Alleviation of Chemotherapy-Induced Peripheral Neuropathy**; Renny Shang-Lun Lan[1]; Manchao Zhang[2]; Wuying Du[2]; Xin Zhao[2]; Samuel Mackintosh[2]; Ricky Edmondson[2]; Reid D Landes[2]; Aaron Storey[2]; Alan J Tackett[2]; Fen Xia[2]; *[1]University of Arkansas for Medical Sciences, Little Rock, AR; [2]University of Arkansas for Medical Sciences, Little Rock, Arkansas*

ThP 789 **Proteome Reveals the Regulation of Broilers Hypothalamus Under Acute Heat Stress Based on iTRAQ-Coupled 2D-LC-MS/MS Analysis**; Yan Xiong[1, 2]; Ying Zhou[1]; Qingshi Meng[1]; Zhen Liu[1]; Qixiang Miao[1]; Jie Gao[1]; Xiaohui Feng[1]; Minhong Zhang[1]; Hongfu Zhang[1]; Xiangfang Tang[1]; *[1]State Key Laboratory of Animal Nutrition, Institute of Animal Science; Chinese Academy of Agricultural Sciences, Beijing, China; [2]Analytical and Testing Center, Beijing Institute of Technology, Beijing, China*

ThP 790 **Mass Spectrometry Based Quantitative Map of Human Tissue Proteome**; Lihua Jiang[1]; Meng Wang[1]; Shin Lin[2]; Ruiqi Jian[1]; Joanne Chan[1]; Xiao Li[1]; Huaying Fang[1]; Hua Tang[1]; Michael Snyder[1]; *[1]Stanford University, School of Medicine, Department of Genetics, Stanford, California; [2]University of Washington, Seattle, WA*

ThP 791 **Proteomics Analysis Reveals Cecum Nutritional Regulation in Response to Piglet-Weanling Stress**; Dan Feng[1]; Qingshi Meng[1]; Xiaohui Feng[1]; Xiangfang Tang[1]; Hongfu Zhang[1]; *[1]State Key Laboratory of Animal Nutrition, Institute of Animal Science; Chinese Academy of Agricultural Sciences, Beijing, China*

ThP 792 **Probing the Molecular Regulation of Lipopolysaccharide Stress in Piglet Liver by Comparative Proteomics Analysis**; Bing Xia[1]; Qingshi Meng[1]; Xiaohui Feng[1]; Xiangfang Tang[1]; Sheng Zhang[2]; Hongfu Zhang[1]; *[1]State Key Laboratory of Animal Nutrition, Institute of Animal Science; Chinese Academy of Agricultural Sciences, Beijing, China; [2]Institute of Biotechnology, Cornell University, Ithaca, NY*

PROTEOMICS: TOP DOWN ANALYSIS II
793-815

ThP 793 **Quantitative Top Down Proteomics of Histone H4**; Matthew V. Holt[1]; Tao Wang[1]; Nicolas L. Young[1]; *[1]Baylor College of Medicine, Houston, TX*

ThP 794 **Multi-Dimensional Liquid Chromatography Enabled Top-Down Proteomics for Comprehensive Analysis of Cancer Proteome**; Samantha J. Knott[1]; Trisha Tucholski[1]; David Inman[2]; Suzanne Ponik[2]; Ying Ge[2, 3]; *[1]The University of Wisconsin Madison-Department of Chemistry, WI; [2]The University of Wisconsin Madison- Department of Cell and Regenerative Biology, WI; [3]The University of Wisconsin Madison - Human Proteomics Training Program, WI*

ThP 795 **Automatic Selection of Discriminative Top-Down Mass Spectra with Diagno-Top: Application to the Differentiation of Enterobacterial Pathogens**; Diogo Borges Lima[1]; Mathieu Dupré[1]; André R F Silva[2]; Christian Malosse[1]; Magalie Duchateau[1]; Valmir C Barbosa[3]; Paulo C Carvalho[2, 4]; Julia Chamot-Rooke[1]; *[1]Mass Spectrometry for Biology Unit, CNRS USR 2000, Institut Pasteur, France; [2]Group for Computational Mass Spectrometry & Proteomics, Carlos Chagas Institute, Fiocruz, Brazil; [3]Systems Engineering and Computer Science Program, Federal University of Rio de Janeiro, Brazil; [4]Laboratory of Toxinology, Fiocruz, Brazil*

ThP 796 **Determination of Neuropeptides-Human Brain Gangliosides Noncovalent Interactions by Microfluidics Tandem Mass Spectrometry**; Adrian-Cristian Robu[1, 2]; Mirela Sarbu[1]; Željka Vukelić[3]; Alina D. Zamfir[1]; *[1]Mass Spectrometry Laboratory, National Institute for Research and Development in Electrochemistry and Condensed Matter, Timisoara, Romania, Timisoara, Romania; [2]Faculty of Physics, West University of Timisoara, Timisoara, Romania, Timisoara, Romania; [3]Department of Chemistry and Biochemistry, Faculty of Medicine, University of Zagreb, Zagreb, Croatia, Zagreb, Croatia*

ThP 797 **Deep Top-Down Proteomics Using Capillary Zone Electrophoresis-Tandem Mass Spectrometry: Identification of 5 700 Proteoforms from the *Escherichia coliproteome***; Eli McCool[1]; Liangliang Sun[1]; *[1]Michigan State University, East Lansing, MI*

ThP 798 **Supercharging and Multiple Reaction Mode Optimization of High Molecular Weight Intact Proteins Using Triple Quadrupole Mass Spectrometry**; Kevin A. Schug[1]; Durga D. Khanal[1]; Yehia Z. Baghdady[1]; Benjamin J. Figard[2]; *[1]Department of Chemistry and Biochemistry, The University of Texas at Arlington, TX; [2]Shimadzu South Central Region (SCN), Houston, TX*

ThP 799 **Top-Down Mass Spectrometry Analysis of Branched Proteins**; Fabio Gomes[1]; Dapeng Chen[1]; Dulith Abeykoon[1]; Betsegaw Lemma[1]; Yan Wang[2]; David Fushman[1]; Catherine Fenselau[1]; *[1]Department of Chemistry and Biochemistry, University of Maryland, College Park, MD; [2]Proteomic Core Facility, University of Maryland, College Park, MD*

ThP 800 **Hybrid ECD Methods for Middle-Down And Top-Down Proteomics Implemented in a Benchtop Quadrupole-Orbitrap Mass Spectrometer**; Yury V. Vasil'ev[1, 2]; Valery G. Voinov[1, 2]; Neha Malhan[3]; Nathan I. Lopez[1, 2]; Joseph S. Beckman[1, 2]; Jared B. Shaw[3]; *[1]Linus Pauling Institute, Oregon State University, Corvallis, OR; [2]e-MSion, Inc., Corvallis, OR; [3]PNNL, Richland, WA*

ThP 801 **Top-Down Proteomics of Large Proteins Enabled by Serial Size Exclusion Chromatography and Ultra-high Resolution Mass Spectrometry**; Trisha Tucholski[1]; Samantha J. Knott[1]; Ying Ge[1]; *[1]University of Wisconsin-Madison, Wisconsin*

ThP 802 **pTop 2.0 Enables Precise Identification and Quantification for Large-Scale Proteoforms in Top-Down Proteomics**; Ruixiang Sun[1]; Ruimin Wang[1]; Zhenzhen Wang[1]; Chao Liu[1]; Hao Chi[1]; Simin He[1]; *[1]Institute of Computing Technology, Chinese Academy of Sciences, Beijing, China*

ThP 803 **Novel Bridged Hybrid Monoliths Coupled to Mass Spectrometry for Top-Down Proteomics**; Yu Liang[1, 2]; Trisha Tucholski[2]; Ci Wu[1]; Xudong Zhu[1]; Zhen Liang[1]; Lihua Zhang[1]; Ying Ge[2]; Yukui Zhang[1]; *[1]CAS Key Lab of Separation Sciences for Analytical Chemistry, National Chromatographic Research and Analysis Center, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China; [2]Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI*

ThP 804 **Enhancing Sensitivity of Top-Down LC/MS-Based Cardiac Troponin Assay**; Yanlong Zhu[1]; Yutong Jin[1]; Ziqing Lin[1]; Bifan Chen[1]; Ying Ge[1]; *[1]University of Wisconsin-Madison, Madison, Wisconsin*

ThP 805 **Capillary amideHILIC-HRMS: A New Sensitive Tool for Top-Down/Middle-Up Analysis of Complex Protein Mixtures and Glycoproteins**; Andrea Gargano[1, 2]; Thomas Senard[3]; Gestur Vidarsson[4]; Guusje van Schaick[2]; Manfred Wuhrer[3]; Elena Domínguez-Vega[3]; David Falk[3]; Govert W. Somsen[1, 2]; *[1]Center for Analytical Science Amsterdam, Amsterdam, Netherlands; [2]Vrije Universiteit Amsterdam, Amsterdam, Netherlands; [3]Center for Proteomics and Metabolomics, Leiden University, Leiden, Netherlands; [4]Dept. Experimental Immunohematology, Sanquin Research and Landsteiner Laboratory, Academic Medical Center, Amsterdam, Netherlands*

ThP 806 **Enhanced Sequence Coverage of Proteins and Novel Fragmentation Pathways in Electron Directed Ion Activation on the Omnitrap Platform**; Dimitris Papanastasiou[1]; Alexander Lekkas[1]; Emmanuel Raptakis[1]; Luciano Di Stefano[2]; Roman Zubarev[2]; *[1]Fasmatech, Athens, Greece; [2]Karolinska Institutet, Stockholm, Sweden*

ThP 807 **Evaluation of Novel FAIMS Technology for Intact Protein Detection and Characterization by Infusion**; Susan E. Abbatiello[1]; Jason Neil[1]; William McGee[1]; Scott Kronewitter[1]; Michael Belford[2]; Jim Stephenson[1]; Mary Blackburn[2]; *[1]Thermo Scientific, Cambridge, MA; [2]Thermo Scientific, San Jose, CA*

ThP 808 **Top-Down Proteomics in Biotherapeutics: Characterization of Intact Nanobodies**; Mar Vilanova[1]; Salvador Guardiola[1]; Monica Varese[1]; Laura Villarreal[1]; Mireia Díaz-Lobo[1]; Macarena Sanchez-Navarro[1]; Meritxell Teixidó[1]; Ernest Giralt[1, 2]; Marina Gay[1]; Marta Vilaseca[1]; *[1]Institute for Research in Biomedicine (IRB Barcelona), The Barcelona Institute of Science and Technology, Barcelona, Spain; [2]Department of Organic Chemistry, University of Barcelona, Spain*

ThP 809 **Exploitation of the Aspartic Acid Effect in Top-Down Protein Identification**; David Foreman[1]; Eric Dziekonski[2]; Scott A McLuckey[1]; *[1]Purdue University, West Lafayette, IN; [2]Sciex, Concord, ON, Canada*

ThP 810 **21T Space Charge and Peak Capacity Enables Mixed (Chimeric) Ion Loading for Top-down Proteomics**; Chad R. Weisbrod[1]; Lissa C Anderson[1]; Greg T. Blakney[1]; Caroline J. DeHart[2]; Christopher L Hendrickson[1, 3]; *[1]National High Magnetic Field Laboratory, Tallahassee, FL; [2]Northwestern University, Evanston, IL; [3]Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL*

ThP 811 **Combining Top-Down and Bottom-Up Proteomic Approaches for Comprehensive Analysis of Allergenic Nut Extracts**; Natalia Gasilova[1]; Mikaël Frossard[2]; Hubert H. Girault[2]; Laure Menin[3]; *[1]EPFL SB ISIC-GE, Sion, Switzerland; [2]EPFL Valais, Sion, Switzerland; [3]EPFL SB ISIC-GE, Lausanne, Switzerland*

ThP 812 **Relative Quantitation of Proteoforms Secreted by Mechanical Stimulation of Mouse Skin Using Complementary Top Down Mass Spectrometry Analysis Workflows**; Francie Moehring[1]; Matthew Waas[1]; Theodore R. Keppel[1]; Deepali Rathore[1]; Ashley M. Cowie[1]; Cheryl L. Stucky[1]; Rebekah L. Gundry[1]; *[1]Medical College of Wisconsin, Milwaukee, WI*

ThP 813 **Crotoxin Multiproteoform Complexes by Top-Down Proteomics**; Larissa D A Silva[1]; Fabio C S Nogueira[1]; Gilberto B Domont[1]; Rafael D Melani[1]; *[1]Proteomics Unit, Universidade Federal do Rio de Janeiro, Rio de Janeiro, Brazil*

ThP 814 **Method Development for Quantitation of Oxidative Proteomics- A Top Down Approach**; Surendar Tadi[1]; Joshua S. Sharp[1]; *[1]UNIVERSITY OF Mississippi, Oxford, MS*

ThP 815 **High pH for Reversed Phase Separation of Intact Proteins in Top-Down Proteomics**; Yehia Z. Baghdady[1]; Kevin A. Schug[1]; *[1]Department of Chemistry and Biochemistry, The University of Texas at Arlington, TX*

SMALL MOLECULES: QUALITATIVE ANALYSIS
816-837

ThP 816 **Improved Orbitrap Tribrid MS for PharmaceuticalImpurity Identification**; Fenghe Qiu[1]; Kate Comstock[2]; Seema Sharma[2]; Graeme McAlister[2]; *[1]Boehringer Ingelheim Pharmaceuticals, Inc., Ridgefield, CT; [2]Thermo Fisher Scientific, San Jose, CA*

ThP 817 **Microsampling, DART-MS, and GC-MS of Metal Soap Protrusions on Aged Oil Paintings**; G. Asher Newsome[1];

Christine Romano[1]; Thomas F. Lam[1]; Jia-Sun Tsang[1]; *[1]Smithsonian Institution Museum Conservation Institute, Suitland, MD*

ThP 818 **Towards the Improvement of the Stability of 2-Thioxothiazolidine-4-Carboxylic Acid Metabolite of Carbon Disulfide Exposure**; Katharine G Roland[1]; Deepak Bhandari[1]; Víctor R. De Jesús[1]; Benjamin C. Blount[1]; *[1]Division of Laboratory Sciences, National Center for Environmental Health, U.S. Centers for Disease Control & Prevention, Atlanta, GA*

ThP 819 **Characterization of Sulfonated Oleic Acid Products and Determination of the Concentration of Oligomers by Liquid Chromatography-High Resolution Mass Spectrometry**; Xiaodong Huang[1]; Jianjun Liu[1]; *[1]Ecolab, Naperville, IL*

ThP 820 **Development of a Non-Targeted UPLC/HR-MS Screening Approach for the Analysis of Tattoo INKS**; Christine M. Fisher[1]; Clark D. Ridge[1]; Caitlin N. Kneapler[1]; Timothy R. Croley[1]; Ann M. Knolhoff[1]; *[1]FDA-CFSAN, College Park, MD*

ThP 821 **Class-Targeted Metabolic Profiling Approach for Determination of Known and Novel Ergot Alkaloids Produced by Atypical Ergot Fungi Collected from Ethiopia**; Asnake Desalegn[1, 2]; Dawit Abate[1]; Kris Audenaert[2]; Sarah De Saeger[2]; José Diana Di Mavungu[2]; *[1]Addis Ababa University, Addis Ababa, Ethiopia; [2]Ghent University, Ghent, Belgium*

ThP 822 **Subcritical Water Processing of Proteins: Identification of antioxidant products by tandem mass spectrometry**; Thomas Powell[1]; Helen J Cooper[1]; Steve Bowra[2]; *[1]University of Birmingham, Birmingham, UK; [2]Phytatec UK, Aberystwyth, UK*

ThP 823 **An Extractable and Leachable Approach to Understanding Potential Chemical Exposure From Consumer Goods**; Vincent P. Sica[1]; Kady L Krivos[1]; Songtao Zhou[1]; Carrie Spitzmueller[2]; Kara Woeller[2]; Joan M. Abbinante-Nissen[2]; Susan P. Felter[1]; Timothy R. Baker[1]; Kenneth R. Wehmeyer[1]; *[1]Procter and Gamble, Mason, Ohio; [2]Procter and Gamble, Cincinnati, Ohio*

ThP 824 **Metabolic Profiling and Footprinting of Hydrophilic Metabolites In Cancer Cells by Ion Chromatography Coupled With High Resolution Mass Spectrometry**; Masatomo Takahashi[1]; Yoshihiro Izumi[1]; Takahiro Suzuki[2]; Kousuke Hata[1]; Kohta Nakatani[1]; Kiyotaka Oshikawa[1]; Kentaro Takahara[2]; Masaki Matsumoto[1]; Takeshi Bamba[1]; *[1]Medical Institute of Bioregulation, Kyushu University, Fukuoka, Japan; [2]Thermo Fisher Scientific Japan, Shibaura Minato-ku, Japan*

ThP 825 **Impurity Profiling of Amiodarone Stability Study Samples Using DAD and Accurate Mass Analysis with Automated Software Processing**; Daniel Warren[1]; Robert Proos[1]; Ian Moore[2]; Matthew Thompson[3]; *[1]Sciex, Framingham, MA; [2]Sciex, Concord, ON, Canada; [3]Alphora Research Inc, Mississauga, ON, Canada*

ThP 826 **Characterization of Glutathione Adducts of Chalcones and Quinolinone-Chalcones by Liquid Chromatography–Electrospray Ionization Mass Spectrometry**; Giulio Demetrius Creazzo d'Oliveira[1]; Pál Perjési[2]; Caridad Noda Pérez[1]; Laszlo Prokai[3]; *[1]Universidade Federal de Goiás, Goiânia, Brazil; [2]University of Pécs, Pécs, Hungary; [3]University of North Texas Health Science Center, Fort Worth, TX*

ThP 827 **Structure Elucidation of Challenging Synthetic Molecules to Drive Process Development and Critical Impurity Characterization and Control**; Steve A Osgood[1]; Tawnya Flick[1]; *[1]Amgen, Inc., Thousand Oaks, CA*

ThP 828 **Optimized MSn Workflow for Improved Structure Elucidation of Pharmaceutically Relevant Extractables and Leachables**; Seema Sharma[1]; Kate Comstock[1]; Douglas E. Kiehl[2]; Graeme McAlister[1]; Ryo Komatsuzaki[1]; Caroline Ding[1]; Ralf Tautenhahn[1]; Derek J. Bailey[1]; Linda Lin[1]; Tim Stratton[1]; Shannon Eliuk[1]; Iman Mohtashemi[1]; Jonathan L. Josephs[1]; Vlad Zabrouskov[1]; Jenny Berryhill[1]; *[1]Thermo Scientific, San Jose, CA; [2]Eli Lilly and Company, IN*

ThP 829 **Pharmaceutical Stability Testing by Online Electrochemistry-LC-MS**; Hendrik-Jan Brouwer[1]; Jean-Pierre Chervet[1]; Martin Eysberg[2]; *[1]Antec Scientific, Zoeterwoude, Netherlands; [2]Antec Scientific, Boston, MA*

ThP 830 **Applying an Untargeted LC-MS Metabolomic Data Mining Platform to a Bottom-up Epitranscriptomic Study of Established Disease Models**; Jennifer H. Simpson[1]; Daniel A. Todd[1]; Joseph N Mwangi[1]; Jian Teng[2]; Bakhos Tannous[2, 3]; Norman H. L. Chiu[1]; *[1]The University of North Carolina at Greensboro; [2]Massachusetts General Hospital, Charlestown, MA; [3]Harvard Medical School, Boston, MA*

ThP 831 **Real-Time Collisional Energy Optimization on the Orbitrap Fusion Platform for confident unknown identification**; Derek J Bailey[1]; Graeme C McAlister[1]; Seema Sharma[1]; Philip M Remes[1]; Ralf Tautenhahn[1]; Ioanna Ntai[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

ThP 832 **Employing the Sciex All in One High Resolution MS/MS Spectral Library to Expand Nontargeted Analyses**; Katherine Hyland[1]; Oscar Cabrices[2]; *[1]Sciex, Redwood City, CA; [2]Sciex, Redwood City, California*

ThP 833 **Comparison of Structure Elucidation Software for Small Molecule Impurity Identification**; Sarah J Robinson; *Genentech, Inc, San Francisco, CA*

ThP 834 **Improved Ranking of Putative Candidates Through Hybrid in Silico / Real Fragmentation Technique**; Tim Stratton[1]; Michal Raab[2]; Robert Mistrik[2]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]HighChem, Bratislava, Slovakia*

ThP 835 **A Facile Screening Method Based-On LC-MS for Discovery of New Strigolactones in Rice**; Shuang Fang[1]; Jinfang Chu[1]; *[1]Institute of Genetics and Developmental Biology Chinese Academy of Sciences, Beijing, China*

ThP 836 **Simultaneous Multi-Site Measurements of Several Neuromodulators in Behaving Macaque Brain Using Solid-Phase Microextraction Recessed Microprobe Coupled with LC-MS**; Sofia Lendor[1]; Seyed-Alireza Hassani[2, 3]; Varoon Singh[1]; Ezel Boyaci[1]; Thilo Womelsdorf[2, 3]; Janusz Pawliszyn[1]; *[1]University of Waterloo, Department of Chemistry, ON, Canada; [2]Vanderbilt University, Department of Psychology, Nashville, TN; [3]York University, Department of Biology, Centre for Vision Research, Toronto, ON, Canada*

ThP 837 **Identification of Silane Oligomers by Electrospray Quadrupole Mass Spectrometry**; Ahmed A Issa[1]; Khalid A. Al-Saad[1]; *[1]Qatar University, Doha, Qatar*

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Short Courses June 1 and 2