



Welcome to the 63rd ASMS Conference on Mass Spectrometry and Allied Topics. Conference program activities and exhibit booths are in America's Center. Corporate Member hospitality suites are located in the Renaissance Grand Hotel.

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Opening Reception



Closing Event

Waters

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Closing Event

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

The PDF document of proceedings submissions for orals and posters may be viewed online one day after presentation at the conference.

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GENERAL INFORMATION

REGISTRATION is open 10:00 am - 8:00 pm on Sunday and 7:30 am - 5:00 pm on Monday through Thursday.

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

4:00 - 4:45 pm, Sunday, Ballroom 220/221

Plan Your Strategy: What to See and Do at ASMS

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

Hall 5, level 1



5:00 - 5:45 pm
**Statistical Experimental Design:
The Building Blocks of a Good
Experiment**

Ann L. Oberg
Mayo Clinic



5:45 - 6:30 pm
**Metabolite Profiling at the 'Omic'
Scale: Untargeted Does not Mean
Unplanned**

Gary Patti
Washington University, St Louis

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

Hall 5, level 1



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



**The Human Gut Microbiome and
Healthy Growth**

Jeffrey L. Gordon
Washington University, St. Louis School
of Medicine

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

Poster/Exhibit Hall. Conference name badge is required.

PLENARY SESSIONS

MONDAY, 4:45 - 5:30 PM

AWARD LECTURE

Hall 5, level 1



**Award for a Distinguished
Contribution in Mass Spectrometry**

Brian T. Chait
The Rockefeller University

TUESDAY, 4:45 - 5:30 PM

AWARD LECTURE

Hall 5, level 1



Biemann Medal

Michael J. MacCoss
University of Washington

THURSDAY, 4:45 - 5:30 PM

PLENARY LECTURE

Hall 5, level 1



**The Evolution of Modern
Neurosurgery: A History of Trial and
Error, Success and Failure**

G. Michael Lemole, Jr.
The University of Arizona College of
Medicine

DON'T MISS

• ASMS MEETING, WEDNESDAY, 4:45 - 5:30 PM

Ballroom 222/224, level 2

Enjoy a beverage while you applaud awards, hear about new initiatives, and more!

• CLOSING EVENT, THURSDAY, 6:30 - 9:00 PM City Museum

Let's celebrate! Your adventure begins with a maze of turrets and open "tunnels" that lead to views of fantastic structures and sculptures. Try your skills of balance and courage, through caves and impossible slides. End with a surprise "artist" and St. Louis buffet. Buses will depart from the convention center, Washington Avenue entrance. Ticket is required, \$30.





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

Level 1

Session A (MOA, TOA, WOA, ThOA)..... Hall 5
 Session B (MOB, TOB, WOB, ThOB) Room 130/132
 Session C (MOC, TOC, WOC, ThOC) Room 123/124
 Session D (MOD, TOD, WOD, ThOD) Room 120/127
 Session E (MOE, TOE, WOE, ThOE) Theater
 Session F (MOF, TOF, WOF, ThOF)..... Room 106

Level 2

Session G (MOG, TOG, WOG, ThOG) . Ballroom 222/224
 Session H (MOH, TOH, WOH, ThOH) .. Ballroom 220/221

ORAL PRESENTATIONS are projected from ASMS computers running Microsoft Office 2010. Speakers are required to use the ASMS computers for their presentations.

SPEAKERS must load presentations at least one day prior to their talks. The speaker room is 116, level 1 between Hall 4 and 5. 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 Reception7:45 pm - 9:00 pm

Monday - Wednesday7:30 am - 8:00 pm

Thursday7:30 am - 3:00 pm

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

POSTER SESSIONS are 10:30 am - 2:30 pm, Monday through Thursday.

POSTER AUTHORS must be present at posters on scheduled days at these times.

10:30 am - 1:00 pm Odd-numbered posters

12:00 - 2:30 pm Even-numbered posters

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

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

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

EXHIBITORS must staff exhibit booths as follows:

Sunday Reception7:45 pm - 9:00 pm

Monday - Thursday 10:30 am - 2:30 pm

WORKSHOPS are 5:45 - 7:00 pm on Monday, Tuesday, and Wednesday. Light refreshments are provided in the pre-function areas on level 1 and outside ballroom on level 2.

DINNER BREAK, 7:00 - 8:00 PM is time for a breath of fresh air before the opening of hospitality suites at 8:00 pm.

SPECIAL PROGRAM FOR UNDERGRADUATE STUDENTS

- **Sunday, 7:30 - 9:00 pm, Poster competition,** Poster/Exhibit Hall
- **Monday, 11:30 am - 1:00 pm, Meet the Experts.** lunch tables reserved for undergraduate students in the Poster/Exhibit Hall, Free vouchers for lunch will be provided at the tables. Arrive promptly at 11:30 am to obtain your voucher.
- **Wednesday, 5:45 - 7:00 pm, Workshop: Getting the Most out of Undergraduate Research in Mass Spectrometry,** Room 230

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

CONFERENCE PROCEEDINGS will be published online. Visit www.asms.org after July 6 to view or download the Proceedings. Submission to the Proceedings does not constitute publication and does not jeopardize the rights of authors to publish contents of their submissions. **Speaker web casting slides will be printed to PDF and used for speakers who fail to submit.**

WEB CASTING includes tutorial lectures, plenary lectures, and oral sessions. Web casting will be available to conference attendees for three months after the conference. ASMS does not retain rights to material included in web castings. To access the presentations, go to www.asms.org and log in. After login, go to annual conference page and select "web casting." Web casting button is visible only to conference registrants.

CORPORATE HOSPITALITY SUITES may be open 8:00 - 11:00 pm, Monday through Wednesday. Suites are located in the **Renaissance Grand Hotel.**

CAREER CENTER is located near the Washington Avenue entrance. 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.

Sunday7:45 - 9:00 pm

Monday – Wednesday.....7:30 am - 5:00 pm

Thursday7:30 am - 2:30 pm

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

CONCIERGE DESK in the conference registration area offers information on transportation, attractions and restaurants.

GENERAL INFORMATION

CORPORATE BREAKFAST SEMINARS are hosted by some Corporate Members. Breakfast seminars are located on level 2 of the convention center and seats must be reserved in advance. **Please reserve at company exhibit booths.**

CORPORATE MEDIA EVENTS are for members of the press and financial institutions. All will be held in the Renaissance Grand Hotel.

| MONDAY | |
|--|------------------------|
| Company | Convention Center Room |
| Advanced Chemistry Development (ACD) | Room 242 |
| Agilent Technologies | Room 276 |
| Bruker Daltonics | Room 263/264 |
| LECO | Room 241 |
| SCIEX | Room 265/266 |
| SCIEX | Room 275 |
| Shimadzu | Room 274 |
| Thermo Scientific (in Renaissance Hotel) | Landmark 4-7 |
| Waters | Room 230 |
| Waters | Room 231 |
| TUESDAY | |
| Company | Convention Center Room |
| Agilent Technologies | Room 276 |
| Biotage | Room 231 |
| Bruker Daltonics | Room 263/264 |
| EMD Millipore | Room 240 |
| GL Sciences | Room 265/266 |
| LECO | Room 241 |
| New Objective | Room 242 |
| Phenomenex | Room 230 |
| Promega | Room 261/262 |
| Prosolia | Room 232 |
| SCIEX | Room 275 |
| SCIEX (in Renaissance Hotel) | Majestic D |
| Shimadzu | Room 274 |
| Thermo Scientific (in Renaissance Hotel) | Landmark 4-7 |
| Waters | Room 260/267 |
| WEDNESDAY | |
| Company | Convention Center Room |
| Agilent Technologies | Room 276 |
| Bruker Daltonics | Room 263/264 |
| LECO | Room 241 |
| New Objective | Room 242 |
| Promega | Room 261/262 |
| SCIEX | Room 265/266 |
| SCIEX | Room 275 |
| Shimadzu | Room 274 |
| Thermo Scientific (in Renaissance Hotel) | Landmark 4-7 |
| Waters | Room 230 |
| Waters | Room 231 |
| THURSDAY | |
| Company | Convention Center Room |
| Shimadzu | Room 274 |
| Thermo Scientific | Room 276 |

| Company | Monday | Renaissance Hotel Location |
|----------------------|-----------------|----------------------------|
| Shimadzu | 8:00-9:00 am | Majestic F-H |
| Bruker | 9:30-10:30 am | Majestic A-C |
| SCIEX | 11:00 -12:00 pm | Majestic D |
| Agilent Technologies | 1:30-2:30 pm | Landmark 1-3 |
| Thermo Scientific | 3:00-4:00 pm | Landmark 4-7 |
| Waters Corporation | 4:30-5:30 pm | Majestic E |

CONFERENCE REGULATIONS

- Name badge is required for all conference sessions, including the Poster/Exhibit Hall and the employment center.
- No smoking is permitted in the convention center.
- Cell phones must be turned off in oral sessions.
- No photography or recording is allowed in oral sessions or in the poster/exhibit Hall.
- 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 the express written authority of the author of the material presented. Such materials that are published in print or online must contain appropriate credits for all quotations and photographs.
- The placement of advertising in the meeting area is prohibited. There are poster boards and tables in the Poster/Exhibit Hall for approved announcements. No signs on easels are permitted.
- Hardware, accessories or any items for sale may be displayed only in corporate exhibit booths and hospitality suites.
- No organized activities (even off-site) other than those approved by ASMS are allowed during the conference week (5:00 pm on Sunday through 6:00 pm on Thursday).
- Corporate or institutional logos on slides or posters may appear only one time in the presentation.

HOTELS



CONFERENCE HOTELS

| Hotel | Telephone | Hotel | Telephone |
|-----------------------------|--------------|---|--------------|
| *Crowne Plaza Downtown | 314-621-8200 | Holiday Inn (formerly Ramada Plaza) | 314-421-5974 |
| *Drury Plaza at the Arch | 314-231-3003 | *Hyatt Regency | 314 655 1234 |
| Drury Inn & Suites Conv Ctr | 314-231-8100 | Magnolia | 314-436-9000 |
| Embassy Suites | 314-269-5900 | *Union Station St. Louis - A Doubletree by Hilton Hotel | 314-621-5262 |
| *Hampton Inn Gateway Arch | 314-621-7900 | Renaissance Grand | 314-621-9600 |
| *Hilton Ballpark | 314-421-1776 | | |
| *Hilton Downtown | 314-436-0002 | | |

**Shuttle service to/from the convention center and hospitality suites will be provided from these hotels.*



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CONGRATULATIONS

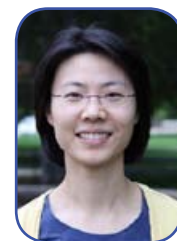
to these members who were elected to the ASMS Board

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Advion, Quintiles and Cornell University
Ithaca, NY

Secretary



Yu Xia
Purdue University
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Cindi Pettit, Miquela Sena
Marin Walker, Brent Watson

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| | |
|--|--|
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| <i>Biotherapeutics</i> | Alain Balland Jason Hogan Damian Houde |
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| <i>DNA/RNA</i> | Balasubrahmanyam Addepalli Michael McGinley |
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| <i>Environmental Applications</i> | Marc Engel Chris Gill |
| <i>Exposomics</i> | Anthony Macherone Skip Kingston |
| <i>Flavor, Fragrance and Foodstuff</i> | Timothy Croley Walter Hammock |
| <i>Forensics & Homeland Security</i> | Glen Jackson Guido Verbeck |
| <i>FTMS</i> | Nathan Kaiser Don Smith |
| <i>Fundamentals</i> | Alessandra Ferzoco Jos Oomens |
| <i>H/D Exchange, Covalent Labeling & Cross Linking</i> | Joshua Sharp David Weis |
| <i>Imaging MS</i> | Vilmos Kertesz Zoltan Takats |
| <i>Ion Mobility MS</i> | Erin Baker Stephen Valentine |
| <i>Ion Trap MS</i> | Daniel E. Austin |
| <i>Lipids & Lipodomics</i> | Stephen Blanksby |
| <i>LC/MS Related Topics</i> | Michael Bereman Helene Cardasis |
| <i>Metabolomics</i> | Andrew Patterson Sunia Trauger |
| <i>Metal Ion Coordination Chemistry</i> | Benjamin Bythell Alex Shvartsburg |
| <i>Pharmaceuticals</i> | Christine Gu Shawna Hengel |
| <i>Photoionization MS</i> | Jack Syage Ralf Zimmerman |
| <i>Polymeric Materials</i> | Stephen Rumbelow Gyorgy Vas |
| <i>Regulated Bioanalysis</i> | Jian Wang |
| <i>Undergraduate Research in MS</i> | Elaine Marzluff J.C. Poutsma |
| <i>Young Mass Spectrometrists</i> | Olga Friese Kristin Wildsmith |

COMMITTEES

| | |
|-----------------------------------|---|
| <i>Asilomar Conference (ACMS)</i> | Sharon Pitteri, Chair Hao Chen Julian Ryan Susan Weintraub |
| <i>Corporate Liaison</i> | Gary Valaskovic, Chair Susan Weintraub Karen Anspach, Phenomenex Johnny Cardenas, SCIEX Lindsay Farnum, Agilent Lance Nicolaysen, Waters Qihui Ni, EMD Millipore Bobbie Jo Seyler, Sigma Aldrich |
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| <i>Sanibel Conference</i> | JC Poutsma, Chair Erin Baker Patrick Griffin Fanyu Meng |

ARCHIVIST

Michael Grayson

AWARD FOR A DISTINGUISHED CONTRIBUTION IN MASS SPECTROMETRY

2015 RECIPIENT: BRIAN T. CHAIT

AWARD LECTURE: 4:45 PM, MONDAY, HALL 5, LEVEL 1



Dr. Brian T. Chait is awarded the 2015 ASMS Award for a Distinguished Contribution in Mass Spectrometry for the recognition and demonstration of the link between protein structure and conformation and electrospray ionization mass spectra. His discovery that a protein's solution phase conformation impacts its electrospray ionization mass spectrometry (ESI-MS) charge state distribution (CSD) blasted away the barriers isolating mass spectrometry from its ability to probe higher order macromolecular structures and fostered a continuing deluge of applications of MS to noncovalent assemblies, hydrogen/deuterium exchange, probes of gas-phase protein structure, and ultimately "native mass spectrometry."

Today, interpreting ESI-MS and MS/MS data for proteins examined from native solutions often begins from NMR or crystal structures, based on assumptions that the gas-phase structure will not be too distant. But 24 years ago there was no expectation that relationships from higher order solution structure could be retained in the gas phase and any such assumption would have been foolhardy. The Chait laboratory opened the world to this possibility, first by demonstrating that electrosprayed cytochrome *c* molecules assumed about twice as much charge when

sprayed from pH 2.6 than from pH 5.2 H₂O (*J. Am. Chem. Soc.* 112, 9012 (1990)), by probing conformational changes in proteins via hydrogen/deuterium exchange (*Rapid Commun. Mass Spectrom.* 5, 214 (1991)), and by monitoring solution-phase thermal denaturation processes by ESI-MS (*Anal. Chem.* 65, 1, (1993)).

Dr. Chait's achievement must be viewed from the perspective of mass spectrometry in 1990 when few of us were capable of spraying 100% aqueous solutions, or did we see a need for it. For some of us an organic sheath solvent (or make-up flow) reduced surface tension enough to complete our analyses; others simply added methanol directly. However, Chowdhury and Chait (*Anal. Chem.* 63, 1660 (1991)) demonstrated that electropolished needles could electrospray water at voltages sufficiently below those inducing dielectric breakdown. That ability to electrospray 100% H₂O was key to observing the charge state distribution differences associated with natively folded proteins. Equally important was Dr. Chait's ability to rationalize and prove that the source of the observed CSD difference had to be solution-phase structure.

We know so little about electrospray ionization today; we knew even less 25 years ago, yet the ideas that Dr. Chait precisely articulated about the electrospray CSD/conformation relationship were a turning point for biological mass spectrometry.

Dr. Brian T. Chait is the Head of the Laboratory of Mass Spectrometry and Gaseous Ion Chemistry and a Camille and Henry Dreyfus Professor at The Rockefeller University, New York, NY.

RON A. HITES AWARD OUTSTANDING RESEARCH PUBLICATION IN JASMS

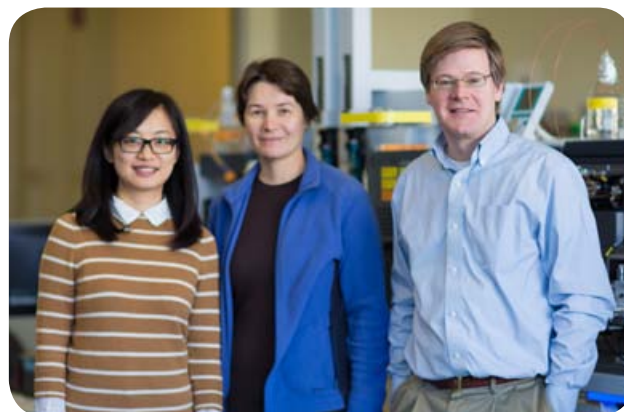
AWARD PRESENTATION: ASMS MEETING, 4:45 PM, WEDNESDAY, BALLROOM 222/224



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

The 2015 award recognizes **John Klassen**, University of Alberta, and, co-authors Lan Liu, Alyson Baergen, Klaus Michelsen, Elena N. Kitova, and Paul D. Schnier; for their paper Energetics of Intermolecular Hydrogen Bonds in a Hydrophobic Cavity: *JASMS*, 2014, 25, 742-750.

Left to right: Lan Liu, Elena Kitova, and John Klassen





BIEMANN MEDAL

2015 RECIPIENT: MICHAEL J. MACCOSS

AWARD LECTURE: 4:45 PM, TUESDAY, HALL 5, LEVEL 1



Dr. Michael J. MacCoss has made a number of contributions of serious and long lasting impact to the field of proteomics. Chief among these is software development that has greatly facilitated proteomics. Dr. MacCoss' philosophy on making software freely available and continually supporting this software so that it enables others has greatly benefitted the proteomic sciences.

Bioinformatics tools developed by the MacCoss laboratory facilitate many different aspects of mass spectrometry data analysis. This includes tools for liquid chromatography mass spectrometry (LC-MS) feature finding, spectrum library searching, peak detection, post-processors for peptide database searching, and more. An important early contribution from his lab, the Percolator algorithm, improved peptide identifications from proteomic analyses through semi-supervised machine learning (Käll *et al.* "Semi-supervised learning for peptide identification from shotgun proteomics datasets," *Nature Methods*, 2007). Percolator became widely adopted partially because of its use of a liberal open source license that encouraged companies to build on Percolator and incorporate into commercial packages (e.g. Mascot and Proteome Discoverer). Another high-impact contribution from the MacCoss laboratory is the development and continued support of an integrated set of software

tools called Skyline (MacLean *et al.* "Skyline: an open source document editor for creating and analyzing targeted proteomics experiments" *Bioinformatics*, 2010; available from <http://skyline.maccosslab.org>). Critically, Skyline is a vendor-neutral toolset, thus enabling methods to be easily transferred and tested across labs, even those that utilize different instrument platforms. Dr. MacCoss has also substantially advanced the new area of data-independent MS analyses. His key contribution in this area has been to develop a multiplexed strategy to better isolate noise and improve signal detection and therefore sensitivity through observational coherence (Egertson *et al.*, *Nature Methods* 2013).

One of the most recent projects championed by Dr. MacCoss is a nonprofit to provide a cost effective mechanism for labs to backup, share, visualize, and analyze data on the cloud called The Chorus Project (<http://chorusproject.org>). They are working with developers in academic labs and companies to offer tools to our community that can process mass spectrometry data stored within Chorus. The hope is to provide a platform where all labs have access to the latest analysis tools and published data can be easily reanalyzed.

Dr. MacCoss is professor in the Department of Genome Sciences, University of Washington, Seattle.

2015 RESEARCH AWARDS

AWARD PRESENTATION: 4:45 PM, TUESDAY, HALL 5

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

Sponsored by
THERMO SCIENTIFIC



Michael Bereman
North Carolina State University

Sponsored by
WATERS CORPORATION



Alexander Ivanov
Northeastern University

ASMS AWARDS

2015 POSTDOCTORAL AWARDS

AWARD PRESENTATION: ASMS MEETING, 4:45 PM, WEDNESDAY, BALLROOM 222/224

Three 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.



Martin Paine
Georgia Institute of Technology



Valentina Pirro
Purdue University



Gloria Sheynkman
Harvard Medical School

STUDENT AWARDS

AWARD PRESENTATION: ASMS MEETING, 4:45 PM, WEDNESDAY, BALLROOM 222/224

2015 inaugurates two student conference travel awards. There are seven 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

Benjamin Diner
Princeton University

Albert Konijnenberg
University of Antwerp

Xin Liu
University of Notre Dame

Mandy Phelps
University of North Texas

Nicholas Riley
University of Wisconsin-Madison

Vincent Sica
University of North Carolina-Greensboro

Chih-Chiang Tsou
University of Michigan

UNDERGRADUATE STUDENT AWARDS

Quintin Ferraris
Kean University

Joshua Fischer
Wayne State University

James Keating
University of Michigan

James Matilla
James Madison University

Danielle McDougall
University of Florida

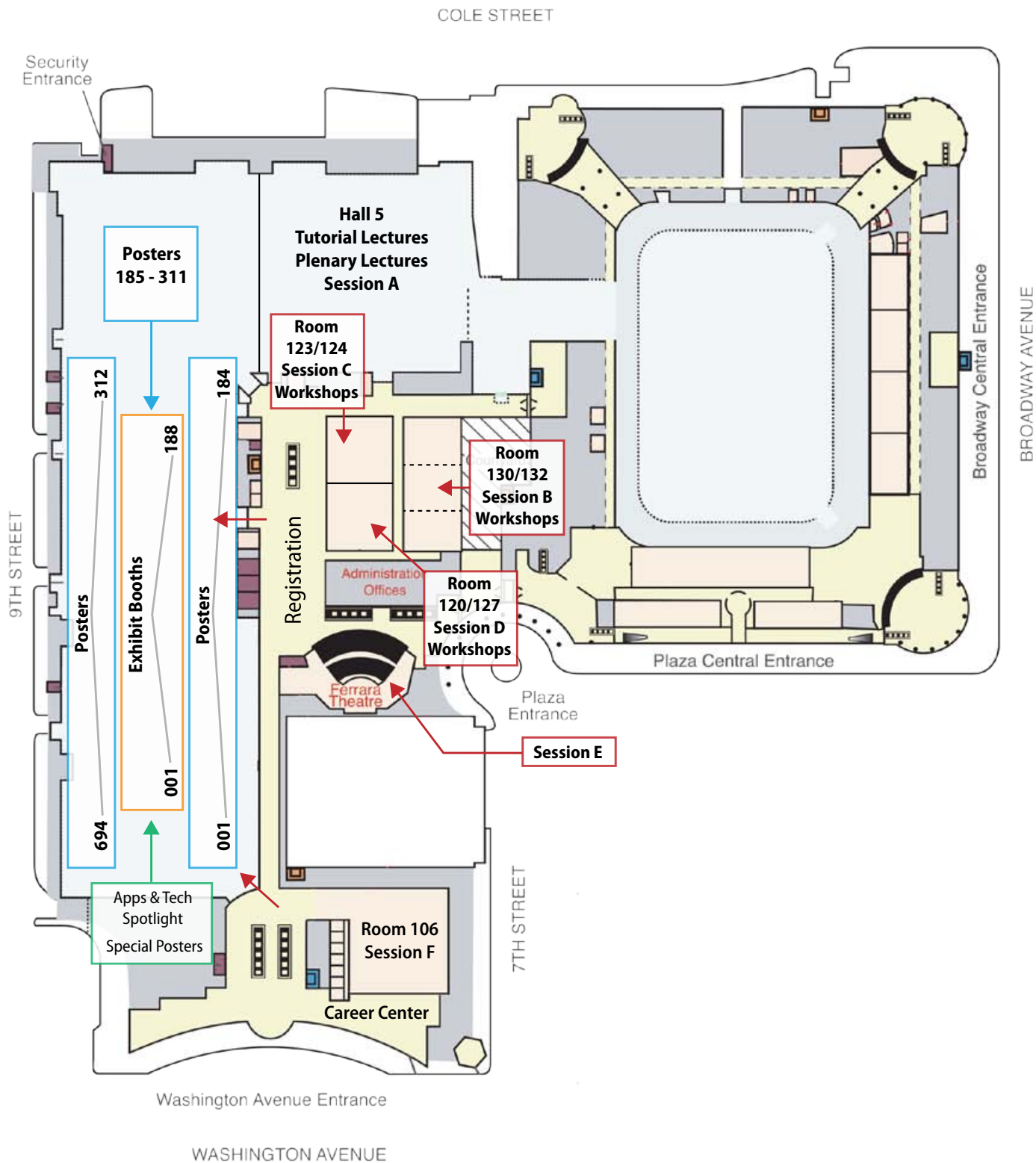
Haley Miller
Bowdoin College

Sydney Morris
George Washington University

Alexandra Plaviak
Duquesne University

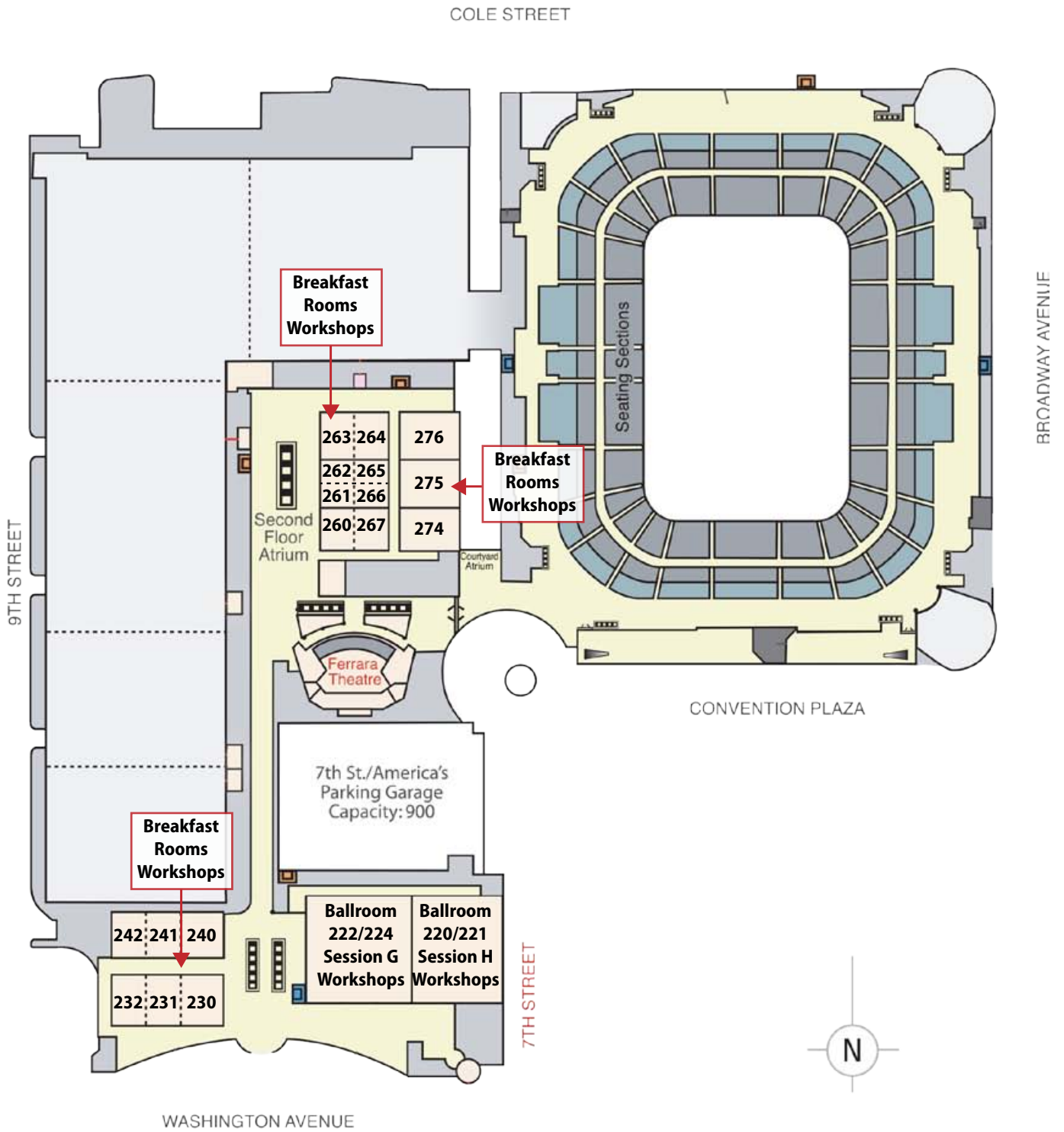
Cheylene Tanimoto
Stanford University

Nick van Huizen
Erasmus MC



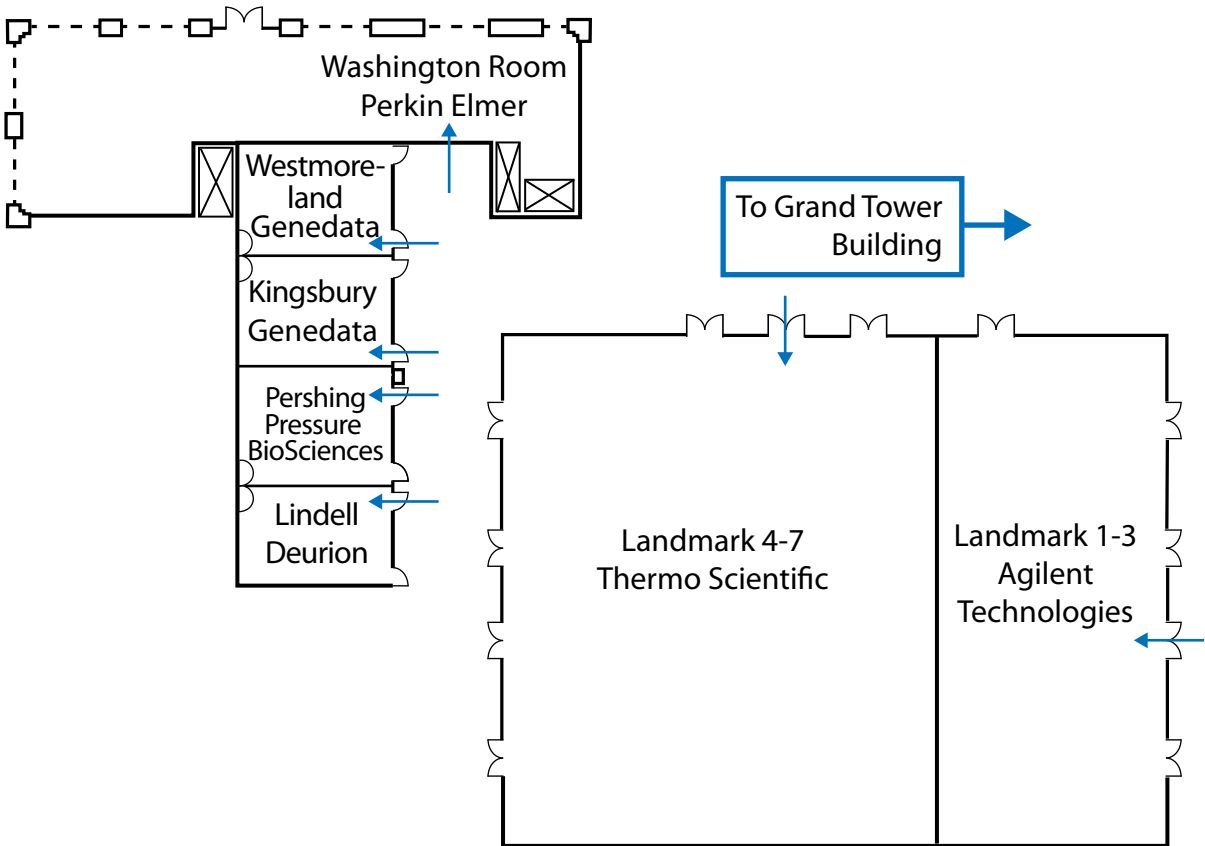


AMERICA'S CENTER, LEVEL 2

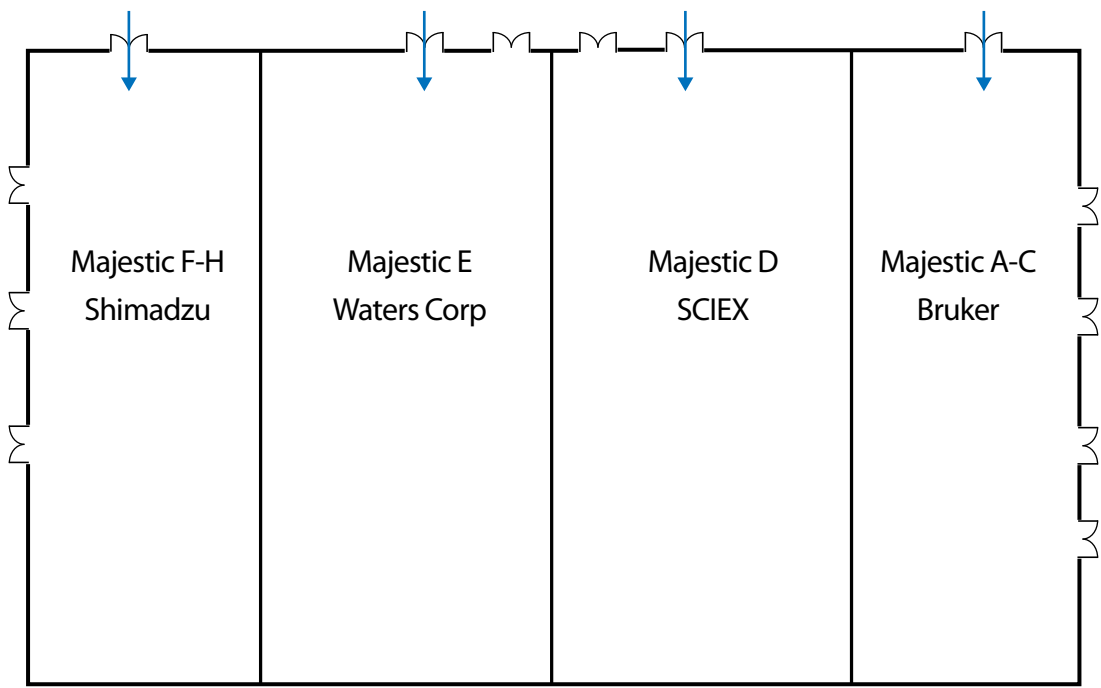




Ballroom Complex – Lobby Level



Ballroom Complex – Second Floor



ASMS CORPORATE MEMBERS

| COMPANY | POSTER / LIBRARY | BOOTH | SUITE IN RENAISSANCE HOTEL | BREAKFAST |
|---|------------------|-------|----------------------------|-------------------------------------|
| ACS Publications | Library | | | |
| Advanced Chemistry Development (ACD/Labs) | Poster | 83 | | Room 242, Monday (6/1) |
| Advanced Chromatography Technologies Ltd | | 52 | | |
| Advanced Energy | | 19 | | |
| Advion Inc. | | 171 | | |
| Agilent Technologies | Poster | 141 | Landmark 1-3 | Room 276, Mon - Wed (6/1 - 6/3) |
| AIM Research Company | | 106 | | |
| American Pharmaceutical Review | Library | | | |
| Amsterdam Scientific Instruments | | 36 | | |
| Analytical Sales and Services, Inc. | | 22 | | |
| Anasys Instruments | | 32 | | |
| Antec | Poster | 61 | | |
| Apricot Designs, Inc. | | 155 | | |
| Ardara Technologies LP | Poster | 103 | | |
| Atlas Antibodies AB | | 107 | | |
| Avanti Polar Lipids, Inc. | | 79 | | |
| BaySpec, Inc. | | 97 | | |
| BIOCRATES Life Sciences AG | | 102 | | |
| Biognosys | | 132 | | |
| Bioinformatics Solutions Inc. | Poster | 151 | | |
| BioPharma Services, Inc. | | 54 | | |
| Biotage | | 121 | | Room 231, Tuesday (6/2) |
| Biotech Support Group | | 73 | | |
| Bruker Daltonics | | 40 | Majestic A-C | Room 263/264, Mon - Wed (6/1 - 6/3) |
| Busch Vacuum Pumps and Systems | | 48 | | |
| CAMAG Scientific, Inc. | | 145 | | |
| Cambridge Isotope Labs | | 179 | | |
| Canadian Life Science | Poster | 162 | | |
| CAS | | 55 | | |
| Cayman Chemical Company | | 175 | | |
| Cell Signaling Technology | | 51 | | |
| Cerilliant | Poster | 33 | | |
| Cerno Bioscience | | 178 | | |
| CovalX | | 81 | | |
| CSS Analytical Co. Inc. | | 11 | | |
| CTC Analytics AG | | 117 | | |
| Denator AB | | 146 | | |
| Detector Technology, Inc. | | 27 | | |

ASMS CORPORATE MEMBERS



| COMPANY | POSTER / LIBRARY | BOOTH | SUITE IN RENAISSANCE HOTEL | BREAKFAST |
|--|------------------|-------|----------------------------|-----------------------------|
| Deurion | | | Lindell | |
| Dikma Technologies, Inc | | 68 | | |
| Drummond Scientific | | 105 | | |
| Edwards Vacuum | | 114 | | |
| Elforlight Ltd. | | 12 | | |
| EMD Millipore | | 84 | | Room 240, Tuesday (6/2) |
| EPREP | | 62 | | |
| ES Industries | | 136 | | |
| ESI Source Solutions | | 50 | | |
| ETP Electron Multipliers | | 44 | | |
| Excellims Corporation | Poster | 59 | | |
| Exelis | Poster | 87 | | |
| Expedeon | | 126 | | |
| Extrel | | 38 | | |
| FLIR Systems, Inc. | Poster | 37 | | |
| Fluid Management Systems | Poster | 10 | | |
| Fortis Technologies Ltd | Poster | 177 | | |
| GAA Custom Engineering | Poster | 3 | | |
| Genedata | | 119 | Westmoreland/ Kingsbury | |
| Genetic Engineering & Biotechnology News | Library | | | |
| Genovis | Poster | 90 | | |
| GenTech Scientific, Inc. | | 17 | | |
| GERSTEL, Inc. | Poster | 94 | | |
| GL Sciences Inc. | | 39 | | Room 265/266, Tuesday (6/2) |
| Glygen Corp. | | 99 | | |
| Golden West Biologicals, Inc. | | 158 | | |
| Hamamatsu Corporation | Poster | 148 | | |
| Hamilton Robotics | | 71 | | |
| Harvard Apparatus | | | | |
| Hecate Software, Inc. | | 3 | | |
| Horizon Technology, Inc. | | 77 | | |
| HTX Technologies, LLC | | 78 | | |
| Hudson Surface Tech | Poster | 35 | | |
| iChrom Solutions | | 9 | | |
| IDEX Health & Science | Poster | 180 | | |
| iLab Solutions | | 6 | | |
| Imtakt USA | | 159 | | |
| Institute for Systems Biology | | 56 | | |
| INTAVIS Bioanalytical Instruments AG | | 95 | | |
| Integrated Engineering Software | | 74 | | |



ASMS CORPORATE MEMBERS

| COMPANY | POSTER / LIBRARY | BOOTH | SUITE IN RENAISSANCE HOTEL | BREAKFAST |
|--|---------------------|-------|-------------------------------|----------------------------------|
| Integrated Proteomics Applications | | 89 | | |
| International Ceramic Engineering | | 29 | | |
| International Equipment Trading Ltd. | | 150 | | |
| ionBench | | 1 | | |
| Ionicon | Poster | 163 | | |
| IONICS Mass Spectrometry | | 134 | | |
| IonSense, Inc. | Poster | 110 | | |
| IsoSciences | | 7 | | |
| JEOL USA, Inc. | | 65 | | |
| JPT Peptide Technologies | | 69 | | |
| LEAP Technologies | Poster | 30 | | |
| LECO Corporation | Poster | 139 | | Room 241, Mon - Wed (6/1 - 6/3) |
| Linden CMS | | 131 | | |
| Mac-Mod Analytical | | 28 | | |
| Markes International | Poster | 53 | | |
| MasCom Technologies | | 8 | | |
| MassTech Inc. | | 70 | | |
| Matrix Science | | 166 | | |
| Matsusada Precision Inc. | | 80 | | |
| McKinley Scientific | | 137 | | |
| MeCour Temperature Control | | 174 | | |
| Microliter Analytical Supplies (A WHEATON Company) | | 93 | | |
| Microsaic Systems | | 45 | | |
| Moeller Medical GmbH | | 176 | | |
| Molecular Discovery, Ltd | | 125 | | |
| Morpho Detection Inc. | Poster | 133 | | |
| MS Bioworks | | 112 | | |
| MS Noise | | 170 | | |
| MS Vision | | 130 | | |
| MSParts | | 135 | | |
| mSPEC group | | 18 | | |
| MStm | | 156 | | |
| Nacalai USA, Inc. | | 104 | | |
| nanoLiter, LLC | Poster | 57 | | |
| Nest Group, The | Poster | | | |
| New England Biolabs | | 66 | | |
| New England Peptide, Inc. | | 153 | | |
| New Objective, Inc. | Poster | 138 | | Room 242, Tues - Wed (6/2 - 6/3) |
| NexTech Science Innovations, LLC | | 172 | | |
| NIST | | 25 | | |
| Novilytic | | 72 | | |

ASMS CORPORATE MEMBERS



| COMPANY | POSTER / LIBRARY | BOOTH | SUITE IN RENAISSANCE HOTEL | BREAKFAST |
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| Oerlikon Leybold Vacuum | | 109 | | |
| OmicScouts GmbH | Poster | 88 | | |
| Omni International | | 124 | | |
| OPOTEK, Inc. | | 67 | | |
| Optimize Technologies, Inc. | Poster | 144 | | |
| Owlstone, Inc. | | 165 | | |
| Pall Laboratory | | 43 | | |
| Parker Hannifin | Poster | 91 | | |
| PEAK Scientific | Poster | 143 | | |
| Perfinity Biosciences | | 157 | | |
| PerkinElmer | | 161 | Washington (Mon, Tues only) | |
| Pfeiffer Vacuum | Poster | 20 | | |
| Phenomenex | | 173 | | Room 230, Tuesday (6/2) |
| Phoenix Pharmaceuticals, Inc. | | 127 | | |
| Phoenix S&T, Inc. | | 101 | | |
| PHOTONIS | Poster | 41 | | |
| Phytronix Technologies, Inc. | | 24 | | |
| PREMIER Biosoft | | 100 | | |
| Pressure BioSciences, Inc. | | 147 | Pershing | |
| Promega Corporation | | 111 | | Room 261/262, Tues - Wed (6/2 - 6/3) |
| Prosolia, Inc. | | 64 | | Room 232, Tuesday (6/2) |
| Protea Biosciences, Inc. | | 123 | | |
| Protein Metrics Inc. | | 116 | | |
| Proteinaceous | Poster | | | |
| Proteome Software Inc. | | 31 | | |
| Proton Onsite | | 122 | | |
| Prozyme, Inc. | | 49 | | |
| PTM Biolabs, Inc. | | 129 | | |
| Pursuits Instrument Limited | | 115 | | |
| Resolution Systems, Inc. | | 108 | | |
| Restek Corporation | | 152 | | |
| RMI Laboratories | | 164 | | |
| Sage Science, Inc. | | 16 | | |
| Samin Science Co., Ltd | | 15 | | |
| Science/AAAS | Library | | | |
| Scientific Instrument Services | Poster | 2 | | |
| Scientific Systems, Inc. | | 34 | | |
| SCIEX | | 21 | Majestic D | Room 275, Mon - Wed (6/1 - 6/3); Rm 265/266, Mon & Wed (6/1, 6/3); Renaissance Hotel Majestic D, Tues (6/2) |
| Shimadzu Scientific Instruments, Inc. | Poster | 120 | Majestic F-H | Room 274, Mon - Thurs (6/1 - 6/4) |

ASMS CORPORATE MEMBERS

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| Shrader Software Solutions | Poster | 75 | | |
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| Silantes GmbH | | 5 | | |
| Sound Analytics | | 14 | | |
| Spark Holland | Poster | 167 | | |
| SpectralWorks Limited | Poster | 118 | | |
| Spectroscopy | | 142 | | |
| Spellman High Voltage | | 58 | | |
| Springer Science + Business Media | | 149 | | |
| SunChrom GmbH | | 98 | | |
| Supelco | Poster | 92 | | |
| Tandem Labs | | 169 | | |
| Tecan | | 46 | | |
| The Analytical Scientist | Library | | | |
| Thermo Scientific | | 140 | Landmark 4-7 | Renaissance Hotel Landmark 4-7, Mon-Wed (6/1-6/3); Room 276, Thursday (6/4) |
| Tofwerk AG | | 23 | | |
| Tomtec | | 13 | | |
| Tosoh Bioscience | | 168 | | |
| Trajan Scientific and Medical | | 26 | | |
| TSI Inc. | | 96 | | |
| United Science Corp. | | 154 | | |
| Veritomyx | | 113 | | |
| VICI Valco Instruments | | 85 | | |
| VRS | | 42 | | |
| WarpLCMS | | 86 | | |
| Waters Corporation | Poster | 160 | Majestic E | Room 260/267, Tues (6/2); Room 230, Mon & Wed (6/1, 6/3); Room 231 Mon & Wed (6/1, 6/3) |
| Wiley | Library | | | |
| Worldwide Clinical Trials | | 47 | | |
| XPC Corporation | | 60 | | |
| YMC America, Inc. | Poster | 82 | | |
| Zef Scientific Inc. | | 63 | | |
| Zhejiang Haochuang Biotech Co., Ltd | | 76 | | |



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

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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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Nathan Yates



PROGRAM OVERVIEW

SATURDAY

| | |
|--------------------------|----------------------|
| 9:00 AM - 4:30 PM | SHORT COURSES |
| 2:00 - 5:00 PM | REGISTRATION |

SUNDAY

| | |
|---------------------------|--|
| 9:00 AM - 4:30 PM | SHORT COURSES |
| 10:00 AM - 8:00 PM | REGISTRATION |
| 4:00 - 4:45 PM | ATTENTION: FIRST-TIME GRADUATE STUDENTS AND UNDERGRADUATE STUDENTS Plan your Strategy: What to See and Do at ASMS |
| 5:00 - 6:30 PM | <p>TUTORIAL LECTURES, Hall 5, level 1</p> <div style="display: flex; align-items: flex-start; margin-top: 10px;"> <div style="flex: 1;">  </div> <div style="flex: 2; padding-left: 10px;"> <p>5:00 - 5:45 pm Statistical Experimental Design: The Building Blocks of a Good Experiment</p> <p>Ann L. Oberg Mayo Clinic</p> </div> </div> <div style="display: flex; align-items: flex-start; margin-top: 10px;"> <div style="flex: 1;">  </div> <div style="flex: 2; padding-left: 10px;"> <p>5:45 - 6:30 pm Metabolite Profiling at the 'Omic' Scale: Untargeted Does not Mean Unplanned</p> <p>Gary Patti Washington University, St Louis</p> </div> </div> |
| 6:45 - 7:45 PM | <p>CONFERENCE OPENING, Hall 5, level 1 Vicki Wysocki, <i>ASMS Vice President for Programs</i></p> <div style="display: flex; align-items: flex-start; margin-top: 10px;"> <div style="flex: 1;">  </div> <div style="flex: 2; padding-left: 10px;"> <p>7:00 - 7:45 pm The Human Gut Microbiome and Healthy Growth</p> <p>Jeffrey L. Gordon Washington University St. Louis School of Medicine</p> </div> </div> |
| 7:45 - 9:00 PM | RECEPTION IN THE POSTER/EXHIBIT HALL Undergraduate Student Poster Competition |

PROGRAM OVERVIEW



MONDAY

| | |
|---------------------------|--|
| 7:30 AM - 5:00 PM | REGISTRATION |
| 8:30 - 10:30 AM | <p>ORAL SESSIONS</p> <ul style="list-style-type: none"> • MOA am: Instrumentation: New Developments in Ionization & Sampling, Hall 5 • MOB am: Informatics: Algorithmic and Statistical Advances, Room 130/132 • MOC am: Protein Complexes: Activation & Dissociation, Room 123/124 • MOD am: Glycopeptides and Glycoproteins, Room 120/127 • MOE am: Metabolomics: New MS Technologies and Applications, Theater • MOF am: Quantitative Proteomics in Systems Biology/Cellular Pathway Analysis, Room 106 • MOG am: Energy, Petroleum, & Biofuels: Advances in MS Design & Informatics, Ballroom 222/224 • MOH am: Advances in Software and Hardware to Improve DMPK Workflows, Ballroom 220/221 |
| 10:30 AM - 2:30 PM | <p>POSTER SESSION AND EXHIBITS, Poster/Exhibit Hall, level 1</p> <p>Monday posters 11:30 – 1:00 pm: Undergraduate students – look for reserved tables and free lunch vouchers to <i>Meet the Experts</i></p> |
| 2:30 - 4:30 PM | <p>ORAL SESSIONS</p> <ul style="list-style-type: none"> • MOA pm: Ion Mobility, FAIMS & DMS: New Developments & Applications, Hall 5 • MOB pm: Informatics: Metabolomics, Room 130/132 • MOC pm: Top-Down Protein Analysis, Room 123/124 • MOD pm: Plant-omics, Room 120/127 • MOE pm: Clinical Diagnostics, Theater • MOF pm: PTMs: Advances in Isolation, Enrichment, Derivatization & Separation, Room 106 • MOG pm: Imaging: Biomedical Applications, Ballroom 222/224 • MOH pm: Quantitative Analysis in Drug Discovery for Small Molecules, Ballroom 220/221 |
| 4:45 - 5:30 PM | <p>AWARD LECTURE, Hall 5, level 1</p> <p>Award for a Distinguished Contribution in Mass Spectrometry</p> <div style="display: flex; align-items: center;">  <div> <p>Brian T. Chait The Rockefeller University</p> </div> </div> |
| 5:45 - 7:00 PM | <p>WORKSHOPS There are light refreshments in common areas.</p> <ol style="list-style-type: none"> 01. Has Photoionization Reached its Potential? Focus on APPI, Room 130 02. Enabling Proteomics Informatics on the Amazon Cloud, Room 131 03. Advanced MS and Separation Approaches for Biofuels and Petroleum, Room 132 04. The Galaxy Framework for MS-based Informatics, Room 123/124 05. Defining Resolution in Imaging MS - A Quest for Solid Ground, Room 120/127 06. Ion Traps: New Experiments and Old Tricks, Room 260/267 07. Metal Cationization of Biomolecules and its Analytical Applications, Room 274 08. Methods and Tools for Intra- and Inter-Experiment LC MS Performance Tracking, Room 275 09. Challenges and progress towards the Site-Specific Characterization of Glycoprotein Heterogeneity, Room 230 10. Mass Spectrometry Applications in Art, Cultural Heritage, and Natural History, Room 231 11. More DMPK Knowledge from Less Sample: Leveraging Modern LC-MS Instruments for Small Sample Amounts, Room 232 12. Metabolomics: Emerging Technologies for Continued Innovation, Ballroom 222/224 13. Which Career Path is Right for Me? Ballroom 220/221 |
| 7:00 - 8:00 PM | DINNER BREAK |
| AFTER 8:00 PM | CORPORATE HOSPITALITY SUITES , Renaissance Grand Hotel |



PROGRAM OVERVIEW

TUESDAY

| | |
|---------------------------|--|
| 7:30 AM - 5:00 PM | REGISTRATION |
| 8:30 - 10:30 AM | ORAL SESSIONS <ul style="list-style-type: none"> • TOA am: Instrumentation: Time-of-Flight and QTOF, Hall 5 • TOB am: Informatics: Multi-omics Integration, Room 130/132 • TOC am: Imaging: Instrumentation & Method Development, Room 123/124 • TOD am: Membrane Proteins, Room 120/127 • TOE am: Lipidomics: New MS Technologies and Applications, Theater • TOF am: Phosphoproteomics in Disease, Room 106 • TOG am: Emerging Environmental Contaminants, Ballroom 222/224 • TOH am: LC-MS Approaches to Combine Translational PK/PD Biomarkers with Small Molecule ADME Workflows, Ballroom 220/221 |
| 10:30 AM - 2:30 PM | POSTER SESSION AND EXHIBITS , Poster/Exhibit Hall Tuesday posters |
| 2:30 - 4:30 PM | ORAL SESSIONS <ul style="list-style-type: none"> • TOA pm: New Developments in High Resolution and Mass Accuracy, Hall 5 • TOB pm: Data Independent Acquisition: Innovative Methods and Applications, Room 130/132 • TOC pm: Ion Spectroscopy, Room 123/124 • TOD pm: Proteomics: Infectious Disease, Room 120/127 • TOE pm: Lipids and Profiling, Theater • TOF pm: Protein-Protein and Protein-Ligand Interactions, Room 106 • TOG pm: Environmental MS: Instrumental Challenges and Solutions, Ballroom 222/224 • TOH pm: Imaging: Pharmaceuticals and Metabolites, Ballroom 220/221 |
| 4:45 - 5:30 PM | AWARD LECTURE , Hall 5, level 1  Biemann Medal Michael J. MacCoss University of Washington |
| 5:45 - 7:00 PM | WORKSHOPS There are light refreshments in common areas <ol style="list-style-type: none"> 01. Laboratory Developed Test Guidance and Mass Spectrometric Diagnostics: Impact and Expectations, Room 130 02. Current Trends, Gaps, and Needs in Workflows for Targeted Protein Quantitation by LC/MS, Room 131 03. ProteomicsDB, Room 132 04. FTMS: MS/MS at High Resolution, Room 123/124 05. Identifying Tandem Mass Spectra of Lipids and Carbohydrates, Room 120/127 06. MS Analysis of Antibody-Drug Conjugates, Room 260/267 07. Measuring the Exposome: Strategies and Preliminary Results, Room 274 08. Advancements and Discussion of Mass Spectrometry Technology and Challenges within the Polymer and Material Fields, Room 275 09. The ABCs of Being a Great Reviewer for Scientific Journals, Room 230 10. How to Network without Really Trying, Room 231 11. Room 232 12. Invalidating your Cores Data: Examples on How to Check your Data and Report Results and Communicate Invalid or Bad Results to your Customers, Room 222/224 13. How Can Ion Mobility Spectrometry Separations Help your Research? Room 220/221 |
| 7:00 - 8:00 PM | DINNER BREAK |
| AFTER 8:00 PM | CORPORATE HOSPITALITY SUITES , Renaissance Grand Hotel |

PROGRAM OVERVIEW



WEDNESDAY

| | |
|---------------------------|--|
| 7:30 AM - 5:00 PM | REGISTRATION |
| 8:30 - 10:30 AM | ORAL SESSIONS <ul style="list-style-type: none"> • WOA am: Ambient and Atmospheric Pressure Generation of Multiply-Charged Ionic Species, Hall 5 • WOB am: Informatics: PRM & DIA, Room 130/132 • WOC am: Ion Mobility: Structures, Room 123/124 • WOD am: Carbohydrates, Room 120/127 • WOE am: FT, Ion Traps, and Hybrid Instruments, Theater • WOF am: Mass Spectrometry in Structural Biology, Room 106 • WOG am: Epigenetic Modifications and Mechanisms, Ballroom 222/224 • WOH am: Application of Stable Isotope Labeling in MS Analysis of Small Molecules and Proteins, Ballroom 220/221 |
| 10:30 AM - 2:30 PM | POSTER SESSION AND EXHIBITS , Poster/Exhibit Hall Wednesday posters |
| 2:30 - 4:30 PM | ORAL SESSIONS <ul style="list-style-type: none"> • WOA pm: Ambient Ionization: Instrumentation & Applications, Hall 5 • WOB pm: Informatics: Protein Identification and Quantification, Room 130/132 • WOC pm: Reactions, Dynamics & Theory of Gas Phase Ions, Room 123/124 • WOD pm: Nucleic Acids, Room 120/127 • WOE pm: Food Chemistry and Safety, Theater • WOF pm: H/D Exchange: Technologies and Applications, Room 106 • WOG pm: Energy, Petroleum, & Biofuels :Sample Preparation & MS Interface Design, Ballroom 222/224 • WOH pm: Antibodies and Anti-body Drug Conjugates, Ballroom 220/221 |
| 4:45 - 5:30 PM | ASMS MEETING , Ballroom 222/224, level 2 Awards, board reports, wine, beer, soft drinks - and more! |
| 5:45 - 7:00 PM | WORKSHOPS There are light refreshments in common areas. <ol style="list-style-type: none"> 01. The Role of High Resolution Mass Spectrometry in the Regulatory Environment, Room 130 02. Emerging Contaminants for Emerging Scientists, Room 131 03. Mass Spectrometry Instrumentation at the Forefront of Technology as Miscible Tools for Forensic and Security Evidence, Room 132 04. Gas-Phase Ion Chemistry: Thermodynamics, Kinetics, Structures and Spectroscopy, Room 123/124 05. Emerging Technologies Advancing Mass Spectrometry Research: 3D Printing, Room 120/127 06. CHORUS - A Community Solution for the Storage Visualization, Sharing, and Analysis of Mass Spectrometry Data on the Cloud, Room 260/267 07. The Big Fat Questions: The Future for Lipidomics in Cell Biology and Clinical Diagnostics? Room 274 08. Characterization of Protein Therapeutics by Mass Spectrometry, Room 275 09. Getting the Most out of Undergraduate Research in Mass Spectrometry, Room 230 10. Working with Federal Agencies to Obtain Research Support : Mock NIH Study Section and Q&A with Agency Staff, Room 231 11. Room 232 12. Ligand Binding Assays (LBA) and LC-MS/MS Integrated Antibody-Drug Conjugate (ADC) Bioanalysis -Immuno-capture LC-MS/MS Hybrid Assays: Challenges, Solutions, and Complementarity with LBA, Ballroom 222/224 13. Hydrogen-Deuterium Exchange, Covalent Labeling and Crosslinking, Ballroom 220/221 |
| 7:00 - 8:00 PM | DINNER BREAK |
| AFTER 8:00 PM | CORPORATE HOSPITALITY SUITES , Renaissance Grand Hotel |



PROGRAM OVERVIEW

THURSDAY

| | |
|---------------------------|---|
| 7:30 AM - 5:00 PM | REGISTRATION |
| 8:30 - 10:30 AM | ORAL SESSIONS <ul style="list-style-type: none"> • ThOA am: Mini/Portable/Fieldable MS, Hall 5 • ThOB am: Informatics: Peptide Identification and Quantification, Room 130/132 • ThOC am: New and Developing Ion Activation Methods, Room 123/124 • ThOD am: Nano-Scale & Microfluidic Separations & MS, Room 120/127 • ThOE am: Structure/Reactivity and Energetics of Gas-Phase Ions and Complexes, Theater • ThOF am: MS in Protein Footprinting: Michael Gross 75th Birthday, Room 106 • ThOG am: Targeted Quantification of Proteins & Post-Translational Modifications, Ballroom 222/224 • ThOH am: Ion Mobility: Small Molecules, Pharmaceuticals, and DMPK, Ballroom 220/221 |
| 10:30 AM - 2:30 PM | POSTER SESSION AND EXHIBITS , Poster/Exhibit Hall Thursday posters |
| 2:30 - 4:30 PM | ORAL SESSIONS <ul style="list-style-type: none"> • ThOA pm: MS in Surgery, Hall 5 • ThOB pm: Mult-PTMs: Comprehensive Analysis, Room 130/132 • ThOC pm: Peptide Fragmentation and Peptidomics, Room 123/124 • ThOD pm: Forensic Applications, Room 120/127 • ThOE pm: Synthetic Polymers, Theater • ThOF pm: Chemical Cross-linking and Covalent Labeling, Room 106 • ThOG pm: Ecological and Human Health Environmental Chemistry and Toxicology, Ballroom 222/224 • ThOH pm: Applying New LC/MS Techniques to Solve Challenging Drug Metabolism Problems, Ballroom 220/221 |
| 4:45 - 5:30 PM | PLENARY LECTURE , Hall 5, level 1  <p>The Evolution of Modern Neurosurgery: A History of Trial and Error, Success and Failure</p> <p>G. Michael Lemole, Jr. The University of Arizona College of Medicine</p> |
| 6:30 - 9:00 PM | CLOSING EVENT, City Museum. Ticket required |



There are light refreshments in common areas.

MONDAY WORKSHOPS, 5:45 - 7:00 PM

01. Has Photoionization Reached its Potential?

Focus on APPI

Photoionization Interest Group

Ralf Zimmerman and Jack Syage presiding

Room 130

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

In this third year we will focus on the topic of whether PI has reached its potential. This is an important topic because there are strong opinions that it is not used as much as its benefits warrant due to the entrenched use of common commercial ionization sources such as ESI and APCI. One can say that PI is late to the game. On the other hand PI and APPI are finding unique uses in high volume applications, most specifically explosives detection in security environments for its unique benefits that are not provided by competing ionization methods.

We have gotten some feedback discouraging us from trying to include both APPI and SPI topics because they are practiced by very different groups of users. So Ralf and I have decided to emphasize one or the other on alternate years. Not totally exclusive, but a strong emphasis and this year the emphasis will be on APPI.

02. Enabling Proteomics Informatics on the Amazon Cloud

Eric Deutsch, Luis Mendoza, David Shteynberg presiding

Room 131

The workshop will begin with a basic overview of the Trans-Proteomic Pipeline (TPP) and its newest features including new compute cloud concepts and services, primarily those offered by Amazon Web Services (AWS). We will describe the amztp platform, which facilitates the usage of AWS in the context of database searching using open-source engines as well as validation and analysis via the TPP; we will also conduct a live demo of the software. During the evening, we will conduct an open discussion on what other software tools and pipelines the community feels should be integrated into the amztp infrastructure (e.g. RNA-Seq analysis, SWATH data processing), and how to best provide an API and framework for others to incorporate their own tools that they wish to launch on the cloud.

03. Advanced MS and Separation Approaches for Biofuels and Petroleum Energy, Petroleum & Biofuels Interest Group

Patrick Hatcher presiding

Room 132

04. The Galaxy Framework for MS-based Informatics

Tim Griffin presiding

Room 123/124

The Galaxy framework for informatic workflow management has emerged as a useful tool for informatics and analysis of biological MS data. Originally focused on genomic informatics, Galaxy enables deployment of disparate software programs into a user-friendly environment, where software tools can be integrated into useful workflows. Once developed, the complete workflows and software tools can be easily shared with other Galaxy users. Given these advantages, Galaxy has great potential to solve a variety of informatics challenges in biological MS.

This workshop will provide attendees a look at some emerging applications in biological MS that are challenging to researchers, and where Galaxy offers an informatics solution. Informal presentations will be given by experts on these applications, with a focus on providing useful details on how these software and workflows can be accessed and used immediately. Audience questions and discussion on usability and other issues will be fielded and facilitated. An informal panel discussion with the presenters will follow the presentations.

Presenters and expected topics will include:

- Gerben Menschaert (Ghent University) - "The Proteoformer Pipeline for RiboProfiling and MS-based Proteomics"
- Ira Cooke (La Trobe University)/Pratik Jagtap (University of Minnesota) - "Galaxy-based PeptideShaker tools and applications, with a focus on downstream applications"
- Shyamasree Saha (Queen Mary University of London) - "Targeted Proteomics tools in Galaxy"

Ample time will be offered for questions from attendees and discussion. Presenters will be available for an informal panel discussion in the final part of the workshop.

05. Defining Resolution in Imaging MS:

A Quest for Solid Ground

Imaging MS Interest Group

Zoltan Takats and Vilmos Kertesz presiding

Room 120/127

The central envisioned topic of the workshop will be "Spatial Resolution in Mass Spectrometry". Due to the recent introduction of a number of new technologies into Mass Spectrometric Imaging, a 'War of Numbers' broke out on the field, where individual research groups keep claiming better and better spatial resolution for their techniques or experimental setups. In order to establish a solid ground, the workshop makes an attempt to come up with a widely acceptable definition (and associated method of determining it!) for spatial resolution claimed in a scientific publication. Furthermore, we are planning to discuss the limitations on spatial resolution (and the associated relationship between sensitivity and resolution) in case of commercially available techniques. We are also planning to include a structural biology expert and end the workshop with a discussion on the concept of 'Necessary Resolution', i.e. the spatial resolution required to answer certain biological questions.

MONDAY WORKSHOPS, 5:45 - 7:00 PM continued

Structure of the workshop is planned to follow these topics:

- Which resolution ? - the variety of definitions and protocols
- Discussion - coming to a commonly acceptable definition
- Resolution of commercially available techniques - trends and limitations
- The Necessary Resolution - what feature resolution and sensitivity is needed for answering biological questions?
- Discussion - Do MSI techniques meet these criteria?

06. Ion Traps: New Experiments and Old Tricks
Ion Trap MS Interest Group
Dan Austin presiding
Room 260/267

Short talks and group discussion will focus on two topics:

1. exciting new experiments
2. tutorial/perspective talks about challenging aspects of trap design and operation.

07. Metal Cationization of Biomolecules and its Analytical Applications
Metal Ion Coordination Chemistry Interest Group
Benjamin Bythell and Alex Shvartsburg presiding
Room 274

Mass spectrometry has been revolutionized since the 1980-s by the invention of soft sources such as electrospray ionization (ESI) and matrix-assisted laser desorption ionization (MALDI) that enabled intact ionization of increasingly large macromolecules. While ionization via attachment or withdrawal of one or more protons has been typical, addition of other charged groups (such as metal cations) is equally possible. Metalated biomolecules differ substantially from their protonated analogs in terms of isotopic distribution and thus MS spectral pattern, conformation, and hence ion mobility separation properties, and/or dissociation chemistry and consequently the products in MS/MS, which may have important analytical benefits. In particular, electron-transfer dissociation and similar direct mechanisms may fragment biomolecules cationized by a multiply-charged metal in a different manner than their polyprotonated analogs of same total charge. This workshop will encourage the discussion and adoption of novel analytical strategies that leverage metal cationization as an alternative to protonation in biological mass spectrometry.

08. Methods and Tools for Intra- and Inter-Experiment LC MS Performance Tracking
LC/MS & Related Topics Interest Group
Michael S. Bereman and Brent Dixon presiding
Room 275

The liquid chromatography mass spectrometry interest group aims to provide a collaborative atmosphere for research scientists, applications chemists, biologists and mass spectrometrists to share/discuss concepts for successful technology application. A major effort in the LC MS/MS community is harmonization and application of quality control metrics to provide confidence and reproducibility in published laboratory results. The chair and co-chair will provide an interactive workshop with insights from experience while engaging the audience. Performance tracking is a key component of transferable science which is strengthened through quality metrics. Confidence in results both within and across experiments lends itself to further application of discoveries to current and future work.

With active input from the audience, the chair and co-chair will discuss methods for monitoring LC MS/MS performance including: acquisition method type (targeted vs. DDA), metrics monitored (fundamental ID free vs. ID metrics), frequency of evaluation, and type of standard employed (simple vs. complex). In addition, an emphasis will be placed on available tools and software for tracking LC MS/MS performance in a longitudinal fashion.

09. Challenges and Progress towards the Site-Specific Characterization of Glycoprotein Heterogeneity
Ron Orlando presiding
Room 230

An early step typically employed in the characterization of glycoprotein glycans involves the liberation of the glycans from the peptide backbone. While this process facilitates the characterization of the glycans, information on the glycan distribution at each site is lost. This workshop focuses on approaches that are used to characterize intact glycoproteins/glycopeptides so that information on the attachment points of each glycan is obtained. The discussion will include: "top down" approaches and enzymatic digestion(s) followed by gas-phase or solution phase separations both condensed and gas phase separations. The use of targeted SRM approaches will also be presented and discussed, as these allow site-specific heterogeneity to be determined in complex mixtures. Methods that permit isomeric structural determination, such as MSⁿ, will also be discussed.

10. Mass Spectrometry Applications in Art, Cultural Heritage, and Natural History
Mehdi Moini presiding
Room 231

The purpose of this workshop is to discuss the application of mass spectrometry (MS) to art and cultural heritage objects, as well as natural history specimens. This will be an interactive workshop in which various subjects relevant to the application of MS to art and natural history 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 and aging of natural history and art 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) Forensic archeology. 5) Determination of the authenticity of art objects.

11. More DMPK Knowledge from Less Sample: Leveraging Modern LC-MS Instruments for Small Sample Amounts
DMPK Interest Group
Mustafa Varoglu and Kevin Bateman presiding
Room 232

Mass spectrometer performance has dramatically improved over the past several years, however sampling techniques for bioanalytical and drug metabolism studies have remained much the same. This DMPK-IG workshop will explore combining mass spectrometer improvements with microsampling of plasma, tissues and miniaturized assays to create better workflows to increase the quality of the DMPK data, and advance drug discovery and development projects. Topics to be explored by panel members and the workshop participants include microsampling blood for

MONDAY WORKSHOPS, 5:45 - 7:00 PM *continued*

plasma or dried blood spot analysis, the translational advantages of serial microsampling vs. traditional sampling methods and the ability to miniaturize assays. In addition, the opportunities for obtaining early tissue distribution data from low amounts of tissue either by homogenization or microdialysis in discovery vs. waiting for comprehensive imaging via MS-imaging or QWBA techniques will be examined. This workshop will explore the opportunities and barriers of leveraging the full abilities of our modern mass spectrometers to take advantage of limited sample amounts.

12. Metabolomics: Emerging Technologies for Continued Innovation

Metabolomics Interest Group
Sunia Trauger and Andrew Patterson presiding
Ballroom 222/224

The workshop will begin with brief presentations to stimulate discussion among the workshop participants. Emerging tools to facilitate metabolomics research and new technologies will be discussed. The moderators will highlight 2-3 recent developments in the field and survey the audience for their opinions. A panel of

invited scientists with expertise in field will be available to answer questions posed by the moderators and attendees. The workshop will close with a discussion where attendees can ask questions of the panelists. Some of the topics addressed will be: (i) new software tools for post-processing of untargeted metabolomics data, (ii) innovative experimental designs (iii) shotgun approaches with ion mobility, and (iv) metabolite identification by *in silico* fragmentation.

13. Which Career Path is Right for Me?
Young Mass Spectrometrists Interest Group
Olga Friese and Dian Su presiding
Ballroom 220/221

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

There are light refreshments in common areas.

TUESDAY WORKSHOPS, 5:45 - 7:00 PM

01. Laboratory Developed Test Guidance and Mass Spectrometric Diagnostics: Impact and Expectations

Clinical Chemistry Interest Group
Brain Rappold presiding
Room 130

In July 2014, the Food and Drug Administration released draft guidance on the use of laboratory developed tests (LDT's). With few exceptions, the use of mass spectrometry testing in patient care is performed by LDT's. The guidance requirements will impact all aspects of mass spectrometric testing in the clinic, from therapeutic drug monitoring to companion diagnostics. Additionally, the proposed guidance will affect the evolution of new biomarkers and new testing, particularly that of multi-index analyte tests. Representatives from manufacturing, industry, regulatory bodies and advocacy groups will deliver brief presentations on their considerations of the proposed directives, followed by an open forum in which the expectations for the industry to deliver on the submission of analytical platforms and assays to the agency will be discussed.

02. Current Trends, Gaps, and Needs in Workflows for Targeted Protein Quantitation by LC/MS

Nalini Sadagopan, Sue Abbatiello, and Dawn Dufield presiding
Room 131

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

We conducted this workshop at ASMS 2014 in Baltimore for the first time and was very successful. We sent out a survey with the participants prior to ASMS and the summary of the survey results were presented. We had about 150 attendees. Panel discussion with industry experts and thought leaders with the audience engagement was valuable. There was interest in continuing this workshop for 2015.

03. ProteomicsDB
Bernhard Kuster and Mathias Wilhelm presiding
Room 132

There is a growing landscape of various databases and repositories for MS and proteomics. In this workshop, we would like to present recent and future developments ProteomicsDB, a free, professionally developed solution to store and analyze mass spectrometry-based proteomics data. ProteomicsDB has a strong focus on functionality and secondary use of proteomics and mass spectrometry data. Following up on a successful workshop at ASMS 2014, we would like to encourage the involvement from the ASMS community, demonstrate typical use-cases for the web interface and API and describe our short and long-term plans.

04. FTMS: MS/MS at High Resolution
FTMS Interest Group
Nathan Kaiser and Don Smith presiding
Room 123/124

The workshop will focus on the practical aspects of tandem MS coupled to high resolution FTMS instruments. FTMS enables tandem MS experiments that are only capable on high resolution instruments. Applications that highlight these unique advantages will be discussed, such as top-down mass spectrometry by electron based methods (ETD/ECD), photo dissociation (UVPD), and collisional based methods (CID/CAD). The workshop will be open for discussion on applications, instrumentation, method development, and data analysis for high resolution tandem MS.

TUESDAY WORKSHOPS, 5:45 - 7:00 PM *continued*

05. Identifying Tandem Mass Spectra of Lipids and Carbohydrates
Bioinformatics Interest Group
Sangtae Kim and David Tabb presiding
Room 120/127

In shotgun proteomics, the identification of tandem mass spectra is taken as a given, and database search algorithms have occupied center stage for two decades. Tandem mass spectra from lipids and carbohydrates, on the other hand, have enjoyed considerably less bioinformatics support. In this panel, the Bioinformatics Interest Group features an introduction to these classes of data from two researchers who have recently published algorithms to automate identification. Dr. Haixu Tang will discuss his efforts to recognize the structures of glycans and glycopeptides. Tomas Cajka will discuss the creation of the LipidBlast spectral library as a tool for recognizing lipids from LC-MS/MS experiments in multiple instrument platforms.

06. MS Analysis of Antibody-Drug Conjugates
Pharmaceuticals Interest Group
Shawna Hengel and Christine Gu presiding
Room 260/267

Due to the success and of the 2013 and 2014 pharmaceutical interest group workshops, and continued interest in MS analysis of antibody-drug conjugates (ADCs), we propose a similar workshop for 2015. After a short informal presentation, less than ten minutes, the majority of the workshop would include an audience driven discussion with the opportunity to ask questions to a panel of experts. The organizers will have backup questions prepared for the panel to start or prompt the discussion if needed. The short presentation will provide an update on current workflows for ADC MS analysis and discuss details of the large range of characterization required for ADCs from initial MAb assessment to bioanalytical assay development. To identify potential panelists, gauge the level of interest of the ASMS community, and tailor the discussion we will send out a survey of open ended questions in April.

07. Measuring the Exposome: Strategies and Preliminary Results
The Exposomic Interest Group
Anthony Macherone and Skip Kingston presiding
Room 274

Genome-wide association studies (GWAS) rarely report relative risks greater than 1.2 for significant SNPs and estimates determined via mining of published data reveal overall genetic risks of about 5% for cancer and 12% for heart disease. These data suggest that the majority of causative factors for chronic human disease is not genetic but rather exposures or some combination of exposures and the genome (G). The exposome (E) is defined as the lifetime sum of these external and internal exposures. Accordingly, 80% - 90% of chronic human diseases is determined by E and GxE (including epigenetics).

The exposome encompasses the other "omes." For example, when one measures the transcriptome, proteome, or metabolome, they are measuring a slice of the exposome. Moreover, the exposome seeks the causative factors of disease to mitigate and prevent disease from occurring. The exposome is therefore a quantity of critical interest if we are to discover the non-genetic causative factors of chronic human diseases in a comprehensive manner. Mass spectrometric and other technologies such as spectroscopy and remote ("smart") sensors will characterize the exposome in large, prospective cohorts and provide reliable information on

exposure-risk relationships. The exposome paradigm will facilitate the translation of applied research into educational, behavioral and policy-based, risk mitigating interventions.

This workshop will review mass spectrometric based assays designed to measure the exposome both from a discovery and from a targeted perspective and present real data from case / control studies for discussion.

08. Advancements and Discussion of Mass Spectrometry Technology and Challenges within the Polymer and Material Fields
Polymer and Material MS Interest Group
Stephen Rumbelow and Gyorgy Vas presiding
Room 275

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

09. The ABCs of Being a Great Reviewer for Scientific Journals
Jenny Brodbelt presiding
Room 230

The peer review process is a critical step in the evaluation of original scientific manuscripts. This workshop will cover the nuts-and-bolts of the publication workflow with an emphasis on the peer review process. A panel of Editors will provide an inside look at how manuscripts are handled after submission, how reviewers are selected, and the role of the both authors and reviewers in the process. Tips for being a top reviewer will be covered, as well as how to become involved as a new reviewer.

10. How to Network without Really Trying: A Forum for Current (and Future) Mass Spectrometrists in Industry
Lucinda Cohen presiding
Room 231

Building on last year's successful "How to Succeed in Pharma without Really Trying" this workshop is designed to bring together mass spectrometrists from all environments including, but not limited to, mass spectrometry vendors, chemical, pharmaceutical, forensic and academic scientists. Attendees will be divided into small groups for break-out discussions on topics such as career transitions, work-life balance and mentoring. Participants will have the opportunity to rotate through these small group sessions in a "speed dating" format to discuss as many topics of interest as possible and enhance networking. Each small group will have an experienced scientist and facilitator. All are welcome. Attendees should bring business cards for distribution if possible.

TUESDAY WORKSHOPS, 5:45 - 7:00 PM continued

12. Invalidating your Cores Data: Examples on How to Check your Data and Report Results and Communicate Invalid or Bad Results to your Customers

**Analytical Laboratory Managers Interest Group
Brett Phinney and Chris Colangelo presiding
Ballroom 222/224**

One of Richard Feynman's more famous quotes involved integrity of scientific data: "If you're doing an experiment, you should report everything that you think might make it invalid -- not only what you think is right about it; other causes that could possibly explain your results; and things you thought of that you've eliminated by some other experiment, and how they worked -- to make sure the other fellow can tell they have been eliminated."

This workshop will present strategies, examples (both good and bad) and discussion on how to report data from analytical core facilities to customers and collaborators including potential problems and caveats that might make the data invalid. Often this challenging aspect is overlooked and under appreciated. Collaborators often have only a cursory understanding of what you did and communicating what may be wrong with the data you generated can be daunting.

Examples presented during this workshop may include

- Examples on communicating potential problems with your data

- How to temper expectations of collaborators when they get excited over initial results
- How to report inconclusive or odd results
- Examples on when your data was wrong and how you fixed it (or did not fix it)
- Examples where initial results conflict with subsequent results, and how you handled it

13. How Can Ion Mobility Spectrometry Separations Help Your Research?

**Ion Mobility Interest Group
Stephen Valentine, Matthew Bush and
Erin Baker presiding
Ballroom 220/221**

Over the last 20 years, ion mobility spectrometry (IMS) separations have been incorporated in many different instrument technologies such as DMA, FAIMS, drift tube IMS, traveling wave IMS, TIMS, SLIM, etc. With all of these different variations, many people have found confusion as to when to apply each technology. This workshop will focus on explaining several of the currently available IMS technologies and delve into the present applications being performed by each such as standalone IMS measurements and MS coupled metabolomic analyses, proteomic studies, and ion/ion reactions.

There are light refreshments in common areas.

WEDNESDAY WORKSHOPS, 5:45 - 7:00 PM

01. The Role of High Resolution Mass Spectrometry in the Regulatory Environment

**Flavor Fragrance and Foodstuff Interest Group
Walter Hammack and Tim Croley presiding
Room 130**

Last year the discussion centered around GC/MS, specifically high resolution options for GC/MS, which remains a staple of the food and food-related laboratories. This year, we propose to continue where we left off last year and focus on the role that high resolution mass spectrometry will play in the regulatory environment. The FDA has issued a guidance document for the use of high resolution data and a number of state and local labs are also beginning to look at HR data as a possible tool. In addition, a number of people are using the term, "non-targeted screening" and we would like to address this term, and, hopefully, come to a consensus on the use of this language. As in the past two years we intend to invite researchers from local, state, academic and government to share their experiences and then have a group discussion.

02. Emerging Contaminants for Emerging Scientists

**Environmental Interest Group
Chris Gill and Marc Engel presiding
Room 131**

This workshop will consist of up to 5 brief presentations from undergraduates, graduates and first-time post-doc researchers from industry, government and academia. The workshop will provide a forum to discuss their work, goals and any problems (up to 5 slides maximum). The forum is aimed at providing positive mentoring and feedback from the working group for the new generation of environmental mass spectrometrists.

03. Mass Spectrometry Instrumentation at the Forefront of Technology as Miscible Tools for Forensic and Security Evidence

**Forensics and Homeland Security Interest Group
Guido Verbeck and Glen Jackson presiding
Room 132**

Mass Spectrometry is arguably one of the most definitive techniques used to confirm the constituents of illicit drugs, energetic materials, urine, blood and other forensic evidence. It is because of the high sensitivity, high peak capacity, and low identification error that mass spectrometry has exploded into portable and imaging applications, as well as shotgun databasing of potential new illicit chemistries. The recent introduction of ambient ionization techniques—which differ somewhat from traditional GC/MS—has raised questions about the admissibility of different MS methods in courtroom battles. For example, are forensic and security applications of ambient ionization held to a different standard than GC/MS or LC/MS counterparts? When developing these instruments and applications, is there sufficient method validation conducted to provide sufficient confidence in analyses? In the proposed workshop, we offer a panel discussion of new mass spectrometric methods and technologies for forensics and security applications, and how we can satisfy the scientific and legal requirements in this important and rapidly developing area. We will also discuss the developments of mass spectrometric standards and recommendations in the various NIST-OSAC forensic science subcommittees.



WEDNESDAY WORKSHOPS, 5:45 - 7:00 PM *continued*

04. Gas-Phase Ion Chemistry: Thermodynamics, Kinetics, Structures and Spectroscopy Fundamentals Interest Group **Jos Oomens and Alessandra Ferzoco presiding** **Room 123/124**

The Fundamentals Interest Group has a long tradition of organizing the Fundamentals of Ion chemistry Workshop, which is well attended each year. We gladly extend this tradition at the upcoming ASMS conference.

As was commonly done at workshops in the recent past, we intend to invite several especially junior researchers to give a brief and informal presentation on their recent work (5 slides max). These short presentations should address unpublished work, work in progress and focus on aspects of the work such as unsolved questions, difficulties, mysteries, etc. The last slide should not so much contain conclusions, but rather open questions, which serve as introduction to a discussion on the subject. From previous experience, this usually leads to interesting, thoughtful and entertaining discussions, often providing novel insights to the presenter.

05. Emerging Technologies Advancing Mass Spectrometry Research: 3D Printing **Vincent Sica and Vilmos Kertesz presiding** **Room 120/127**

This workshop series concerns the use of technologies that support advancements in the field of mass spectrometry. With 3D printers becoming more accurate, reliable, and affordable, they are quickly finding their way into laboratories. This year's discussion will focus on the implementation of 3D printing to support mass spectrometry research.

A couple of 5-minute presentations showcasing applications of this technology will be followed by the discussion of the following topics:

1. Choice of hardware (Cost, Precision, Ease of use)
2. Choice of software (Design & Slicing)
3. Choice of material (Chemical compatibility, Durability, etc.)
4. Micro or macro applications (Are your prints designed for your lab or the MS community?)
5. Tips and tricks (Software or hardware related)
6. What improvements to 3D printing are necessary to further impact MS (New filament types? Higher resolution? etc.)

These discussions aim to not only educate on how to improve their research through 3D printing, but also to spark ideas on what the future may bring to the growing technologies of both 3D printing and mass spectrometry.

06. CHORUS - A Community Solution for the Storage Visualization, Sharing, and Analysis of Mass Spectrometry Data on the Cloud **Andrey Bondarenko, Michael MacCoss, Christine Wu, and Nathan Yates presiding** **Room 260/267**

The sharing, public dissemination, and analysis of mass spectrometry data has become a major challenge. We would like to present a community effort to provide a sustainable and professionally developed solution to the mass spectrometry field's needs. The application provides an intuitive graphical user interface specifically developed to organize and visualize mass spectrometry data. Data can be uploaded and kept private, shared with a group of collaborators, or made entirely public. Over the

last two years CHORUS has gained almost 1000 users and these users have placed >55,000 data files into the service. We are now in the process of releasing new tools that will enable the analysis of data stored within CHORUS and improving the interaction of our data with existing client and server tools.

We have received a lot of feedback from our users and we have used this feedback to alter our development efforts. We would like to discuss improvements made to CHORUS over the last year and what new analysis capabilities have and are being added. We will discuss our goals and get feedback from the community on our current and long-term priorities.

07. The Big Fat Questions: The Future for Lipidomics in Cell Biology and Clinical Diagnostics? **Lipids and Lipidomics Interest Group** **Stephen Blanksby and Christer Ejsing presiding** **Room 274**

Innovation in mass spectrometry has fueled the rapid expansion of lipidomics research over the last decade. Increasingly powerful instrumentation and accompanying software tools are now available to wide range of researchers around the world. This workshop will reflect on some of the big research questions in cell biology, biotechnology and clinical medicine and ask whether current mass spectrometry-based lipidomics can underpin future breakthroughs in these disciplines. The discussion will be led by a panel of experts who will opine on current impediments to development in their respective fields. Panellists will challenge participants to consider how lipid mass spectrometry can breakthrough such roadblocks and drive innovation in biochemical understanding, clinical diagnosis or novel therapeutics. Conceptual discussion will then be facilitated on whether currently available lipid mass spectrometry approaches can provide these answers or whether new technology is required.

08. Characterization of Protein Therapeutics by Mass Spectrometry **Biotherapeutics Interest Group** **Damian Houde, Alain Balland, and Jason Hogan presiding** **Room 275**

This workshop will be a forum to discuss the current technical challenges and solutions for the characterization of protein therapeutics by mass spectrometry. Mass spectrometry is now used for protein characterization from discovery through product development. The workshop will lead off with a short background overview of a few topics ranging from protein modifications, higher-order structure characterization, protein batch comparability and biosimilarity, or protein production lot release to initiate a discussion. Recent advancements in instrumentation and software for data analysis and reporting may also be discussed.

09. Getting the Most out of Undergraduate Research in Mass Spectrometry **Undergraduate Research in MS Interest Group** **Elaine Marzluff presiding** **Room 230**

This panel discussion, aimed at undergraduate students and their mentors, will focus on helping undergraduate students leverage their undergraduate research in mass spectrometry into successful experiences in graduate school and industry.



WEDNESDAY WORKSHOPS, 5:45 - 7:00 PM continued

10. Working with Federal Agencies to Obtain Research Support : Mock NIH Study Section and Q&A with Agency Staff
Charles G. Edmonds and Douglas M. Sheeley presiding
Room 231

12. Ligand Binding Assays (LBA) and LC-MS/MS Integrated Antibody-Drug Conjugate (ADC) Bioanalysis -Immuno-capture LC-MS/MS Hybrid Assays: Challenges, Solutions, and Complementarity with LBA Regulated Bioanalysis Interest Group
Jian Wang presiding
Ballroom 222/224

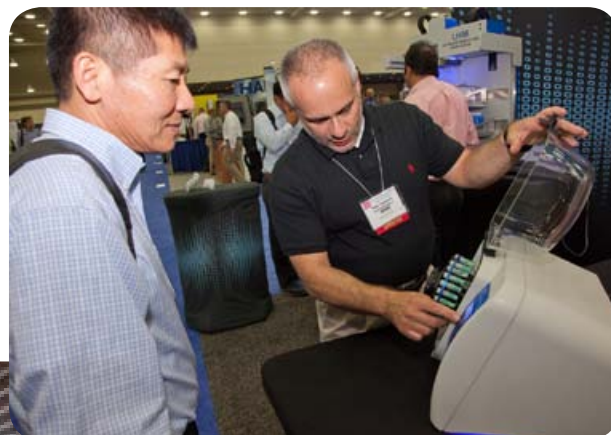
Antibody-drug conjugates (ADCs) consist of a cytotoxic drug covalently bound to an antibody (mAb) via a linker. The complex structure of ADCs presents unique bioanalytical challenges and requires novel strategies. Multiple analytes in the heterogeneous mixture may contribute to the efficacy and safety of ADCs. Four quantitative assays are considered essential, industry-wide, in ADC PK bioanalysis, (1) total-antibody, (2) conjugated-antibody, (3) conjugated-payload, and (4) unconjugated-payload. Immuno-capture LC-MS/MS hybrid assays are required for the analysis of conjugated-payload and are viable alternatives or complementary to ligand binding assays (LBA) for the analysis of total-antibody and conjugated-antibody.

Each hybrid assay involves three essential experimental steps: capture, enzymatic cleavage or digestion, and LC-MS/MS detection. After the initial immuno-capture of the ADC, the conjugated-payload assays proceed with the cleavage of the payload using Cathepsin B enzyme and LC-MS measurement of the released payload, while the conjugated-antibody and total-antibody assays measure the signature peptides generated by trypsin digestion of the mAb. Immuno-capture with either anti-id or anti-payload capture reagents could be conducted using magnetic beads or cartridges formats.

This workshop will focus on current hybrid assay strategies, applications, and their complementarity to ligand binding assays. Technical details of hybrid assay development and validation will be discussed. The capability of hybrid assays to appropriately quantify mixtures of analytes with different Drug to Analyte Ratio (DAR) will be addressed as well.

13. Hydrogen-Deuterium Exchange, Covalent Labeling and Crosslinking Interest Group
Joshua Sharp and David Weis presiding
Ballroom 220/221

The workshop will provide a forum for discussing the latest HDX, covalent labeling and crosslinking methods for protein analysis. The program will provide an opportunity to discuss MS-based methods, data analysis routines and applications with the attendees. The goal of the program will be to stimulate discussion and convey useful experimental detail you can take back to your lab.



SUNDAY EVENING AND MONDAY MORNING ORAL SESSIONS

4:00 – 4:45 PM, SUNDAY

Attention First-time Graduate Students and Undergrads
Plan your Strategy: What to See and Do at ASMS
Elaine Marzluff and JC Poutsma, presiding
Ballroom 220/221

5:00 – 6:30 PM, SUNDAY

TUTORIAL SESSION
Vicki Wysocki (The Ohio State University) presiding
Hall 5



5:00 – 5:45 pm
Statistical Experimental Design:
The Building Blocks of a Good Experiment

Ann L. Oberg
Mayo Clinic



5:45 – 6:30 pm
Metabolite Profiling at the 'Omic' Scale:
Untargeted Does not Mean Unplanned

Gary Patti
Washington University, St Louis

6:45 – 7:45 PM, SUNDAY

Conference Opening
Vicki Wysocki (The Ohio State University) presiding
Hall 5

Welcome, Vicki Wysocki
ASMS Vice President for Programs



The Human Gut Microbiome and Healthy
Growth

Jeffrey L. Gordon
Washington University, St. Louis School of
Medicine

7:45 – 9:00 PM, SUNDAY

WELCOME RECEPTION
Poster/Exhibit Hall
Conference name badge is required

8:30 – 10:30 AM, MONDAY MORNING

INSTRUMENTATION: NEW DEVELOPMENTS IN
IONIZATION AND SAMPLING

Peter Nemes (George Washington University) presiding
Hall 5

- MOA am 08:30 **Matrix Assisted Ionization: Enhancing Mass Spectrometry through Proper Sampling Conditions on Small Portable to High Performance Mass Spectrometers;** Sarah Trimpin^{1,2}; Christian Reynolds^{1,2}; Casey Foley¹; Shubhashis Chakrabarty^{1,3}; Daniel Woodall¹; Jessica DeLeeuw¹; Joshua Fischer¹; Shameemah Thawoos¹; Zachary Devereaux¹; Bryan Harless¹; Claudio Verani¹; Mathew Allen¹; Thomas Sanderson²; Karin Przyklenk²; Paul Stemmer⁴; ¹Department of Chemistry, Wayne State University, Detroit, MI; ²Cardiovascular Research Institute, Wayne State Uni, Detroit, MI; ³MSTM LLC, Wayne State University, Detroit, MI; ⁴Institute of Environmental Health Science, WSU, Detroit, MI
- MOA am 08:50 **Infrared, Visible, and and Ultraviolet Laser Ablation for High Spatial Resolution Sampling Mass Spectrometry;** Chinthaka A. Seneviratne; Suman Ghorai; Kermit K. Murray; Louisiana State University, Baton Rouge, LA
- MOA am 09:10 **Hybrid Optical Microscope/Laser Ablation Liquid Capture Mass Spectrometry System Providing Co-Registered Optical Bright Field, Fluorescence and Mass Spectral Images;** Gary J. Van Berke¹; John Cahill¹; Vilmos Kertesz¹; Thomas Covey²; Julian Burke³; ¹Oak Ridge National Laboratory, Oak Ridge, TN; ²ABSciex, Concord, Ontario, Canada; ³Leica Microsystems Group, Cambridge, UK
- MOA am 09:30 **T-probe: a Novel Device to Implement Online in situ single Cell Analysis Using Mass Spectrometry;** Renmeng Liu; Ning Pan; Zhibo Yang; University of Oklahoma, Norman, OK
- MOA am 09:50 **Fabrication of Silica Multi-nozzle Emitters for Multiple Electrospray Ionization by Selective Etching of a Microstructured Fiber with Doped Regions;** Yueqiao Fu¹; Timothy Hutama¹; Graham Gibson¹; Steeve Morency²; Jean-Francois Viens²; Younes Messaddeq²; Richard Oleschuk¹; ¹Queen's University, Kingston, Canada; ²COPL at Université Laval, Quebec City, Canada
- MOA am 10:10 **Square-Wave Facilitated Electroosmosis in a Theta Glass nESI Emitter: Improved Turbulent Mixing on the Milliseconds Timescale;** Christine Fisher; Ryan T. Hilger; Feifei Zhao; Scott A. McLuckey; Purdue University, West Lafayette, IN

8:30 – 10:30 AM, MONDAY MORNING

INFORMATICS: ALGORITHMIC AND STATISTICAL ADVANCES

Oliver Serang (Thermo Fisher Scientific) presiding
Room 130/132

- MOB am 08:30 **The Midpoint Mixed Model with a Missingness Mechanism: A Likelihood Based Framework for Relative Quantification of Mass Spectrometry Data;** Jonathon O'Brien; Harsha P. Gunawardena; Bahjat Qaqish; University of North Carolina at Chapel Hill, Chapel Hill, NC
- MOB am 08:50 **Comparative Study of Automated Feature Selection and Classification Techniques For Detection of Histological Features by Mass Spectrometry Imaging;** Nazanin Zounemat Kermani¹; Ottmar Golf²; Sabine Guenther¹; Robert D. Goldin¹; James Kinross¹; Abigail V. M. Speller¹; Kirill Veselkov¹; Zoltan Takats¹; ¹Imperial College London, London, UK; ²Justus Liebig University, Giessen, Germany



- MOB am 09:10 **Multi-species Identification of Polymorphic Peptide Variants via Propagation in Spectral Networks**; [Seungjin Na](#)¹; Sam Payne²; Nuno Bandeira¹; ¹University of California, San Diego, La Jolla, CA; ²Pacific Northwest National Lab, Richland, WA
- MOB am 09:30 **Clustering Spectra Based on Fragment Rarity**; [Matthew The](#); Lukas Käll; *Royal Institute of Technology - KTH, Stockholm, Sweden*
- MOB am 09:50 **Improved Computational Demultiplexing for Data Independent Acquisition Data Acquired by MSX or with Overlapping Windows**; [Jarrett Egerton](#)¹; Richard S. Johnson¹; Yue Xuan²; Philip M Remes³; Brendan Maclean¹; Gennifer Merrihew¹; Olga Vitek⁴; Vlad Zabrouskov³; Markus Kellmann²; Michael J. Maccoss¹; ¹Univ of Washington, Seattle, WA; ²Thermo Fisher Scientific, Bremen, N/A; ³Thermo Fisher Scientific, San Jose, CA; ⁴Northeastern University, Boston, MA
- MOB am 10:10 **Improved Computational Analysis of Imaging Mass Spectrometry Data through Sparse Intensity Variation De-noising**; [Yousef El Aalamat](#)^{1,2}; Nico Verbeeck^{1,2}; Junhai Yang⁴; Bart De Moor^{1,2}; Richard M. Caprioli⁴; Etienne Waelkens^{5,6}; Raf Van De Plas^{3,4}; ¹KU Leuven, ESAT-STADIUS, 3001 Leuven, Belgium; ²iMinds Medical IT, 3001 Leuven, Belgium; ³Delft University of Technology, Delft, Netherlands; ⁴Vanderbilt University, Nashville, TN; ⁵KU Leuven, Dept. of Cellular and Molecular, 3000 Leuven, Belgium; ⁶KU Leuven, SybioMa, 3000 Leuven, Belgium

**8:30 – 10:30 AM, MONDAY MORNING
PROTEIN COMPLEXES: ACTIVATION & DISSOCIATION**
[Michal Sharon](#) (Weizmann Institute of Science) presiding
Room 123/124

- MOC am 08:30 **Assembly and Disassembly of Protein Complexes Involved in Complement Activation Monitored by Q-ToF and Orbitrap Analyzers with Extended Mass Ranges**; Guanbo Wang; Andrey Dyachenko; [Albert J.R. Heck](#); *Utrecht University, Utrecht, Netherlands*
- MOC am 08:50 **On and Off: Probing Aβ Peptide Association with Aggregation Inhibiting Peptides and Small Molecules via Dissociation**; [Ashley S. Phillips](#)¹; Harriet L. Cole²; Mark Taylor³; Isabel Riba-Garcia¹; Cait E. MacPhee²; Richard D. Unwin¹; Garth J. S. Cooper¹; David Allsop³; Perdita E. Barran¹; ¹University of Manchester, Manchester, UK; ²University of Edinburgh, Edinburgh, UK; ³University of Lancaster, Lancaster, UK
- MOC am 09:10 **Laser Activation of Soluble and Membrane Protein Assemblies for Structural Biology**; [Victor A. Mikhailov](#); Ildir Liko; Todd Mize; Carol Robinson; *University of Oxford, Oxford, UK*
- MOC am 09:30 **Surface Induced Dissociation Reveals Substructural Information Consistent With The Interfacial Analysis Of Protein Complexes**; [Sophie R. Harvey](#); Royston S. Quintyn; Yang Song; Jing Yan; Aniruddha N. Sahasrabudhe; Vicki H. Wysocki; *The Ohio State University, Columbus, Ohio*
- MOC am 09:50 **Determining Iron-Binding Motifs in Biological Macromolecular Assemblies with IR-Induced Native Electron Capture Dissociation**; [Owen Skinner](#); Michael McAnally; Richard Van Duyn; Philip Compton; Neil L. Kelleher; *Northwestern University, Evanston, IL*

- MOC am 10:10 **Structural Interpretation of Gas-phase Protein Unfolding: New Applications in Structural Biology and Protein Engineering**; [Joseph Eschweiler](#); Brandon Ruotolo; *University of Michigan, Ann Arbor, MI*

**8:30 – 10:30 AM, MONDAY MORNING
GLYCOPEPTIDES AND GLYCOPROTEINS**
[Xiaoping Hironowski](#) (Biogen, Inc.) presiding
Room 120/127

- MOD am 08:30 **Isotope Targeted Glycoproteomics (IsoTaG): A Chemical Proteomics Platform for N- and O-Glycopeptide Discovery**; [Christina Woo](#); Anthony Iavarone; Carolyn Bertozzi; *UC Berkeley, Berkeley, California*
- MOD am 08:50 **Integrated Bottom-Up and Middle-Down Glycoproteomics**; Kshitij Khatri; Joshua Klein; Yi Pu; Catherine E. Costello; Cheng Lin; [Joseph Zaia](#); *Boston University, Boston, MA*
- MOD am 09:10 **O-GlcNAc Modification Site-Specific Characterization of ABL2 Produced from a ΔNagZ E. coli Co-Expression System by Tandem Mass Spectrometry**; [Kelin Wang](#)¹; Octavia Y. Goodwin¹; Fabrizio Donnarumma¹; Behrooz Zekavat²; Touradj Solouki²; Megan A. Macnaughtan¹; Kermit K. Murray¹; ¹Louisiana State University, Baton Rouge, LA; ²Baylor University, Waco, TX
- MOD am 09:30 **Glazer: An Integrated Software Platform for interpretation of N-glycopeptide MS/MS Data with Robust FDR Control, without ExD Dissociation**; [John Froehlich](#); Peter Warren; Richard Lee; *Children's Hospital Boston, Boston, MA*
- MOD am 09:50 **Analysis of the Cell Surface N-Glycoproteome by Integrating Metabolic Labeling, Copper-free Click Chemistry and LC-MS/MS**; [Johanna Smeekens](#); Weixuan Chen; Ronghu Wu; *Georgia Institute of Technology, Atlanta, GA*
- MOD am 10:10 **Top-down and Middle-Down CE-MS for Deep Characterization of Biopharmaceuticals with Glycan Heterogeneity: Identification of Interferon-β1 and Monoclonal Antibody Proteoforms**; [David R. Bush](#)¹; Arseniy M. Belov¹; Li Zang²; Alexander R. Ivanov¹; Barry L. Karger¹; ¹Northeastern University, Boston, MA; ²Biogen Idec, Inc., Cambridge, MA

**8:30 – 10:30 AM, MONDAY MORNING
METABOLOMICS:**
NEW MS TECHNOLOGIES AND APPLICATIONS
[Ian Blair](#) (University of Pennsylvania) presiding
Theater

- MOE am 08:30 TBD
- MOE am 08:50 **The Human Plasma REDOXOME: A Broad Compendium of Oxidative Stress Biomarkers**; [Miriam Sindelar](#); Qiuying Chen; Darya Akimova; Ronald G Crystal; Steven S Gross; *Weill Medical College of Cornell, New York, NY*
- MOE am 09:10 **Metabolic Changes and Oxidative Stress Pathways in a Novel Patient Derived IDH1-R132H Mutant Oligodendroglioma Xenograft Assessed by Mass Spectrometry Imaging**; [Guillaume Hochart](#)¹; Fred Fack²; Fabien Pamelard¹; Jonathan Stauber¹; Simone P. Niclou²; ¹ImaBiotech, MS Imaging Dept., Loos, France; ²Luxembourg Institute of Health, Luxembourg, Luxembourg

MONDAY MORNING ORAL SESSIONS

- MOE am 09:30 **Highly Reproducible and Robust LC-MS/MS Assay for Targeted Profiling of 180 Metabolites Using a Single HILIC Chromatography Method;** Danijel Djukovic¹; Jiangjiang Zhu¹; Haiwei Gu¹; Farhan Himmati¹; Daniel Raftery^{1,2}; ¹University of Washington Medicine, Seattle, WA; ²Fred Hutchinson Cancer Research Center, Seattle, WA
- MOE am 09:50 **Simultaneous Targeted Quantification and Untargeted Metabolomics of Meconium Steroid Content;** Nathaniel Snyder; Alexander Frey; Bo Young Park; *Drexel University, Philadelphia, PA*
- MOE am 10:10 **Effect of Controlled Diet on Biomarker Measurements in the Clinic;** Petia Shipkova; Serhiy Hnatyshyn; Michael Reily; Yi Luo; Rose Christian; *Bristol Myers Squibb, Princeton, NJ*

8:30 – 10:30 AM, MONDAY MORNING QUANTITATIVE PROTEOMICS IN SYSTEMS BIOLOGY/CELLULAR PATHWAY ANALYSIS

**Lan Huang (University of California, Irvine) presiding
Room 106**

- MOF am 08:30 **PALM (Pulse Azidohomoalanine Labeling in Mammals) Analysis for Global Analysis of Newly-Synthesized Proteins in Animal Models of Disease;** John Yates¹; Daniel Mclatchey¹; Yuanhui Ma¹; Reuben Shaw²; ¹The Scripps Research Institute, La Jolla, CA; ²The Salk Institute, LaJolla, CA
- MOF am 08:50 **Refining the Human Proteome: Integrated Analysis of Human Tissues by RNAseq, Proteomics, Phosphoproteomics and Antibodies;** Hannes Hahne¹; Dongxue Wang¹; Björn Hallström²; Lihua Li¹; Anna Asplund³; Mathias Wilhelm¹; Harald Marx⁴; Frederik Ponten³; Mathias Uhlen²; Bernhard Kuster¹; ¹Technical University Munich, Freising, Germany; ²KTH Royal Institute of Technology, Stockholm, Sweden; ³Uppsala University, Uppsala, Sweden; ⁴University Wisconsin-Madison, Madison, WI
- MOF am 09:10 **An ORFeome-based, Mass Spectrometry-driven Human Protein Interaction Network;** Edward L. Huttlin¹; Lily Ting¹; Raphael Bruckner¹; Fana Gebreab¹; Melanie Gygi¹; John Szpyt¹; Stanley Tam¹; Gabriela Zarraga¹; Gregory Colby¹; Kurt Baltier¹; Rui Dong²; Virginia Guarani¹; Laura Pontano Vaites¹; Alban Ordureau¹; Ramin Rad¹; Brian Erickson¹; Martin Wuehr¹; Joel Chick¹; Bo Zhai¹; Deepak Kolipakkam¹; Julian Mintseris¹; Robert Obar¹; Tim Harris³; Sypros Artavanis-Tsakonas³; Mathew Sowa¹; Pietro DeCamilli²; Joao Paulo¹; J. Wade Harper¹; Steven Gygi¹; ¹Harvard Medical School, Boston, MA; ²Yale School of Medicine, New Haven, CT; ³Biogen Idec, Cambridge, MA
- MOF am 09:30 **A Sentinel Protein Assay for the Simultaneous Quantification of Cellular Processes;** Martin Soste¹; Rita Hrabakova²; Stefanie Wanka³; Andre Melnik¹; Paul Boersema¹; Christian von Mering³; Paola Picotti¹; ¹ETH Zurich, Zurich, Switzerland; ²Academy of Sciences of the Czech Republic, Libechov, Czech Republic; ³University of Zurich, Zurich, Switzerland
- MOF am 09:50 **Systems Biology Approach Reveals Drug Resistance Mechanism in Multiple Myeloma;** Junmin Peng; *St. Jude Children's Research Hospital, Memphis, TN*
- MOF am 10:10 **Mapping the Sites of Interaction of a Hub Protein in a Transcription Factor Protein Interaction Network using the HaloTag;** Charles Banks; Gina Boanca; Zachary Lee; Laurence Florens; Michael

Washburn; Stowers Institute for Medical Research, Kansas City, MO

8:30 – 10:30 AM, MONDAY MORNING ENERGY, PETROLEUM, AND BIOFUELS: ADVANCES IN MS DESIGN AND INFORMATICS

**Matthew Hurt (Chevron) presiding
Ballroom 222/224**

- MOG am 08:30 **Comparison of Atmospheric Solid Analysis Probe with Other Atmospheric Pressure Ionization Sources by Ion Mobility-Mass Spectrometry using PetroOrg Software;** Mathilde Farenc^{1,5}; Yuri E. Corilo^{2,3}; Priscila M. Lalli³; Eleanor Riches⁴; Ryan P. Rodgers²; Carlos Afonso¹; Pierre Giusti⁵; ¹University of Rouen, Mont Saint Aignan, FRANCE; ²National High Magnetic Field Laboratory, Tallahassee, FL; ³Future Fuels Institute, Tallahassee, FL; ⁴Waters Corporation, Wilmslow, UK; ⁵TOTAL Refining and Chemicals, Gonfreville l'Orcher, France
- MOG am 08:50 **Dissociation of Petroleum Components using Fourier Transform Ion Cyclotron Resonance Mass Spectrometry;** Juan Wei; Simona Gherghel; Mark Barrow; *University of Warwick, Coventry, UK*
- MOG am 9:10 **APCI and APPI-GC/MS-MS for Characterization of the Macondo Crude Oil and the Oil Spill;** Vladislav Lobodin^{1,2}; Ryan P. Rodgers^{1,2}; ¹National High Magnetic Field Laboratory, Tallahassee, FL; ²Future Fuels Institute, Tallahassee, FL
- MOG am 09:30 **Alicyclic Structures in Sediments and Kerogens: Potential Sources of Petroleum;** Patrick Hatcher; Blaine Hartman; Nicole Didonato; Derek Waggoner; *Old Dominion University, Norfolk, VA*
- MOG am 09:50 **Algae Biomass Characterization by Traveling Wave Ion Mobility Mass Spectrometry;** Maira Fasciotti¹; Ingrid Chastinet Ribeiro¹; Paulo Roque Martins Silva¹; Thays V. Monteiro¹; Gustavo H. M. F. Souza²; Julia Itacolomy da Silva¹; Romeu J. Daroda¹; Valnei S. Cunha¹; Claudia Maria Luz Lapa Teixeira³; Amarjit S. Sarpal¹; ¹INMETRO, Duque De Caxias, Brazil; ²Waters Corporation, Rio de Janeiro, Brazil; ³National Institute of Technology, INT, Rio de Janeiro, Brazil
- MOG am 10:10 **Identification of the Phenol Functionality in Monomeric Lignin Degradation Products via Negative Ion-Molecule Reactions with Diethylmethoxyborane;** Hanyu Zhu; Hilikka Kenttämäa; *Purdue University, West Lafayette, IN*

8:30 – 10:30 AM, MONDAY MORNING ADVANCES IN SOFTWARE AND HARDWARE TO IMPROVE DMPK WORKFLOWS

**Hongying Gao (Pfizer, Inc.) presiding
Ballroom 220/221**

- MOH am 08:30 **Automated LC/MS Quantitation Method Development Using a Hybrid Quadrupole-Orbitrap Mass Spectrometer;** Jonathan L. Josephs; Keeley Murphy; Hongxia (Jessica) Wang; David Brant; Jamie K Humphries; Kristi Akervik; Nicholas Duczak, Jr; Mark Sanders; *Thermo Fisher Scientific, San Jose, CA*
- MOH am 08:50 **Utilization of MassMetaSite for in vitro and in vivo Metabolite Identification of Complex Therapeutic Peptides;** Heather Trexler¹; Kevin Bateman¹; Richard Gundersdorf¹; Fabien Fontaine²; Rodger Tracy¹; Kenneth Koeplinger¹; Ismael Zamora²; Mark Cancilla¹; ¹Merck & Co., West Point, PA; ²Lead Molecular Design, S.L., Sant Cugat Del Valles, Spain

MONDAY MORNING AND AFTERNOON ORAL SESSIONS

- MOH am 09:10 **Fully Integrated Novel IMS-QToF Informatics Platform for Rapid Drug Screening and Elucidation**; Russell Mortishire-Smith¹; Jayne Kirk¹; Nick Tomczyk¹; Martin Palmer¹; Richard Denny¹; Alan Prile¹; Simon Cubbon¹; Yun Alelyunas²; Mark Wrona²; ¹Waters MS Technologies, Wilmslow, UK; ²Waters Corporation, Milford, MA
- MOH am 09:30 **A Novel Platform for Automated High-Throughput LC-MS/MS Analysis of *In Vitro* ADME and *In Vivo* ADME PK Samples**; Andreas Luippold; Wolfgang Joerg; Klaus Klinder; Daniel Bischoff; *Boehringer Ingelheim Pharma GmbH & Co KG, Biberach, GERMANY*
- MOH am 09:50 **Untargeted and Rapid Detection and Characterization of Modified Monoclonal Antibodies using LC-TripleTOF and Multivariate Statistical Analysis**; Ming Yao¹; Xu Wang²; Weiping Zhao¹; Li Ma¹; John T. Mehl¹; Yi Zhang²; Sahana Mollah²; W. Griff Humphreys¹; Mingshe Zhu¹;
- MOH am 10:10 **Advances in HRMS and *in vitro* Systems Provide an Option to Detect and Characterize Human Disproportionate Metabolites of Loratadine**; Ragu Ramanathan¹; Cornelia Smith²; Lakshmi Ramanathan²; Caroline Lee³; Helen Shen²; Zamas Lam²; ¹Pfizer, Groton, CT; ²QPS, Newark, DE; ³Ardea Biosciences, San Diego, CA

10:30 AM – 2:30 PM, MONDAY
MONDAY POSTER SESSION
Poster/Exhibit Hall
Lunch concessions are open 11:00 am – 2:00 pm

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

MONDAY AFTERNOON ORAL SESSIONS

2:30 – 4:30 PM, MONDAY AFTERNOON
ION MOBILITY, FAIMS & DMS:
NEW DEVELOPMENTS AND APPLICATIONS
Melvin Park (Bruker Daltonics, Inc.) presiding
Hall 5

- MOA pm 2:30 **Very Long Path Length High Resolution Ion Mobility Separations using Structures for Lossless Ion Manipulations (SLIM)**; Richard D. Smith; Ian K. Webb; Ahmed Hamid; Sandilya V. B. Garimella; Yehia M. Ibrahim; Aleksey V. Tolmachev; Spencer A. Prost; Gordon A. Anderson; Erin S. Baker; *Pacific Northwest National Laboratory, Richland, WA*
- MOA pm 2:50 **3D Printed Concentric Ring Drift Tube with Nanoelectrospray Ionization Source for ion Focusing, Separation, and Detection under Ambient Conditions**; Zane Baird; Adam Hollerbach; R. Graham Cooks; *Purdue University, West Lafayette, IN*
- MOA pm 3:10 **Improvement of Resolution and Peak Capacity for Differential Ion Mobility Spectrometry Scans using Linked Helium and Compensation Field Scans**; Brandon G. Santiago; Rachel A. Harris; Gary L. Glush; *The University of North Carolina at Chapel Hill, Chapel Hill, NC*
- MOA pm 3:30 **A Polarizable Projection Approximation Method to Predict Molecular Cross Section for Use in Ion Mobility / Mass Spectrometry Studies.**; Christian Bleiholder; *Florida State University, Tallahassee, FL*
- MOA pm 3:50 **Differential Photofragmentation Patterns for Mobility Selected Glycans**; Kelsey A. Morrison; Enamul H. Khan; Brian H. Clowers; *Washington State University, Pullman, WA*
- MOA pm 4:10 **Coupling FAIMS and LESA for the Analysis of Proteins Directly from Biological Substrates**; Andrew Creese¹; Joscelyn Sarsby¹; Rian Griffiths¹; Elizabeth Randall¹; Alan Race²; Josephine Bunch²; Helen Cooper¹; ¹University of Birmingham, Birmingham, United Kingdom; ²The National Physical Laboratory, Teddington, N/A

2:30 – 4:30 PM, MONDAY AFTERNOON
INFORMATICS: METABOLOMICS
Alexey Nesvizhskii (University of Michigan) presiding
Room 130/132

- MOB pm 2:30 **Accurate Mass for Improved Metabolite Identification via High-Resolution GC/MS**; Nicholas W. Kwiecien; Derek J. Bailey; Matthew J. P. Rush; Arne Ulbrich; Alexander S. Hebert; Michael S. Westphall; Joshua J. Coon; *University of Wisconsin, Madison, WI*
- MOB pm 2:50 **Exploring Correlation Networks for the Analysis of Metabolomics Data**; Alla Karnovsky¹; Sumanta Basu²; Bill Duren¹; Charles Evans¹; George Michalidis¹; Charles Burant¹; ¹University of Michigan, Ann Arbor, MI; ²University of California, Berkeley, CA
- MOB pm 3:10 **Improving the Efficiency of Feature Annotation in Untargeted Metabolomics: Integrating Metabolic Pathway Analysis with XCMS and METLIN**; Anna Chen^{1,2}; Rebecca Schugar³; Peter Crawford⁴; Gary Patti^{1,2}; ¹Washington University in St. Louis, St. Louis, MO; ²Washington University Medical School, St. Louis, MO; ³Cleveland Clinic Lerner Research Institute, Cleveland, OH; ⁴Sanford-Burnham Medical Research Institute, Orlando, FL
- MOB pm 3:30 **Constructing MSⁿ Mass Spectral Library for More Accurate Metabolite Identification**; Xiaoyu Yang; Pedatsur Neta; Yuxue Liang; Stephen Stein; *NIST, Gaithersburg, MD*
- MOB pm 3:50 **Greazy: Open-Source Software for Automated Phospholipid MS/MS Identification**; Michael Kochen¹; Matthew Chambers¹; Jerry Holman¹; Thomas Metz²; Alexey Nesvizhskii³; Susan T. Weintraub⁴; David Tabb¹; ¹Vanderbilt University, Nashville, TN; ²Pacific Northwest National Laboratory, Richland, WA; ³University of Michigan, Ann Arbor, MI; ⁴Univ. of Texas HSC, San Antonio, TX
- MOB pm 4:10 **Translating Molecular Information from HR Imaging MS data: towards Spatial Annotation of the Cellular Metabolome**; Andrew D. Palmer^{1,2}; Eric Weaver³; Marco Hennrich¹; Jens Fuchser⁴; Michael Becker⁴; Anne-Claude Gavin¹; Amanda B. Hummon³; Theodore Alexandrov^{1,5}; ¹EMBL Heidelberg, Heidelberg, Germany; ²University of Bremen, Bremen, Germany; ³University of Notre Dame, Notre Dame, IN; ⁴Bruker Daltonik GmbH, Bremen, Germany; ⁵SCILS, Bremen, Germany

MONDAY AFTERNOON ORAL SESSIONS

2:30 – 4:30 PM, MONDAY AFTERNOON

TOP-DOWN PROTEIN ANALYSIS

Mark McComb (Boston University School of Medicine) presiding
Room 123/124

- MOC pm 2:30 **Stochastic SILAC for Intact Protein Quantitation in Any Organism Using Any Growth Medium or Feed**; Jared R. Auclair; Joseph Salisbury; Jennifer Quijada; Jeffrey Agar; *Northeastern University, Boston, MA*
- MOC pm 2:50 **Characterizing Protein Complexes and Mapping their Surface and Interfacial Residues in One Native Top-Down MS Experiment with FTICR**; Huilin Li; Rachel R. Ogorzalek Loo; Joseph A. Loo; *University of California, Los Angeles, Los Angeles, CA*
- MOC pm 3:10 **Detailed Characterisation of Photoactivatable Metallo-drug Interactions with Peptides, Proteins, and DNA by High Resolution Tandem FT-ICR MS**; Christopher A. Wootton; Andrea F. Lopez-Clavijo; Evyenia Shaili; Mark P. Barrow; Peter J. Sadler; Peter B. O'Connor; *University of Warwick, Coventry, UK*
- MOC pm 3:30 **Top-Down Proteogenomics of Pathogenic *Helicobacter***; Egor Vorontsov^{1,2}; Frédéric Fischer¹; Christian Malosse^{1,2}; Hilde de Reuse¹; Julia Chamot-Rooke^{1,2}; *Institut Pasteur, Paris, France*; ²CNRS, Paris, France
- MOC pm 3:50 **Integrated Proteogenomic Analysis of CompRef Breast Tumor Xenografts via Top-Down and Bottom-Up Proteomics**; Ioanna Ntai¹; Richard Leduc¹; Ryan Fellers¹; Petra Erdmann-Gilmore²; Sherri Davies²; Jeanne Rumsey²; Bryan Early¹; Paul Thomas¹; Shunqiang Li²; Philip Compton¹; Matthew Ellis³; Kelly Ruggles⁴; David Fenyo⁵; Emily Boja⁶; Henry Rodriguez⁶; Reid Townsend²; Neil Kelleher¹; ¹*Northwestern University, Evanston, IL*; ²*Washington University School of Medicine, St. Louis, Missouri*; ³*Baylor College of Medicine, Houston, TX*; ⁴*NYU Langone Medical Center, New York, NY*; ⁵*New York University, New York, NY*; ⁶*National Cancer Institute, Bethesda, MD*
- MOC pm 4:10 **Intact Protein Profiling: On the Hunt for Wound Healing Factors**; Giuseppe Infusini¹; Condina Mark²; Jemma Evans³; Lois Salamonsen³; Andrew Webb¹; ¹*Walter & Eliza Hall Institute, Parkville, Australia*; ²*Bruker, Preston, Australia*; ³*MIMR-PHI, Clayton, Australia*

2:30 – 4:30 PM, MONDAY AFTERNOON

PLANT-OMICS

A. Daniel Jones (Michigan State University) presiding
Room 120/127

- MOD pm 2:30 **A Family-Wide Phosphoproteomic Study of Leucine-Rich Repeat Receptor-Like Kinase Autophosphorylation in *Arabidopsis thaliana***; Srijeet Mitra¹; Ruiqiayang Chen¹; Murali Dhundaydham¹; Xiaofeng Wang¹; Kevin Blackburn¹; Uma Kota¹; Michael Goshe¹; Daniel Schwartz²; Steven Huber³; Steven Clouse¹; ¹*North Carolina State University, Raleigh, NC*; ²*University of Connecticut, Storrs, CT*; ³*University of Illinois, Urbana, IL*
- MOD pm 2:50 **Rapid and Comprehensive Proteome Profiling in Plants**; Catherine Minogue; Alicia Richards; Harald Marx; Dhileepkumar Jayaraman; Junko Maeda; Shanmugam Rajasekar; Michael S. Westphall; Michael R. Sussman; Jean-Michel Ane; Joshua J. Coon; *University of Wisconsin, Madison, WI*
- MOD pm 3:10 **Metabolic Interplay between the Asian Citrus Psyllid and its *Proffella* Symbiont: An Achilles' Heel of the Citrus Greening Insect Vector**; Michelle Cilia^{1,2}; John Ramsey³; Richard S. Johnson⁴; Jason Hoki³; David Hall⁵; Frank

Schroeder³; Michael J. MacCoss⁴; ¹*United States Department of Agriculture, ARS, Ithaca, NY*; ²*Department of Plant Pathology, Cornell University, Ithaca, NY*; ³*Boyce Thompson Institute for Plant Research, Ithaca, NY*; ⁴*Univ of Washington, Seattle, WA*; ⁵*United States Department of Agriculture, ARS, Fort Pierce, FL*

- MOD pm 3:30 **Integrating Multiple -omic Resources to Better Characterize Photosynthetic Diversity in Constitutive and Facultative Crassulacean Acid Metabolism Plants**; Paul Abraham¹; Hengfu Yin³; Timothy Tschaplinski¹; Gerald Tuskan¹; Xiaohan Yang¹; Bernard W. M. Wone²; Won Cheol Yim²; Karen A. Schlauch²; John C. Cushman²; Robert Hettich¹; ¹*Oak Ridge National Laboratory, Oak Ridge, TN*; ²*University of Nevada, Reno, NV*; ³*Chinese Academy of Forestry, Zhejiang, China*
- MOD pm 3:50 **Using Mass Spectrometry-Based Metabolomics for Chemotaxonomy Studies**; Dominique Ardura; Oliver Fiehn; *Genome Center, University of California, Davis, CA*
- MOD pm 4:10 **Chemical Isotope Labeling LC-MS for Profiling Spatial Distribution of Metabolites in Ginseng Roots**; Chiao-Li Tseng; Liang Li; *University of Alberta, Edmonton, Canada*

2:30 – 4:30 PM, MONDAY AFTERNOON

CLINICAL DIAGNOSTICS

Christine Snozek (Mayo Clinic) presiding
Theater

- MOE pm 2:30 **Personalized Detection of Multiple Myeloma Tumor Burden**; Melissa Hoffman; Saavedra-Roman Luis; Sean Yoder; Rachid Baz; Kaaron Benson; Aunshka Collins; Robert Sprung; Jamie Teer; John Koomen; *Moffitt Cancer Center, Tampa, FL*
- MOE pm 2:50 **Cerebrospinal Fluid Tau Phosphopeptides: Detection, Quantitative Analysis and Assessment for the Diagnosis of Neurological Diseases**; Nicolas R Barthélemy^{1,5}; Christophe Hirtz¹; Martial Seveno³; Susanna Schraen-Maschke²; Randall J Bateman⁵; Audrey Gabelle¹; François Becher⁴; Philippe Marin³; Sylvain Lehmann¹; ¹*LBPC, IRMB, CHU Montpellier St. Eloi, Montpellier, France*; ²*Inserm, UMR 837, IMPRT, Lille, France*; ³*PPF, IGF, CNRS-UMR 5203, Inserm U661, Montpellier, France*; ⁴*CEA, iBiTec-S, SPI, LEMM, Gif-sur-Yvette, France*; ⁵*Washington University School of Medicine, St. Louis, MO*
- MOE pm 3:10 **MALDI Imaging Classification of Tumors in Formalin-Fixed Paraffin-Embedded Tissues.**; Rita Casadonte¹; Mark Kriegsmann²; Jan Hendrik Kobarg³; Dennis Trede³; Michael Becker⁴; Peter Maaß⁵; Sören-Oliver Deininger⁴; Katrin Friedrich⁶; Daniela Aust⁶; Christian Pilarsky⁶; Gustav Baretton⁶; Mike Otto^{1,7}; Jörg Kriegsmann⁷; ¹*Proteopath GmbH, Trier, Germany*; ²*University of Heidelberg, Heidelberg, Germany*; ³*SCiLS GmbH, Bremen, Germany*; ⁴*Bruker Daltonik GmbH, Bremen, Germany*; ⁵*University of Bremen, Bremen, Germany*; ⁶*University of Dresden, Dresden, Germany*; ⁷*Center for Histology, Cytology and Molecular Diagn, Trier, Germany*
- MOE pm 3:30 **Analysis of Urinary Free Oligosaccharides for the Diagnosis of Lysosomal Storage Diseases using UPLC-SRM**; Rongrong Huang; Tim Wood; *Greenwood Genetic Center, Greenwood, SC*
- MOE pm 3:50 **MALDI-TOF Analysis of Whole Blood: Its Usefulness and Potential in the Assessment of HbA1c Levels in Diabetes Mellitus**; Stephen J. Hattan¹; Kenneth Parker¹; Marvin Vestal¹; David Herold³; Jane Yang⁴; Mark W Duncan²; ¹*SimulTOF/*



MOE pm 4:10 VIC Instruments, Sudbury, MA; ²Univ. Colorado, School of Medicine, AURORA, CO; ³VAMC/ UCSD, San Diego, CA; ⁴UCSD, San Diego, CA
Clinical Diagnostics of Rare Kidney Disease with UPLC-MS/MS; Finnur Eiriksson^{1,2}; Hrafnhildur Runolfsson¹; Vidar O. Edvardsson³; Runolfur Palssson^{1,3}; Margret Thorsteinsdottir^{1,2}; ¹University of Iceland, Reykjavik, Iceland; ²ArcticMass, Reykjavik, Iceland; ³Landspítali, Reykjavik, Iceland

**2:30 – 4:30 PM, MONDAY AFTERNOON
 PTMS: ADVANCES IN ISOLATION, ENRICHMENT,
 DERIVATIZATION AND SEPARATION**

**Erik Soderblom (Duke University School of Medicine) presiding
 Room 106**

MOF pm 2:30 **PTM Profiling in Serum & Plasma to Identify Potential Biomarkers by Immunoaffinity LC-MS Methods**; Hongbo Gu; Jian Min Ren; Jeffrey Silva; Cell Signaling Technology, Danvers, MA

MOF pm 2:50 **Optimization of Automated Phosphopeptide Enrichment using Fe3+-NTA IMAC on the Bravo AssayMAP Liquid Handling Robotics Platform**; Jennifer Abelin¹; Caitlin Feeney¹; Jinal Patel¹; Lola Fagbami¹; Xiaodong Lu¹; Daniel Lam¹; Jason Russell²; Steve Murphy²; Gavin Fischer²; Steven A. Carr¹; Jacob D. Jaffe¹; ¹Broad Institute of MIT and Harvard, Cambridge, MA; ²Agilent Technologies, Inc., Madison, WI

MOF pm 3:10 **Quantifying Reversible Oxidation of Protein Thiols in Photosynthetic Organisms**; William Slade¹; Emily Werth¹; Evan McConnell¹; Sophie Alvarez²; Leslie Hicks¹; ¹University of North Carolina, Chapel Hill, NC; ²Danforth Center, St Louis, MO

MOF pm 3:30 **An Integrated Workflow for Enrichment, Separation, and Quantitation of Plasma Glycoproteins in Prostate Cancer and Benign Prostate Hyperplasia**; Sarah Totten; Majlinda Kullolli; Cheylene Tanimoto; James Brooks; Sharon Pitteri; Stanford University School of Medicine, Palo Alto, CA, USA

MOF pm 3:50 **Isobaric Labeling Enables 10-Plex Quantitative Analysis Of Ubiquitylated Peptides: A Diagnostic Ion to Improve Identification and Quantification**; Christopher M. Rose¹; Marta Isasa¹; Sean A. Beausoleil²; Steven P. Gygi¹; ¹Harvard Medical School, Boston, MA; ²Cell Signaling Technology, Danvers, MA

MOF pm 4:10 **A New Method for Enhanced Identification of Citrullinated Peptides using SWATH-MS Technology**; Ronald Holawinski; Justyna Fert-Bober; Jennifer Van Eyk; Cedars Sinai Medical Center, Los Angeles, CA

**2:30 – 4:30 PM, MONDAY AFTERNOON
 IMAGING: BIOMEDICAL APPLICATIONS**

**Jihyeon Lim (Albert Einstein College of Medicine) presiding
 Ballroom 222/224**

MOG pm 2:30 **Direct Structure-Specific Quantitative Molecular Imaging of Neurotransmitters in Experimental Parkinson's Disease**; Mohammadreza Shariatgorji¹; Anna Nilsson¹; Patrik Källback¹; Erwan Bezdard³; Per Svenningsson²; Per E. Andren¹; ¹Uppsala University, Uppsala, Sweden; ²Karolinska Institutet, Stockholm, Sweden; ³Université de Bordeaux, Bordeaux, France

MOG pm 2:50 **Glycopathology and Glycoimmunology of Prostate Cancer Tissues by N-Glycan MALDI Mass Spectrometry Imaging**; Richard R Drake; Ellen Jones; Thomas Powers; Medical University of South Carolina, Charleston, SC

MOG pm 3:10 **Anatomy-guided Differential Analysis of Imaging Mass Spectrometry Data Using the Allen Mouse**

Brain Atlas; Nico Verbeeck^{1,2}; Jeffrey Spraggins⁴; Junhai Yang⁴; Bart De Moor^{1,2}; Richard M. Caprioli⁴; Etienne Waelkens^{5,6}; Raf Van de Plas^{3,4}; ¹ESAT-STADIUS, KU Leuven, Leuven, Belgium; ²iMinds Medical IT, Leuven, Belgium; ³Delft University of Technology, Delft, Netherlands; ⁴Vanderbilt University, Nashville, TN; ⁵Dept. Cellular and Molecular Medicine, KU Leuven, Leuven, Belgium; ⁶Sybioma, Leuven, Belgium

MOG pm 3:30 **Application of MALDI-MSI to Identify Biomarkers of Radiation-Induced Lung Injury and Medical Countermeasure Development**; Claire L. Carter; Jace W. Jones; Isabel L. Jackson; Zeljko Vujaskovic; Sean Kearney; Kory Barrow; Kaitlyn Kieta; Cheryl Taylor-Howell; Allison Gibbs; Ann M. Farese; Thomas J. MacVittie; Maureen A. Kane; University of Maryland, Baltimore, MD

MOG pm 3:50 **Tools for Multivariate Analysis (MVA) of 2D and 3D Mass Spectrometry Images**; Daniel Graham; Lara Gamble; Department of Bioengineering, UW, Seattle, Washington

MOG pm 4:10 **Phospholipid MALDI Imaging Mass Spectrometry Stratification of Colorectal Cancer Liver Metastasis Clinical Biopsies**; Heath Patterson¹; Balqis Alabdulkarim²; Aurélien Thomas³; Martin M. Marcinkiewicz⁴; Anthoula Lazaris²; Peter Metrakos²; Pierre Chaurand¹; ¹Dept. of Chemistry, University of Montreal, Montreal, Quebec, Canada; ²Dept. of Surgery, McGill University, Montreal, Quebec, Canada; ³Unit of Toxicology, CURML, University of Lausanne, Lausanne, Switzerland; ⁴Cytochem Inc., Montreal, Quebec, Canada

**2:30 – 4:30 PM, MONDAY AFTERNOON
 QUANTITATIVE ANALYSIS IN DRUG DISCOVERY FOR
 SMALL MOLECULES**

**Rick King (PharmaCadence Analytical Services) presiding
 Ballroom 220/221**

MOH pm 2:30 **The Evaluation and Development of Automated Workflows in Blood, Plasma and Urine Using Volumetric Absorptive Microsampling (VAMS)**; Leanne Grafmuller; Joseph Tweed; Zhenhua Gu; Mark Wallace; Mark Milisci; Rick Steenwyk; Ragu Ramanathan; Pfizer, Groton, CT

MOH pm 2:50 **Calibration Curve Sensitivity: The Role of Internal Standard on Slope and Precision of Clinical LC-MS/MS Assays**; Brian Rappold; Andrew Lickteig; Matthew Salske; Essential Testing, Collinsville, IL

MOH pm 3:10 **LC-MS/MS and LC-HRMS Approaches to Support Toxicity Studies of a Glycolipid Vaccine Adjuvant**; Kasie Fang; Chester L. Bowen; Jonathan Kehler; Kendal Ryter; GlaxoSmithKline, King of Prussia, PA

MOH pm 3:30 **Improving Quantitative Analysis through Reduction of Matrix Suppression Effects by coupling Multi-Dimensional Chromatography to ESI-MS**; Tom Van De Goor; Stephan Buckenmaier; Agilent Technologies, Waldbronn, GERMANY

MOH pm 3:50 **Whole blood Analysis using New Solid Phase Microextraction Devices and Investigation of the Hematocrit Effect**; Nathaly Reyes Garces; Barbara Bojko; Janusz Pawliszyn; University of Waterloo, Waterloo, CANADA

MOH pm 4:10 **Comparison of Travelling Wave IMS-QToF Geometries and Acquisition Modes for Quantitative Analysis**; Mark Wrona¹; Yun Alelyunas¹; Jayne Kirk²; Martin Palmer²; Nick Tomczyk²; Russell Mortishire-Smith²; ¹Waters Corporation, Milford, MA; ²Waters MS Technologies, Wilmslow, United Kingdom

MONDAY AFTERNOON AND TUESDAY MORNING ORAL SESSIONS

4:45 – 5:30 PM, MONDAY AFTERNOON

AWARD LECTURE

Jenny Brodbelt (University of Texas, Austin) presiding
Hall 5



**Award for a Distinguished Contribution
in Mass Spectrometry**

Brian T. Chait
The Rockefeller University

5:45 – 7:00 PM, MONDAY AFTERNOON
WORKSHOPS

There are light refreshments in the common areas.

01. Has Photoionization Reached its Potential? Focus on APPI, Room 130
02. Enabling proteomics informatics on the Amazon cloud, Room 131
03. Advanced MS and separation approaches for biofuels and petroleum, Room132

04. The Galaxy Framework for MS-based Informatics, Room 123/124
05. Defining Resolution in Imaging MS - A Quest for Solid Ground, Room 120/127
06. Ion Trap Interest Group: new experiments and old tricks, Room 260/267
07. Metal Cationization of Biomolecules and its Analytical Applications, Room 274
08. Methods and Tools for Intra- and Inter-Experiment LC MS Performance Tracking, Room 275
09. Challenges and progress towards the site-specific characterization of glycoprotein heterogeneity, Room 230
10. Mass Spectrometry Applications in Art, cultural Heritage, and Natural History, Room 231
11. More DMPK Knowledge from Less Sample: Leveraging Modern LC-MS Instruments for Small Sample Amounts, Room 232
12. Metabolomics: Emerging Technologies for Continued Innovation, Ballroom 222/224
13. Which Career Path is Right for Me? - Young Mass Spectrometrists Workshop, Ballroom 220/221

AFTER 8:00 PM
CORPORATE HOSPITALITY SUITES
RENAISSANCE GRAND HOTEL

TUESDAY MORNING ORAL SESSIONS

8:30 – 10:30 AM, TUESDAY MORNING
INSTRUMENTATION: TIME-OF-FLIGHT AND QTOF
Jody C. May (Vanderbilt University) presiding
Hall 5

- TOA am 08:30 **High Resolution Multi-Reflecting TOFMS with Multiplexing by Encoded Frequent Pulsing for Increasing the Duty Cycle 10-100 Times;** Peter Willis¹; Viatcheslav Artaev¹; George Tikhonov¹; Kevin Siek¹; Vasily Makarov²; Anatoly Verenchikov²; ¹LECO Corporation, St Joseph, MI; ²MSC-CG, Bar, Montenegro
- TOA am 08:50 **Novel Operating Modes of an Ion Mobility Quadrupole Time-Of-Flight Hybrid Instrument;** Jason L Wildgoose; Kevin Giles; Keith Richardson; Steven Pringle; *Waters Corporation, Manchester, UK*
- TOA am 09:10 **A W-geometry ortho-TOF MS with High Resolution and Up To 100% Duty Cycle for MS/MS;** Samuel Merenbloom¹; Nic Bloomfield¹; Alexandre Loboda²; Igor Chernushevich¹; ¹SCIEX, Concord, Canada; ²Fluidigm Canada Inc., Markham, Canada
- TOA am 09:30 **Inductively Coupled Plasma Distance-Of-Flight Mass Spectrometry with an ionCCD Camera detector;** Elise Dennis¹; Steven J. Ray¹; Christie G. Enke²; Charles J. Barinaga³; David W. Koppelaar³; Gary M. Hieftje¹; ¹Indiana University, Bloomington, IN; ²University of New Mexico, Placitas, NM; ³Pacific NW Nat'l Laboratory, Richland, WA
- TOA am 09:50 **A New Instrument for High Speed, True Pixel and Large Dataset MALDI TOF Imaging;** Jens Höhndorf; Andreas Haase; Arne Fütterer; Michael Becker; Armin Holle; *Bruker Daltonik GmbH, Bremen, Germany*
- TOA am 10:10 **Artificial Intelligent Algorithm, Particle Swarm Optimization (SWARM), Opens a New Era for Mass Spectrometer Application Tune;** Huy Bui¹; Christian Klein¹; Dorothy Yang¹; Yevgeny Kaplun¹; Syed Lateef¹; Gregor Overney¹; Koen Sandra²; ¹Agilent Technologies, Santa Clara, CA; ²Research Institute for Chromatography, Kortrijk, Belgium

8:30 – 10:30 AM, TUESDAY MORNING
INFORMATICS: MULTI-OMICS INTEGRATION
Akhilesh Pandry (Johns Hopkins University) presiding
Room 130/132

- TOB am 08:30 **STATegra – Studying B-Cell Differentiation by Combination of Multiple Omics Datasets;** The STATegra Consortium; Andreas Schmidt; Axel Imhof; *ZFP - LMU Munich, Munich, GERMANY*
- TOB am 08:50 **The Quest for Novel Proteoforms: Integration of Proteomics and Ribosome Profiling Based Translatomics;** Jeroen Crappé; Volodimir Olexiouk; Daria Gawron; Elvis Ndah; Sandra Steyaert; Alexander Koch; Steven Verbruggen; Ellen De Meester; Sarah De Keulenaer; Petra Van Damme; Gerben Menschaert; *Ghent University, Ghent, Belgium*
- TOB am 09:10 **Peptide Search Engine Approach for the Detection Of Translated Mutations Based on Sequencing Data, Mutation Databases and Exhaustive Codon Changes;** Pavel Sinitcyn; Stefka Tyanova; Matthias Mann; Juergen Cox; *Max-Planck-Institute of Biochemistry, Martinsried, Germany*
- TOB am 09:30 **Enosi: A web-accessible Proteogenomic Pipeline for Identification of Proteomic Event using Large-scale NGS Data;** Seong Won Cha; Sunghye Woo; Vineet Bafna; *University of California, San Diego, La Jolla, CA*
- TOB am 09:50 **SearchGUI and PeptideShaker Deployed in the Galaxy Framework: A Powerful Informatics Platform for Protein Identification and Beyond;** Ira Cooke¹; Bjoern Groening²; Harald Barsnes³; Marc Vaudel³; Lennart Martens⁴; James Johnson⁶; Candace Guerrero⁵; Getiria Onsongo⁵; John Chilton⁷; Pratik Jagtap⁸; Tim Griffin⁵; ¹La Trobe University, Melbourne, Australia; ²University of Freiburg, Freiburg, Germany; ³University of Bergen, Bergen, Norway; ⁴Ghent University, Ghent, Belgium; ⁵University of Minnesota, Minneapolis, MN; ⁶University of Minnesota Supercomputing Institute, Minneapolis, MN; ⁷Pennsylvania State



TOB am 10:10 *University, State College, PA; ⁸Center for Mass Spectrometry and Proteomics, UMN, St.Paul, MN*
Mass Spectrometry Centric Analysis of Public Proteomic Data in ProteomicsDB; Mathias Wilhelm¹; Hans-Christian Ehrlich²; Judith Schlegl³; Wilhelm Becker²; Lars Rueckert²; Hannes Hahne¹; Bernhard Kuster¹; ¹Technical University Munich, Freising, GERMANY; ²SAP SE, Innovation Center Potsdam, Potsdam, Germany; ³SAP SE, Walldorf, Germany

8:30 – 10:30 AM, TUESDAY MORNING

IMAGING: INSTRUMENTATION AND METHOD

Gary Van Berkel (Oak Ridge National Laboratory) presiding
 Room 123/124

TOC am 08:30 **Constant-Distance Mode for High-Resolution Ambient Imaging Using Nanospray Desorption Electropray Ionization Mass Spectrometry**; Julia Laskin¹; Ingela Lanekoff²; Andrey Liyu¹; Mathew Thomas¹; ¹Pacific NW National Laboratory, Richland, WA; ²Uppsala University, Uppsala, SWEDEN

TOC am 08:50 **Enhancing the Analytical Capabilities of DESI Imaging using Ion Mobility Separation- Providing Superior Insights of Biological Samples**; Emmanuelle Claude¹; Emrys A Jones^{1,3}; Mark Towers¹; Karolina Skraskova²; Ron M.A. Heeren²; Jim Langridge¹; ¹Waters Corporation, Wilmslow, UK; ²Maastricht University, Maastricht, NL; ³Imperial College London, London, UK

TOC am 09:10 **Best of Both Worlds? - Matrix-enhanced SIMS Reveals New Information in Cerebellum Grey and White Matter**; Masoumeh Dowlatshahi Pour¹; Per Malmberg¹; Andrew Ewing^{1,2}; ¹Chalmers University of Technology, Gothenburg, Sweden; ²University of Gothenburg, Gothenburg, Sweden

TOC am 09:30 **Transmission Geometry MALDI: Assessing Ion Generation/Collection Efficiency at Laser Spot Sizes Down to 1 μm**; Andre Zavalin; Junhai Yang; Richard Caprioli; *Vanderbilt University, Nashville, TN*

TOC am 09:50 **MALDI-2: Sensitive MS Imaging with Laser-Induced Postionization at 5 micrometer pixel size**; Jens Soltwisch¹; Hans Ketting^{1,2}; Simeon Vens-Cappell^{1,2}; Marcel Wiegelmann¹; Johannes Muthing¹; Klaus Dreisewerd^{1,2}; ¹Institute for Hygiene, University of Muenster, Muenster, GERMANY; ²Interdisciplinary Center for Clinical Research, Muenster, Germany

TOC am 10:10 **High Performance MALDI MS Imaging with a Scanning Laser Beam**; Jan Preisler^{1,2}; Antonin Bednarik^{1,2}; Pavel Kuba³; Eugene Moskovets⁴; ¹Chemistry Department, Masaryk University, Brno, Czech Republic; ²CEITEC, Masaryk University, Brno, Czech Republic; ³FME, University of Technology, Brno, Czech Republic; ⁴MassTech, Inc., Columbia, MD

8:30 – 10:30 AM, TUESDAY MORNING

MEMBRANE PROTEINS

Frank Sobott (University of Antwerp) presiding
 Room 120/127

TOD am 08:30 **Structure and Dynamics of a Membrane Protein-Surfactant Assembly Studied by Ion-Mobility Mass Spectrometry and Molecular Dynamics Simulations**; Antoni Borysik; Antoni Borysik; *King's College London, London, UK*

TOD am 08:50 **Probing the Structure & Interactions of Membrane Protein Complexes Using Orbitrap Mass Spectrometry**; Joseph Gault¹; Todd Mize¹; Eugen Damoc²; Mikhail Belov²; Alexander Makarov²;

Carol V. Robinson¹; ¹Oxford University, Oxford, UK; ²Thermo Fisher Scientific, Bremen, Germany

TOD am 09:10 **Membrane Proteins and Complexes: Using an FTMS to "Shake it Off"**; Iain Campuzano²; HuiLin Li¹; Dhanashri Bagal²; Paul Schmier²; Joseph A. Loo¹; ¹UCLA, Los Angeles, CA; ²AMGEN, Thousand Oaks, CA

TOD am 09:30 **Lipid Binding Induces Conformational Changes in the Peripheral Membrane Protein PDZK1**; Jamie A. Moroco¹; Thomas E. Wales¹; Jennifer L. Halford²; Nadine Elowe⁴; Olivier Kocher³; Monty Krieger²; John R. Engen¹; ¹Northeastern University, Boston, MA; ²Massachusetts Institute of Technology, Cambridge, MA; ³Harvard Medical School, Boston, MA; ⁴Broad Institute, Cambridge, MA

TOD am 09:50 **Using Ion Mobility-Mass Spectrometry to Study the Integral Membrane Protein Translocator Protein (TSPO) and its Therapeutic Ligand Binding Behavior**; Shuai Niu¹; Fei Li²; Shelagh Ferguson-Miller²; Brandon Ruotolo¹; ¹University of Michigan, Ann Arbor, MI; ²Michigan State University, East Lansing, MI

TOD am 10:10 **Fast size-exclusion Chromatography Electrospray-Ionization Mass Spectrometry of Integral Membrane Proteins**; Whitaker Cohn; Joseph Capri; Chris Ryan; Julian Whitelegge; *University of California LA, Los Angeles, CA*

8:30 – 10:30 AM, TUESDAY MORNING

LIPIDOMICS: NEW MS TECHNOLOGIES AND APPLICATIONS

David Ford (St. Louis University School of Medicine) presiding
 Theater

TOE am 08:30 **High Mass Resolution Lipid Imaging: A New Workflow for Guiding FTICR Analysis with High-Speed MALDI TOF Data**; Jeffrey Spraggins¹; Raf Van De Plas²; Nico Verbeeck³; Etienne Waelkens³; Shannon Cornett⁴; Richard Caprioli¹; ¹Vanderbilt University, Nashville, TN; ²Delft University of Technology, Delft, Netherlands; ³K.U. Leuven, Leuven, Belgium; ⁴Bruker Daltonics Inc., Billerica, MA

TOE am 08:50 **Abnormal Biogenic Lipid Signalling In Chronic Pain Elucidated With Multimodal Imaging Mass Spectrometry**; Jorg Hanrieder¹; Jie Su³; Lorenz Gerber²; Kim Kultima⁴; Camilla Svensson³; ¹University of Gothenburg, Mölndal, Sweden; ²SLU, Umeå, Sweden; ³Karolinska Institute, Stockholm, Sweden; ⁴Uppsala University, Uppsala, Sweden

TOE am 09:10 **Separating Lipid Isomers with LC-IMS-MS Measurements to Understand Their Role in Biochemical Processes**; Erin S. Baker; Kristin E. Burnum-Johnson; Jennifer E. Kyle; Xing Zhang; Matthew E. Monroe; Yehia M. Ibrahim; Thomas O. Metz; Richard D. Smith; *Pacific Northwest National Laboratory, Richland, WA*

TOE am 09:30 **Multidimensional Mass Spectrometry-based Shotgun Lipidomics Analysis of Vinyl Ether Diglycerides**; Kui Yang; Christopher M. Jenkins; Beverly Dilthey; Richard W. Gross; *Washington University, St. Louis, MO*

TOE am 09:50 **A Shotgun Lipidomics Approach to Study Non-Alcoholic Fatty Liver Disease (NAFLD)**; Amani Batarseh¹; Harry Glickman¹; David Peake³; Alexander Mazur²; Peter Metrakos¹; Tommy Nilsson¹; ¹RI-MUHC, Montreal, CA; ²McGill University, Montreal, CA; ³Thermo Fisher Scientific, San Jose, USA

TUESDAY MORNING ORAL SESSIONS

TOE am 10:10 **Isotopically-labelled TrEnDi: New Technology to Increase the Sensitivity and Selectivity of MS-Based Lipid Analysis of Complex Biological Samples**; Carlos R. Canez; Karl V. Wasslen; Hyunmin Lee; Samuel W. J. Shields; Jeffrey M. Manthorpe; Jeffrey C. Smith; *Carleton University, Ottawa, Canada*

8:30 – 10:30 AM, TUESDAY MORNING PHOSPHOPROTEOMICS IN DISEASE

**Jun Qu (State University of New York, Buffalo) presiding
Room 106**

TOF am 08:30 **Kinome Profiling of Glioblastoma Samples by Mass Spectrometry**; Lennard Dekker¹; Marcel Stoop¹; Jan-Willem Jachtenberg¹; Lona Zenedyepour¹; Noor Abdulhussain¹; Jos Joore²; Sieger Leenstra^{1,3}; Theo Luider¹; ¹*Erasmus Medical Center, Rotterdam, Netherlands*; ²*Pepscope, Utrecht, Netherlands*; ³*Elisabeth Medical Hospital, Tilburg, Netherlands*

TOF am 08:50 **Unravelling Signaling Pathways in Niemann-Pick type C Disease by "in-vivo" Phosphoproteomic Analysis of Mouse Cerebellum**; Nicolas Lebesgue¹; Martin Fitzpatrick¹; Allie Colaco²; Frances Platt²; Albert J.R. Heck¹; Simone Lemeer¹; ¹*Utrecht University, Utrecht, The Netherlands*; ²*Oxford University, Oxford, UK*

TOF am 09:10 **Phosphoproteomic and Proteomic Identification of Oncogenic Pathways in LKB1 Dependent Non-Small Cell Lung Cancer by Two-Dimensional LC-MS/MS**; Nilini Ranbaduge; Joseph Amann; Tadaaki Yamada; Zhen Wang; David Carbone; Vicki Wysocki; *The Ohio State University, Columbus, OH*

TOF am 09:30 **Assessment of Rational Peptide Design for Kinase Activity Assays by Mass Spectrometry**; Marcel Stoop¹; Jetse Scholma²; Maikel Peppelenbosch¹; Jos Joore³; Theo Luider¹; ¹*ErasmusMC, Netherlands, Rotterdam, Netherlands*; ²*University of Twente, Enschede, Netherlands*; ³*Pepscope B.V., Utrecht, Netherlands*

TOF am 09:50 **Advanced Ti⁴⁺-IMAC (phospho)proteomics to Identify Novel Melanoma Companion Drug Targets and Uncover Phosphorylation Dynamics and Pathway Dependence in Senescence Signaling**; Violette Gautier^{1,2}; Gianluca Maddalo^{1,2}; Erik L. de Graaf^{1,2}; Joanna Kaplon³; Marjon A. Smit³; Kristel Kemper³; Daniel S. Peeper³; Albert J.R. Heck¹; A.F. Maarten Altelaar¹; ¹*Utrecht University, Utrecht, Netherlands*; ²*Netherlands Proteomics Center, Utrecht, Netherlands*; ³*The Netherlands Cancer Institute, Amsterdam, Netherlands*

TOF am 10:10 **Characterization of Regulatory Protein Phosphorylations in Dynamic Golgi Reassembly by Quantitative Label-Free Phosphoproteomic Analysis**; Hye Kyong Kweon; Shijiao Huang; Yanzhuang Wang; Philip Andrews; *University of Michigan, Ann Arbor, MI*

8:30 – 10:30 AM, TUESDAY MORNING EMERGING ENVIRONMENTAL CONTAMINANTS

**Susan Richardson (University of South Carolina) presiding
Ballroom 222/224**

TOG am 08:30 **Unequivocal Identification of Detection-Based Transformation Products in Real-World Environmental Samples using High-Resolution MS and NMR**; Damia Barcelo^{1,2}; Bozo Zonja¹; Sandra Perez¹; Antonio Delgado^{3,4}; ¹*Water and Soil Research Group, IDAEA-CSIC, Barcelona, SPAIN*; ²*Catalan Institute of Water Research - ICRA, Girona, SPAIN*; ³*University of Barcelona (UB); Faculty of Pharmacy, Barcelona, SPAIN*; ⁴*Res. Unit on BioActive Molecules(RUBAM), IQAC-CSIC, Barcelona, Spain*

TOG am 08:50 **Systematic Suspect Screening and Identification of Sulfa Drug Metabolites in the Aquatic Environment**; Marius Majewsky¹; Thomas Glauner²; Craig Marvin³; Harald Horn^{1,4}; ¹*Karlsruhe Institute of Technology, Water Chemistry, Karlsruhe, Germany*; ²*Agilent Technologies Sales & Services GmbH, Waldbronn, Germany*; ³*Agilent Technologies Inc., Wilmington, DE*; ⁴*DVGW Research Laboratories, Karlsruhe, Germany*

TOG am 09:10 **Rapid Tracking of ZnO and CeO₂ Nanoparticles through Drinking Water Treatment by Single Particle ICP-MS**; Ariel Donovan^{1,2}; Honglan Shi^{1,2}; Yinfa Ma¹; Craig Adams^{2,3}; Chady Stephan⁴; Todd Eichholz⁵; ¹*Missouri S&T, Rolla, MO*; ²*CS3M, Rolla, MO*; ³*Utah State University, Logan, UT*; ⁴*PerkinElmer, Woodbridge, ON*; ⁵*Missouri Department of Natural Resources, Jefferson City, MO*

TOG am 09:30 **Determination of Urinary Metabolites of Organophosphate Flame Retardants Using Ultra Performance Liquid Chromatography (UPLC) Tandem Mass Spectrometry (MS/MS)**; Ivana Kosarac¹; Cariton Kubwabo¹; Warren Foster²; ¹*Environmental and Radiation Health Sciences Direct, Ottawa, Canada*; ²*McMaster University, Department of Obstetrics and, Hamilton, Canada*

TOG am 09:50 **Multi-residue Analyses of 71 Endocrine Disruptors in Indoor Air by Liquid and Gas Chromatography Mass Spectrometry Methods**; Stéphanie Laborie¹; Elodie Moreau-Guigon¹; Fabrice Alliot¹; Annie Desportes¹; Lucie Ozio²; Marc Chevreuil¹; ¹*EPHE, UMR 7619, Paris, France*; ²*Université Paris sud, UMR 8079, Orsay, France*

TOG am 10:10 **Identification of 3,5-Dichloro-4-hydroxybenzene Sulfonic Acid as an Unknown Persistent Pollutant in Wastewater Effluent and Natural Water**; M. Paul Chiarelli; Qian Wang; Matthew Reichert; Marlon Lutz; Daniel Becker; *Loyola University, Chicago, IL*

8:30 – 10:30 AM, TUESDAY MORNING LC-MS APPROACHES TO COMBINE TRANSLATIONAL PK/PD BIOMARKERS WITH SMALL MOLECULE ADME WORKFLOWS

**Darren Dumlao (Pfizer, Inc.) presiding
Ballroom 220/221**

TOH am 08:30 **LC-MS Determination of Cyclooxygenase, Lipoxygenase Enzymatic Mediating Pathways Biomarkers in Rat Colon Microdialysate During Inflammatory Bowel Disease**; Yunan Wang; Craig Lunte; *Department of Chemistry, University of Kansas, Lawrence, KS*

TOH am 08:50 **Biomarker Identification and Evaluation of Therapeutic Efficacy using in vivo Microdialysis coupled with Mass Spectrometry**; Matthew Buczynski; Cristina Irimia; Luis Natividad; Loren Parsons; *The Scripps Research Institute, La Jolla, CA*

TOH am 09:10 **Exploring Phenotypic Cell Metabolism using a LC-HRAMS Metabolic Flux Infrastructure**; John Meissen¹; Aditi Jatkar²; Emily Miller¹; Russell Miller²; Min Wan²; Matt Blatnik¹; ¹*Pfizer, Groton, CT*; ²*Pfizer, Cambridge, MA*

TOH am 09:30 **Considerations for a New Strategy of Successful Metabolomics Workflow with Reduced Effort**; Alla Kloss¹; Sarah Geller¹; Kristen Randall¹; Harvey Lieberman¹; Aharon Cohen²; ¹*AR&D, LGCR, Sanofi, Waltham, MA*; ²*Waltham, MA*

TOH am 09:50 **Untargeted Stable Isotope Tracing: Establishing A Novel MS-based Strategy for Discovering Metabolic Fate and Flux**; Qiuying Chen; Steven S. Gross; *Weill Medical College of Cornell, New York, NY*



TOH am 10:10 **Quan-Qual in Real-Life Drug Discovery. What Have We Learned and How Do We Move Ahead?**
Anne-Charlotte Dubbelman¹; Lieve Dillen²; Gerhard Gross²; Filip Cuyckens²; Thomas Hankemeier¹; Rob J. Vreeken^{1,2}; ¹LACDR, Leiden University, Leiden, nl; ²Janssen Pharmaceutica, Beerse, Be

10:30 AM – 2:30 PM, TUESDAY
TUESDAY POSTER SESSION
Poster/Exhibit Hall
Lunch concessions are open 11:00 am – 2:00 pm

TUESDAY AFTERNOON ORAL SESSIONS

2:30 – 4:30 PM, TUESDAY AFTERNOON
NEW DEVELOPMENTS IN HIGH RESOLUTION AND
MASS ACCURACY

Carolyn J. Cassady (University of Alabama) presiding
Hall 5

TOA pm 2:30 **Advances in High Field FT-ICR MS: Ultra-High Resolving Power and Mass Accuracy for Environmental and Biological Research;** Jared B. Shaw; Tzu-Yung Lin; Aleksey V. Tolmachev; Errol W. Robinson; David W. Koppenaal; Ljiljana Pasa-Tolic; *Pacific Northwest National Laboratory, Richland, WA*

TOA pm 2:50 **21 Tesla FT-ICR Mass Spectrometer: A National Resource for Ultrahigh Resolution Mass Spectrometry;** Christopher L. Hendrickson^{1,2}; John P. Quinn¹; Nathan K. Kaiser¹; Donald F. Smith¹; Greg T. Blakney¹; Tong Chen²; Alan G. Marshall^{1,2}; ¹National High Magnetic Field Laboratory, Tallahassee, FL; ²FSU Dept of Chemistry and Biochemistry, Tallahassee, FL

TOA pm 3:10 **The New non-FT Method of Super-High Resolution Mass Spectrometry, Based on Measuring of “Antenna” Ion’s Cyclotron Frequency Time Dependence.;** Eugene Nikolaev^{1,2}; Gleb Vladimirov^{1,3}; Oleg Kharybin¹; Igor Popov^{1,2}; ¹Institute for Energy Problems of Chemical Physics, Moscow, Russia; ²Moscow Institute of Physics and Technology, Moscow, Russia; ³Skolkovo Institute of Technology, Moscow, Russia

TOA pm 3:30 **High Resolution on Both Precursor and Fragment Ions in the MS/MS Spectra of Complex Mixtures by Bidimensional FT-ICR MS;** Fabrice bray¹; Lionel Chiron⁴; Matthias Witt³; Marc-André Delsuc²; Christian Rolando¹; ¹Université Lille 1, Villeneuve d’Ascq, France; ²IGBMC, Université de Strasbourg, Strasbourg, France; ³Bruker Daltonik, Bremen, Germany; ⁴CASC4DE, Strasbourg, France

TOA pm 3:50 **High Resolution and Accurate Mass (HRAM) Characterization of Multiply Charged Proteins by Newly Developed Ionization Techniques on CE-LSI/MAIV-LTQ-Orbitrap Platform;** Bingming Chen; Xuefei Zhong; Chirstopher Lietz; Lingjun Li; *University of Wisconsin-Madison, Madison, WI*

TOA pm 4:10 **A Fully Integrated GC Orbitrap System Opens a New Chapter in GC-MS;** Paul Silcock¹; Cristian Cojocariu¹; Dominic Roberts¹; Scott T. Quarmby²; G.Brody Guckenberger²; Jason S. Cole²; John G. Voss²; Amelia Peterson³; Jan-Peter Hauschild³; Oliver Lange³; Nicholas Kwiecien⁴; Michael S. Westphall⁴; Joshua J. Coon⁴; Alexander Makarov³; ¹Thermo Fisher Scientific, Runcorn, United Kingdom; ²Thermo Fisher Scientific, Austin, TX; ³Thermo Fisher Scientific, Bremen, Germany; ⁴University of Wisconsin, Madison, WI

2:30 – 4:30 PM, TUESDAY AFTERNOON
DATA INDEPENDENT ACQUISITION:
INNOVATIVE METHODS AND APPLICATIONS

Alexander Leitner (ETH Zurich) presiding
Room 130/132

TOB pm 2:30 **Evaluate SWATH Quantitation using Local and Extended Libraries;** Xiaomin Song; Jemma Wu; Dana Pascovici; Thiri Zaw; Natasha Care; Mark P. Molloy; *Australian Proteome Analysis Facility, Sydney, Australia*

TOB pm 2:50 **Intrinsic Ratiometric Filters Enhance Precision in Stable Isotope Data-Independent Acquisition Proteomics;** Jaimeen Majmudar; Brent Martin; *University of Michigan, Ann Arbor, MI*

TOB pm 3:10 **Multi Laboratory Reproducibility and Performance of SWATH™ Acquisition for Proteomic Analyses;** Christie Hunter¹; Ben Collins²; Yansheng Liu²; Stefani Thomas³; Dan Chan³; Hui Zhang³; Samuel Bader⁴; Robert Moritz⁴; Birgit Schilling⁵; Bradford Gibson⁵; Christoph Krisp⁶; Mark Molloy⁷; Guixue Hou⁸; Liang Lin⁸; Siqi Liu⁸; Mio Hirayama⁹; Sumio Ohtsuki⁹; Nathalie Selevsek¹⁰; Ralph Schlapbach¹⁰; Shin-Cheng Tzeng¹¹; Jason Held¹¹; Brett Larsen¹²; Anne-Claude Gingras¹²; Ruedi Aebersold²; ¹SCIEX, Redwood City, CA; ²ETH Zurich, Zurich, Switzerland; ³Johns Hopkins University, Baltimore, MD; ⁴Inst Systems Biology, Seattle, WA; ⁵Buck Institute for Research on Aging, Novato, CA; ⁶Australian Proteome Analysis Facility, Sydney, Australia; ⁷Macquarie University, Sydney, Australia; ⁸BGI, Shenzhen, China; ⁹Univ Kumamoto, Kumamoto, Japan; ¹⁰FGCZ, Univ Zurich, Zurich, Switzerland; ¹¹Washington University, St. Louis, MO; ¹²LTRI, Toronto, ON

TOB pm 3:30 **Data-independent Acquisition using Q Exactive HF to Improve Detection of Urinary Diagnostic Biomarkers of Systemic Diseases;** Jan Muntel¹; Yue Xuan²; Sebastian Berger¹; Alex Kentsis⁴; Richard Bachur³; Hanno Steen¹; ¹Harvard Medical School/Children’s Hospital Boston, Boston, MA; ²ThermoFisherScientific, Bremen, Germany; ³Boston Children’s Hospital, Boston, MA; ⁴Cornell University, New York, NY

TOB pm 3:50 **Quantitative Profiling of Circulating Plasma Microparticle Associated Proteins by DDA and DIA nanoLC-MS2;** Manfred Heller; Natasha Buchs; Sophie Braga Lagache; *University of Bern, Bern, Switzerland*

TOB pm 4:10 **Identification of Archaeal Biofilm Marker Candidates by SWATH-LC/MS/MS Analysis of Planktonic and Sessile Cultures of Halobacterium salinarum R1;** Christof Lenz^{1,2}; Gerald Losensky³; Sabrina Froels³; Felicitas Pfeifer³; Henning Urlaub^{1,2}; ¹Max Planck Institute for Biophysical Chemistry, Goettingen, Germany; ²University Medical Center (UMG), Goettingen, Germany; ³Technical University of Darmstadt, Darmstadt, Germany

TUESDAY AFTERNOON ORAL SESSIONS

2:30 – 4:30 PM, TUESDAY AFTERNOON ION SPECTROSCOPY

Jim Prell (University of Oregon) presiding
Room 123/124

- TOC pm 2:30 **Fusion of Spectroscopy and Mass Spectrometry for Structural Identification of Biomolecules;** Vladimir Kopysov¹; Alexander Makarov²; Oleg Boyarkin¹; ¹Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland; ²Thermo Fisher Scientific, Bremen, Germany
- TOC pm 2:50 **Two-Step Energy Transfer Enables Use of Phenylalanine in Action-EET for Distance Constraint Determination in Gaseous Biomolecules;** Nathan Hendricks; Ryan R. Julian; University of California, Riverside, Riverside, CA
- TOC pm 3:10 **Photodissociation Action Spectroscopy of Protonated N-Substituted Aromatics: Vibronic Details from Room Temperature Ions;** Christopher Hansen¹; Stephen J Blanksby²; Adam Trevitt¹; ¹University of Wollongong, Wollongong, Australia; ²Queensland University of Technology, Brisbane, Australia
- TOC pm 3:30 **Peptide Fragmentation Mechanisms by Infrared Ion Spectroscopy: Recent Advances and Application to ETD;** Jonathan Martens¹; Josipa Grzetic¹; Giel Berden¹; Jos Oomens^{1,2}; ¹FELIX Facility - IMM - Radboud University, Nijmegen, The Netherlands; ²University of Amsterdam, Amsterdam, The Netherlands
- TOC pm 3:50 **Infrared Spectroscopy of Mobility-Selected H⁺Gly-Pro-Gly-Gly (GPGG);** Michael Kamrath¹; Antoine Masson¹; Matthew Glover²; David Clemmer²; Thomas Rizzo¹; ¹EPFL, Lausanne, Switzerland; ²Indiana University, Bloomington, IN
- TOC pm 4:10 **Infrared Multiple Photon Dissociation Action Spectroscopy of Mechanically Interlocked Lasso Peptides.;** Kevin Jeanne Dit Fouque¹; Helene Lavanant¹; Severine Zirah²; Vincent Steinmetz³; Philippe Maitre³; Sylvie Rebuffat²; Carlos Afonso¹; ¹University of Rouen, Mont Saint Aignan, France; ²National Museum of Natural History, Paris, France; ³Université Paris Sud, Orsay, France

2:30 – 4:30 PM, TUESDAY AFTERNOON PROTEOMICS: INFECTIOUS DISEASE

Julia Chamot-Rooke (Institut Pasteur) presiding
Room 120/127

- TOD pm 2:30 **Identification of Staphylococcus aureus Isolates by Shotgun Spectral Matching;** Dana Ohana; Hans Dalebout; Martha van der Beek; Ed Kuijper; Magnus Palmblad; Leiden University Medical Centre, Leiden, THE NETHERLANDS
- TOD pm 2:50 **Accurate Characterization of Difficult to Differentiate Pathogens by Intact Protein ESI-HRMS;** Helene Cardasis²; Jason Neil²; Ping Yip²; Eugen Damoc⁴; Roger Grist³; Alexander Cherkassky²; James Stephenson¹; ¹Thermo Fisher Scientific, Raleigh, NC; ²Thermo Fisher Scientific, Cambridge, MA; ³Thermo Fisher Scientific, East Grinstead, UK; ⁴Thermo Fisher Scientific, Bremen, Germany
- TOD pm 3:10 **Proteomic Analysis of the Secretome upon Helicobacter pylori Infection;** Justine Arrington; Xueqin Wang; Daoguo Zhou; Andy Tao; Purdue University, West Lafayette, IN
- TOD pm 3:30 **Profiling of Staphylococcus Aureus Secretomes using Bottom-Up and Top-Down Mass Spectrometry;** Jessica Chapman; Elizabeth Ohneck; Divya Balasubramanian; Kayan Tam; Victor Torres; Beatrix Ueberheide; NYU School of Medicine, New York, NY

- TOD pm 3:50 **Baccus – a Novel Way of using Targeted Mass Spectrometry to Estimate Bacterial Load;** Ola Kilsgård; Johan Teleman; Erik Malmström; Johan Malmström; Lund University, Lund, Sweden
- TOD pm 4:10 **Integrated omics of Influenza A virus: Correlating Glycan Macro and Micro-Heterogeneity with Virus Evolution and Interactions with Host Immune System.;** Kshittij Khatri¹; Mitchell R. White¹; Joshua A. Klein¹; Nancy Leymarie¹; David F. Smith²; Kevan L. Hartshorn¹; Joseph Zaia¹; ¹Boston University School of Medicine, Boston, MA; ²Emory University School of Medicine, Atlanta, GA

2:30 – 4:30 PM, TUESDAY AFTERNOON LIPID AND PROFILING

Kari Green (University of Florida) presiding
Theater

- TOE pm 2:30 **SFC-MS/MS as a New Tool for Global and Quantitative Lipidomics;** Marie Méjean¹; Laurent Laboureur¹; Benoit Colsch²; Alain Brunelle¹; David Touboul¹; ¹Institut de Chimie des Substances Naturelles, CNRS, Gif sur Yvette, France; ²CEA de SACLAY, Gif sur Yvette, France
- TOE pm 2:50 **Large Scale Lipid Profiling of a Human Serum Lipidome Using a High Resolution Accurate Mass LC/MS/MS Approach;** Reiko Kiyonami¹; David A. Peake¹; Xiaodong Liu²; Yingying Huang¹; ¹ThermoFisher Scientific, San Jose, CA; ²Thermo Fisher Scientific, Sunnyvale, CA
- TOE pm 3:10 **Breast Cancer Tissue Analysis using Photochemical Derivatization and Tandem Mass Spectrometry;** Leelyn Chong; Xiaoxiao Ma; Yu Xia; Zheng Ouyang; Purdue University, West Lafayette, IN
- TOE pm 3:30 **Imaging of Changes in Lipids Profile over Time in Traumatic Brain Injury;** Aurelie Roux¹; Ludovic Muller¹; Shelley N Jackson¹; Brian M Cox²; J. Albert Schultz³; Amina S. Woods¹; ¹NIH/NIDA-IRP, Baltimore, MD; ²Uniformed Services University, Bethesda, MD; ³Ionwerks, Inc, Houston, TX
- TOE pm 3:50 **Single Cell Nanomanipulation to Identify Heterogeneity of Fatty Acid Profiles within Healthy and Diseased Breast Tissue at the Cancer Forefront;** Jason Hamilton; Mandy Phelps; Guido Verbeck; University of North Texas, Denton, TX
- TOE pm 4:10 **Assessment of Function of sPLA₂ and Its Receptor PLA2R and Quantification of Intracellular Uptake and Degradation of SPRL by LC-MS/MS;** Ben Nie¹; Brian S. Cummings²; Robert D. Arnold¹; ¹Harrison School of Pharmacy, Auburn University, Auburn, AL; ²Wilson College of Pharmacy, University of Georgia, Athens, GA

2:30 – 4:30 PM, TUESDAY AFTERNOON PROTEIN-PROTEIN AND PROTEIN-LIGAND INTERACTIONS

H. Ewa Witkowska (UCSF) presiding
Room 106

- TOF pm 2:30 **Characterization of Large Transient Protein Complexes using Size Exclusion Chromatography with On-Line Detection by Native ESI-MS;** Khaja Muneeruddin; Honglin Yao; Cedric Bobst; Igor A. Kaltashov; University of Massachusetts, Amherst, MA
- TOF pm 2:50 **Drug Candidate Screening for Inhibitors of Protein Self-Aggregation using ESI-IMS-MS;** Alison E Ashcroft; Lydia M Young; Janet C Saunders; Rachel A Mahood; Charlotte H Revill; Richard J Foster; Sheena E Radford; University of Leeds, Leeds, United Kingdom

- TOF pm 3:10 **A Platform for the Untargeted Analysis of Protein Interactions;** Owen Skinner¹; Luis Do Vale¹; Rafael Melani¹; Pierre Havugimana¹; Mikhail Belov²; Stevan Horning³; Alexander Makarov³; Neil L. Kelleher¹; Philip Compton¹; ¹Northwestern University, Evanston, IL; ²Spectrograph LLC, Kennewick, WA; ³Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany
- TOF pm 3:30 **Time-Resolved Charge Detection Mass Spectrometry of Hepatitis B Virus Capsid Assembly;** Corinne Lutomski; Elizabeth Pierson; Jason Deer; Adam Zlotnick; Martin Jarrold; *Indiana University, Bloomington, IN*
- TOF pm 3:50 **Protein-Glycolipid Interactions Studied *in vitro* using ESI-MS and Nanodiscs. Insights into the Mechanisms and Energetics of Binding;** Ling Han; Elena Kitova; Jun Li; Hong Lin; John Klassen; *University of Alberta, Edmonton, Canada*
- TOF pm 4:10 **Towards a Comprehensive Strategy for Proteome-Wide Characterization of Small Molecule-Protein Interactions.;** Jason Murphy; Scott Brittain; Daniel Palacios; Edmund Harrington; Jason Thomas; Markus Schirle; *Novartis Institutes for BioMedical Research, Inc., Cambridge, MA*
- 2:30 – 4:30 PM, TUESDAY AFTERNOON
ENVIRONMENTAL MS:
INSTRUMENTAL CHALLENGES AND SOLUTIONS**
Lee Ferguson (Duke University) presiding
Ballroom 222/224
- TOG pm 2:30 **High Resolution and Tandem Mass Spectrometry Uncovers Chlorination Reaction Pathways for Transformation of Medical Imaging Compounds in Drinking Water Treatment;** Susan Richardson¹; Cristina Postigo²; Christina Joseph¹; Friedrich Wendel³; Christian Luetke Eversloh³; Thomas Ternes³; Edward Machek⁴; Stephen Duirk⁴; Elizabeth Wagner⁵; Michael Plewa⁵; ¹University of South Carolina, Department of Chemis, Columbia, SC; ²CSIC, Barcelona, Spain; ³Federal Institute of Hydrology, Koblenz, Germany; ⁴University of Akron, Akron, OH; ⁵University of Illinois, Urbana, IL
- TOG pm 2:50 **Discovery, Identification and Investigation of Naturally Occurring Antibiotics in Drinking Water using Differential Ion Mobility and Soft Mass Spectrometry;** Jadwiga Lyczko; Wojciech Gabryelski; *University of Guelph, Guelph, Canada*
- TOG pm 3:10 **Direct On-Line Measurement of PAHs in Complex Aqueous Samples: Condensed Phase Membrane Introduction Mass Spectrometry - Direct Electron Ionization (CP-MIMS-DEI);** Veronica Termopoli¹; Giorgio Famigliani¹; Laura Magrini¹; Pierangela Palma¹; Erik Krogh^{2,3}; Achille Cappiello¹; Christopher G. Gill^{2,3}; ¹University of Urbino, Urbino, Italy; ²University of Victoria, Victoria, BC, Canada; ³Appl. Env. Res. Labs. (AERL), Nanaimo, BC, Canada
- TOG pm 3:30 **Identification of Contaminants In House Dust by Two-Dimensional Gas Chromatography and Liquid Chromatography with Mass Spectrometry and Non-Targeted Data Analytics;** Benjamin Place; Jacolin Murray; *National Institute of Standards and Technology, Gaithersburg, MD*
- TOG pm 3:50 **Coupling Atmospheric Pressure Photoionization with Differential Mobility Analysis – Mass Spectrometry for detection of non-polar environmental analytes within gas-phase samples;** Ross McCulloch; Arturo Álvaro Carballido; *SEADM, Boecillo, Spain*
- TOG pm 4:10 **Chemical Characterization of Organic Contaminants in the Environment near an E-Waste Site in China;** Jonathan Byer³; Ed Sverko¹; Kurunthachalam Kannan²; Qian Wu²; Joe Binkley³; ¹Environment Canada, Burlington, ON; ²Wadsworth Center, New York State Department of Health, Albany, NY; ³LECO Corporation, St. Joseph, MI
- 2:30 – 4:30 PM, TUESDAY AFTERNOON
IMAGING: PHARMACEUTICALS AND METABOLITES**
Steve Castellino (GlaxoSmithKline) presiding
Ballroom 220/221
- TOH pm 2:30 **High Spatial Resolution MALDI Mass Spectrometry Imaging for the Determination of Therapeutic Compound Distribution in Rodent Intestinal Sections;** Anna Nilsson¹; Alexandra Peric²; Marie Strimfors²; Eva Lundborg²; Richard Goodwin³; Martin A. Hayes²; Constanze Hilgendorf²; Per E. Andren¹; ¹Uppsala University, Uppsala, Sweden; ²AstraZeneca, Molndal, SE; ³AstraZeneca, Cambridge, UK
- TOH pm 2:50 **Insects and Plants: Metabolite Studies using High-Performance AP-MALDI Mass Spectrometry Imaging;** Bernhard Spengler; Andreas Römpf; Dhaka Bhandari; Saleh Khalil; *Analytical Chemistry, Giessen, Germany*
- TOH pm 3:10 **Induced Interstitial Pulmonary Fibrosis (IPF) Model: Unlabeled Bleomycin Distribution and Early IPF Markers Identification by MALDI Imaging;** David Bonnel¹; Mary McElroy²; Emeline Falaux¹; Fabien Pamelard¹; Gael Picard de Muller¹; Gregory Hamm¹; Stephen Madden²; Jonathan Stauber¹; ¹ImaBiotech, MS Imaging Dept., Loos, France; ²Charles River Discovery Research Services, Edinburgh, United-Kingdom
- TOH pm 3:30 **Multiplatform Mass Spectrometry Imaging to Detect and Differentiate Nanoparticle Formulated and Released Drug in Preclinical Tumors;** Richard Goodwin¹; John Swales¹; Anna Nilsson²; Per E Andren²; Nicole Strittmatter³; Zoltan Takats³; Susan Ashton⁴; Philip Jewsbury⁴; Peter Webborn⁴; Simon Barry⁴; ¹AstraZeneca, Cambridge, UK; ²Uppsala University, Uppsala, SE; ³Imperial College, London, UK; ⁴AstraZeneca, Macclesfield, UK
- TOH pm 3:50 **The Applications of Single-probe Mass Spectrometry: Single Cell Analysis and Biological Tissue Imaging;** Ning Pan; Wei Rao; Mei Sun; Zhibo Yang; *University of Oklahoma, Norman, OK*
- TOH pm 4:10 **Molecular Imaging of Antibiotic Inhibition of Bacterial Growth and Metabolism by Laser Ablation Electrospray Ionization Mass Spectrometry;** Pranav Balan¹; Hang Li²; Akos Vertes²; ¹Thomas Jefferson HS for Science and Technology, Alexandria, VA; ²George Washington University, Washington, DC

TUESDAY AFTERNOON AND WEDNESDAY MORNING ORAL SESSIONS

4:45 – 5:30 PM, TUESDAY AFTERNOON
AWARD LECTURE

Jenny Brodbelt (University of Texas, Austin) presiding
Hall 5

Presentation of the 2015 Research Awards



Biemann Medal

Michael J. MacCoss
University of Washington

5:45 – 7:00 PM, TUESDAY AFTERNOON
WORKSHOPS
There are light refreshments in the common areas.

01. Laboratory Developed Test Guidance and Mass Spectrometric Diagnostics: Impact and Expectations, Room 130
02. Current Trends, Gaps, and Needs in Workflows for Targeted Protein Quantitation by LC/MS, Room 131
03. ProeomicsDB, Room 132

04. FTMS: MS/MS at High Resolution, Room 123/124
05. Identifying Tandem Mass Spectra of Lipids and Carbohydrates, Room 120/127
06. MS Analysis of Antibody-Drug Conjugates, Room 260/267
07. Measuring the exposome: Strategies and preliminary results, Room 274
08. Advancements and Discussion of Mass Spectrometry Technology and Challenges within the Polymer and Material Fields, Room 275
09. The ABCs of Being a Great Reviewer for Scientific Journals, Room 230
10. How to Network without Really Trying: A Forum for Current (and Future) Mass Spectrometrists in Industry, Room 231
11. Room 232
12. Invalidating your Cores Data: Examples on How to Check your Data and Report Results and Communicate Invalid or Bad Results to your Customers, Ballroom 222/224
13. How Can Ion Mobility Spectrometry Separations Help your research? Ballroom 220/221

AFTER 8:00 PM
CORPORATE HOSPITALITY SUITES
RENAISSANCE GRAND HOTEL

WEDNESDAY MORNING ORAL SESSIONS

8:30 – 10:30 AM, WEDNESDAY MORNING
AMBIENT AND ATMOSPHERIC PRESSURE GENERATION OF
MULTIPLY-CHARGED IONIC SPECIES

Abraham Badu-Tawiah (Ohio State University) presiding
Hall 5

- WOA am 08:30 **How are Nearly Identical Charge States Produced from the Solution (ESI) and Solid (MAIV) States;** Charles N. McEwen^{1,2}; Sarah Trimpin^{3,4}; ¹Univ. of the Sciences, Philadelphia, PA; ²MSTM, Newark, Delaware; ³Cardiovascular Research Center, WSU, Detroit, MI; ⁴Wayne State University, Detroit, MI
- WOA am 08:50 **A Suite of Liquid UV-AP-MALDI Techniques for the Generation of Multiply Charged Ions at High Sensitivity with Stable, Long-Lasting Yield;** Pavel Ryumin¹; Jeff Brown^{1,2}; Mike Morris²; Rainer Cramer¹; ¹University of Reading, Reading, UK; ²Waters Corporation, Wilmslow, UK
- WOA am 09:10 **Improving the Analysis of Proteins by Desorption Electrospray Ionization (DESI) by the Addition of Ammonium Bicarbonate;** Andre Venter; Elahe Honarvar; Western Michigan University, Kalamazoo, MI
- WOA am 09:30 **Effects of Supercharging Reagents on Protein Stability in Bulk Solution and Insight into the Mechanism of Supercharging;** Catherine Going; Beryl Xia; Evan Williams; , Berkeley, CA
- WOA am 09:50 **Molecular Dynamics Simulations Yield Atomistic Insights Into Electrospray Mechanisms: From Salt Clusters to Protein Ions;** Lars Konermann; Robert G. McAllister; Haidy Metwally; Univ. of Western Ontario, London, Canada
- WOA am 10:10 **Particle Size Selected Inlet Ionization;** Kermit K. Murray; Fan Cao; Fabrizio Donnarumma; Louisiana State University, Baton Rouge, LA

8:30 – 10:30 AM, WEDNESDAY MORNING
INFORMATICS: PRM AND DIA

Brendan MacLean (University of Washington) presiding
Room 130/132

- WOB am 08:30 **Targeted Analysis of MS1 Only DIA Data;** Oliver M. Bernhardt¹; Roland M. Bruderer¹; Yue Xuan²; Tejas Gandhi¹; Paul Boersema³; Paola Picotti³; Lukas Reiter¹; ¹Biognosys AG, Zuerich, Switzerland; ²Thermo Fisher Scientific, Bremen, Germany; ³Institute of Biochemistry, ETH, Zuerich, Switzerland
- WOB am 08:50 **Using DIA to Predict High-Responding Peptides for Targeted Proteomics Experiments;** Brian C. Searle^{1,2}; Jarrett D. Egerton¹; James G. Bollinger¹; Michael J. MacCoss¹; ¹University of Washington, Seattle, WA; ²Proteome Software Inc., Portland, OR
- WOB am 09:10 **Making the Transition from Targeted to DIA: Genetic Algorithms Enable Assay Portability;** Jacob D. Jaffe; Jennifer Abelin; Steven A. Carr; The Broad Institute, Cambridge, MA
- WOB am 09:30 **Towards a “Load and Play” Solution for Parallel Reaction Monitoring Assays;** Bruno Doman; Sang Yoon Kim; Daniel Ayoub; Sebastien Gallien; Luxembourg Clinical Proteomics Center, Strassen, Luxembourg
- WOB am 09:50 **Sensitive Peptide Identification in Data-Independent Acquisition by Spectral Library Search;** Jian Wang¹; Monica Tucholska²; Brett Larsen²; Anne-Claude Gingras²; Nuno Bandeira³; ¹UCSD, La Jolla, CA; ²Lunenfeld-Tanenbaum Research Institute, Toronto, Canada; ³University of California, San Diego, La Jolla, CA
- WOB am 10:10 **Toward an Optimal Computational Strategy for DIA Mass Spectrometry Data;** Chih-Chiang Tsou¹; Anne-Claude Gingras²; Alexey Nesvizhskii¹; ¹University of Michigan, Ann Arbor, MI; ²Samuel Lunenfeld Research Institute, Mount Sinai H, Toronto, ON


**8:30 – 10:30 AM, WEDNESDAY MORNING
ION MOBILITY: STRUCTURES**
**Kevin Giles (Waters Corporation) presiding
Room 123/124**

- WOC am 08:30 **Mobility Calculations from Small Ions to Macromolecular Complexes using the Electronic Surface Representation**; Yuri Alexeev¹; Joseph Insley¹; Dmitri Fedorov²; Alexandre Shvartsburg³; ¹Argonne National Laboratory, Argonne, IL; ²Nanosystem Research Institute, Tsukuba, Japan; ³Wichita State University, Wichita, KS
- WOC am 08:50 **Pushing the Boundaries of Small Molecule Analysis: using Ion Mobility MS and Gas-Phase Infrared Spectroscopy To Study Protonation Site Isomers**; Jasper Boschmans¹; Stephan Warnke²; Jongcheol Seo²; Jonathan P. Williams³; Kevin Pagel^{2,4}; Gert von Helden²; Filip Lemièrè¹; Frank Sobott¹; ¹University of Antwerp, Antwerp, Belgium; ²Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany; ³Waters Corporation, Manchester, UK; ⁴Freie Universität Berlin, Berlin, Germany
- WOC am 09:10 **Ion Mobility-Mass Spectrometry Reveals the Energy Landscape of Polyproline Folding**; Liuging Shi¹; Alison Holliday²; Matthew Glover¹; Michael Ewing¹; David Russell³; David Clemmer¹; ¹Indiana University, Bloomington, IN; ²Moravian College, Bethlehem, PA; ³Texas A&M University, College Station, TX
- WOC am 09:30 **Structural Analysis of Monomeric and Dimeric Neuropeptide Y (NPY) with IM-MS, HDX MS, and MD simulations**; Xueqin Pang¹; Christopher B. Lietz²; Lingjun Li¹; ¹School of Pharmacy, University of Wisconsin, Madison, WI; ²Department of Chemistry, University of Wisconsin, Madison, WI
- WOC am 09:50 **HDX-TIMS-MS and Molecular Dynamics Reveal Folding Pathways in DNA-Binding Proteins**; Emily Schenk¹; Frederic Nau¹; Genevieve Gozo¹; Mark Ridgeway²; Melvin A. Park³; Fenfei Leng¹; Francisco Fernandez Lima¹; ¹Florida International University, Miami, FL; ²Bruker Daltonic, Billerica, MA; ³Bruker Daltonics, Inc., Billerica, MA
- WOC am 10:10 **Novel Insights into the Structural Dynamics and Effects of Ligand-Binding on Protein Kinase A using Ion Mobility-Mass Spectrometry**; Matthias Vonderach; Dominic Byrne; Samantha Ferries; Patrick Eyers; Claire Eyers; University of Liverpool, Liverpool, UK

**8:30 – 10:30 AM, WEDNESDAY MORNING
CARBOHYDRATES**
**Robert Chalkley (UCSF) presiding
Room 120/127**

- WOD am 08:30 **Characterization of Highly Heterogeneous Protein-Heparin Complexes using Novel Mass Spectrometry-Based Approaches**; Yunlong Zhao; Rinat Abzalimov; Igor A. Kaltashov; University of Massachusetts, Amherst, MA
- WOD am 08:50 **A New Image of Wheat Cell Walls Revealed through MS Imaging and Ion Mobility**; Dušan Veličković; Fabienne Guillon; Luc Saulnier; Hélène Rogniaux; INRA, Nantes, France
- WOD am 09:10 **Resin-Based and Magnetic Nanoparticle-Based Biomimetic Reagents for Glycan Structure Determination by Mass Spectrometry**; Jinshan Gao; Jungeun Lee; Nikunj Desai; Montclair State University, Montclair, NJ
- WOD am 09:30 **Coupling of FANGS to the INLIGHT™ Strategy for Accurate Relative Quantification of N-Glycans Derived from Minimal Biological Material**; Elizabeth S. Hecht; James P. McCord; Rebecca

Wysocky; James N. Petite; David C. Muddiman; North Carolina State University, Raleigh, NC

- WOD am 09:50 **The Use of Isotopically Labeled IgG for the Relative and Absolute Quantitation of N-linked Glycans**; Ron Orlando^{1,2}; Shujuan Tao¹; Yining Huang¹; Emily Betchy¹; Barry Boyes^{2,3}; Alex Harvey²; ¹Complex Carbohydrate Research Center, UGA, Athens, GA; ²GlycoScientific, LLC, Athens, GA; ³Advanced Materials Technology Inc., Wilmington, DE
- WOD am 10:10 **Integrated Glycomics and Proteomics Study for Astrocytoma from 118 Patient Samples**; Chun Shao; Lilla Turiak; Nancy Leymarie; Joseph Zaia; Boston University School of Medicine, Boston, MA

**8:30 – 10:30 AM, WEDNESDAY MORNING
FT, ION TRAPS AND HYBRID INSTRUMENTS
Eugene Nikolaev (Institute for Energy Problems and Chemical Physics) presiding
Theater**

- WOE am 08:30 **Experimental Investigation of Linear Quadrupole and Octopole Ion Traps for External Ion Accumulation for High Field FT-ICR MS**; Donald E. Smith¹; Nathan K. Kaiser¹; John P. Quinn¹; Steven C. Beu²; Alan G. Marshall^{1,3}; Christopher L. Hendrickson¹; ¹National High Magnetic Field Laboratory, FSU, Tallahassee, FL; ²S C Beu Consulting, Austin, TX; ³Dept. Chem. & Biochem., Florida State University, Tallahassee, FL
- WOE am 08:50 **Towards Parallel Mass Spectrometry with a Novel Multi-Quadrupole Ion Trap (MultiQ-IT)**; Andrew N. Krutchinsky; Herbert Cohen; Brian T. Chait; The Rockefeller University, New York, NY
- WOE am 09:10 **Time-Dependent Modulation of Reflector Plate Potential for Increased Charge Density and Reduced Dephasing in an Electrostatic Linear Ion Trap**; Eric Dziekonski; Scott McLuckey; Purdue University, West Lafayette, IN
- WOE am 09:30 **Middle Down Proteomics by MS3 on a Tribird Mass Spectrometer**; Jolene K. Diedrich; Mathieu Lavallée-Adam; Antonio F. M. Pinto; James J. Moresco; John R. Yates III; The Scripps Research Institute, La Jolla, CA
- WOE am 09:50 **Parallel Detection of Ions with an ICR Cell Array**; Sung-Gun Park¹; Gordon Anderson²; James Bruce¹; ¹University of Washington, Seattle, WA; ²GAA Custom Engineering, LLC, Benton, WA
- WOE am 10:10 **Novel mass analyzers for rapid high-performance FT-ICR MS**; Yury Tsybin^{1,2}; Anton Kozhinov¹; Konstantin Nagornov¹; ¹Ecole Polytechnique Federale, Lausanne, Switzerland; ²Spectroswiss Sàrl, Lausanne, Switzerland

**8:30 – 10:30 AM, WEDNESDAY MORNING
MASS SPECTROMETRY IN STRUCTURAL BIOLOGY
Arthur Laganowsky (Texas A&M Health Science) presiding
Room 106**

- WOF am 08:30 **Measuring the Binding Interfaces of Protein Complexes by Gas-Phase Hydrogen/Deuterium Exchange Mass Spectrometry (Gas-Phase HDX-MS)**; Ulrik H. Mistarż¹; Jeffery M. Brown²; Kim F. Haselmann³; Kasper D. Rand¹; ¹Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark; ²Waters MS Technologies Centre, Wilmslow, U. K; ³Diabetes Protein Engineering, Novo Nordisk A/S, Måløv, Denmark

- WOF am 08:50 **Development of Isotope-Encoded Protein Footprinting for Mass Spectrometry-based Protein Conformational Studies**; Hao Zhang; Haijun Liu; Michael L. Gross; Robert E. Blankenship; *Washington University, Saint Louis, MO*
- WOF am 09:10 **Distinctive Structural Dynamics in Ras and Related Proteins by Hydrogen Exchange Mass Spectrometry**; Rane Harrison¹; Martin Carrasco²; John Hunter²; Anuj Manandhar²; Kenneth Westover²; John Engen¹; ¹*Northeastern University, Boston, MA*; ²*University of Texas Southwestern Medical Center, Dallas, TX*
- WOF am 09:30 **Mass Spectrometry for Monitoring the Transfer of Iron-Sulfur Clusters between Proteins**; William K. Russell; James Vranish; David Barondeau; David Russell; *Texas A&M University, College Station, TX*
- WOF am 09:50 **Structure Elucidation of Toyocamycin Nitrile Hydratase, a Hetero-hexameric Protein Complex, by Mass Spectrometry**; Yang Song¹; Micah Nelp²; Vahe Bandarian²; Vicki H. Wysocki¹; ¹*The Ohio State University, Columbus, OH*; ²*The University of Arizona, Tucson, AZ*
- WOF am 10:10 **Using Cross-Linking Coupled to Mass Spectrometry and Integrated Modeling to Study the Molecular Architecture of Large Protein Assemblies**; Florian Stengel^{1,2}; Erzberger Jan¹; Riccardo Pellarin³; Suyang Zhang¹; Tanja Schaefer¹; Christopher H. S. Aylett¹; Peter Cimermančič³; Daniel Boehringer¹; Andrej Sali³; Ruedi Aebersold¹; Nenad Ban¹; ¹*ETH Zurich, Zurich, Switzerland*; ²*University of Konstanz, Konstanz, Germany*; ³*University of California, San Francisco, CA*

8:30 – 10:30 AM, WEDNESDAY MORNING

EPIGENETIC MODIFICATIONS AND MECHANISMS

Kangling Zhang (University of Texas, Galveston) presiding
Ballroom 222/224

- WOG am 08:30 **Modifications of the Mind: RNA Modifications Profile of Differentiated Human Frontal Cortex Cells**; Maria Basanta-Sanchez¹; Subhrakanti Saha¹; Sally Temple²; Mo Liu²; Paul Agris¹; ¹*The RNA Institute, University at Albany, Albany, NY*; ²*Neural Stem Cell Institute, Rensselaer, NY*
- WOG am 08:50 **Towards Understanding the Dynamics of Histone Combinatorial Proteoforms using a Boosted Middle-Down Proteomics Platform**; Simone Sidoli¹; Chrystian Ruminowicz²; Kelly Karch¹; Shu Lin¹; Benjamin A. Garcia¹; ¹*University of Pennsylvania, Philadelphia, PA*; ²*Private developer, Bialystok, Poland*
- WOG am 09:10 **Analysis of Histone Posttranslational Modifications on Nascent Chromatin**; Constance Alabert¹; Teresa Barth²; Axel Imhof²; Anja Groth¹; ¹*Biotech Research and Innovation Centre (BRIC), Copenhagen, Denmark*; ²*Adolf-Butenandt-Institute, Munich, Germany*
- WOG am 09:30 **A Top-Down Approach to Decoding Histones Using a Modified Tribrid Mass Spectrometer with Improved Vacuum and ETD Performance**; Yupeng Zheng¹; Luca Fornelli¹; Philip D. Compton¹; Seema Sharma²; Jesse D. Canterbury²; Christopher Mullen²; Vlad Zabrouskov²; Jon A. Oyer¹; Jonathan D. Licht¹; Michael W. Senko²; Neil L. Kelleher¹; ¹*Northwestern University, Evanston, IL*; ²*Thermo Fisher Scientific, San Jose, CA*

- WOG am 09:50 **Unraveling Site-Specific Acetylation using High Resolution Mass Spectrometry in HATs and HDACs Mutants of Fission Yeast**; Nebiyu Abshiru^{1,2}; Roshan Rajan^{1,2}; Alain Verreault^{1,2}; Pierre Thibault^{1,2}; ¹*University of Montreal, Montreal, QC, Canada*; ²*Institute for Research in Immunology and Cancer, Montreal, QC, Canada*
- WOG am 10:10 **Mass Spectrometry-Based Characterization of Histone Methylation in Microglia after Ethanol Exposure**; Joao Paulo Costa Pinho¹; Jennifer Guergues¹; Harris Bell-Temin¹; Bin Liu²; Stanley M. Stevens, Jr.¹; ¹*University of South Florida, Tampa, FL*; ²*University of Florida, Gainesville, FL*

8:30 – 10:30 AM, WEDNESDAY MORNING

APPLICATION OF STABLE ISOTOPE LABELING IN MS ANALYSIS OF SMALL MOLECULES AND PROTEINS

Mingshe Zhu (Bristol-Myers Squibb) presiding
Ballroom 220/221

- WOH am 08:30 **LC-MS Methods to Profile the Cow Milk Metabolome and Determine the Effects of Milk Consumption on the Human Urine Metabolome**; Dorothea Mung; Liang Li; *University of Alberta, Edmonton, Canada*
- WOH am 08:50 **Developmental Stage of Tomato Leaves Determines the Diversity and Dynamics of Trichome Specialized Metabolites**; Zhenzhen Wang; A. Daniel Jones; *Michigan State University, East Lansing, MI*
- WOH am 09:10 **Platelet Biomarkers of Metabolic Disturbances in Friedreich's Ataxia**; Andrew J. Worth¹; Sankha S. Basu²; Eric C. Deutsch³; Wei-Ting Hwang¹; Nathaniel W Snyder¹; David R. Lynch³; Ian A. Blair¹; ¹*University of Pennsylvania, Philadelphia, PA*; ²*Brigham & Women's Hospital, Harvard, Boston, MA*; ³*Departments of Neurology and Pediatrics, CHOP, Philadelphia, PA*
- WOH am 09:30 **Hyperplex Amino Acid-based Isobaric Labels for Quantitative Proteomics**; Qing Yu¹; Tyler Greer²; Lingjun Li³; ¹*University of Wisconsin-Madison, Madison, Wisconsin*; ²*University of Wisconsin-Madison, Middleton, WI*; ³*University of Wisconsin, Madison, WI*
- WOH am 09:50 **A Novel Triplex Isobaric Peptide Termini Labeling Approach for Quantitative Proteomics**; Haojie Lu; Hongrui Yin; Lei Zhang; Liqi Xie; Ying Zhang; *Fudan University, Shanghai, CHINA*
- WOH am 10:10 **Large Scale Metabolic Exploration of Human CSF Proteins using Stable Isotope Labeling Amino Acid *in-vivo* (SILAV)**; Sylvain Lehmann¹; Jérôme Vialaret¹; Guillaume Gras Combe²; Luc Bauchet²; Mamadou Lamine Tall³; Olivier Hanon⁴; Audrey Gabelle⁵; Christophe Hirtz¹; ¹*CHRU de Montpellier and Université de Montpellier, Montpellier, France*; ²*Service de Neurochirurgie, CHRU de Montpellier, Montpellier, France*; ³*Pharmacie, Groupement Hospitalier Edouard Herriot, Lyon, France*; ⁴*AP-HP, Hôpital Broca, Service de Gériatrie, Paris, France*; ⁵*Centre Mémoire Ressources CHRU Montpellier, Montpellier, France*

10:30 AM – 2:30 PM, WEDNESDAY

WEDNESDAY POSTER SESSION

Poster/Exhibit Hall

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



**2:30 – 4:30 PM, WEDNESDAY AFTERNOON
AMBIENT IONIZATION: INSTRUMENTATION AND APPLICATIONS**
Douglas F. Barofsky (Oregon State University) presiding
Hall 5

- WOA pm 2:30 **Development of a New Versatile Instrument Combining Laser Ablation Mass Spectrometry and Laser Emission Spectroscopy;** Andreas Bierstedt¹; Ulrich Panne^{1,2}; Jens Riedel¹; ¹BAM Federal Institute for Materials, Berlin, Germany; ²Humboldt University, Berlin, Germany
- WOA pm 2:50 **Species Identification by Chemotaxonomy, Ambient Ionization, and Chemometrics with Hierarchical Clustering.;** Rabi Musah²; Robert B. Cody¹; Edgard Espinoza³; Ashton Lesiak⁴; Earl Christensen⁵; Hannah Moore⁶; Simin D. Maleknia⁷; ¹JEOL USA, Inc., Peabody, MA; ²University at Albany-SUNY, Albany, NY; ³US National Fish and Wildlife Forensics Laboratory, Ashland, OR; ⁴University at Albany, Albany, New York; ⁵National Renewable Energy Laboratory, Golden, CO; ⁶Keele University, Keele, UK; ⁷University of New South Wales, Sydney, Australia
- WOA pm 3:10 **Development of a Solid-Phase Micro Extraction-Dielectric Barrier Discharge Ionization-Mass Spectrometry (SPME-DBDI-MS) Direct Coupling under Ambient Conditions: Approaching ppq Sensitivity;** Mario Francesco Mirabelli; Jan-Christoph Wolf; Renato Zenobi; ETH Zurich, Switzerland, CH
- WOA pm 3:30 **Rapid Discrimination of Human Skin-related Microorganisms *in vitro* by Ambient Ionization Mass Spectrometry;** Pu Wei¹; Alan Jamusch¹; Ahmed M. Hamid¹; Valentina Pirro¹; Rafal M. Pielak²; R. Graham Cooks¹; ¹Purdue University, West Lafayette, IN; ²L'Oréal California Research Center, San Francisco, CA
- WOA pm 3:50 **Coupling Charge Reduction Mass Spectrometry to Liquid Chromatography for Complex Mixture Analysis;** John Stutzman; Matthew Crowe; James Alexander IV; Bruce Bell; The Dow Chemical Company, Collegetown, PA
- WOA pm 4:10 **Demonstrating the use of Surface Acoustic Wave Nebulization (SAWN) on Multiplex Assay of Lysosomal Storage Diseases;** Angelo Condulle; Frantisek Turecek; University of Washington, Seattle, WA

**2:30 – 4:30 PM, WEDNESDAY AFTERNOON
INFORMATICS: PROTEIN IDENTIFICATION AND
QUANTIFICATION**

**Oliver Kohlbacher (Universitat Tübingen) presiding
Room 130/132**

- WOB pm 2:30 **Top-Down Proteogenomics;** Mikhail Kolmogorov; Pavel Pevzner; UCSD, La Jolla, CA
- WOB pm 2:50 **MSPathFinder: An Open Source Proteoform Identification and Quantification Tool for Top-Down Proteomics;** Sangtae Kim; Christopher S. Wilkins; Jungkap Park; Paul D. Piehowski; Anil K. Shukla; Yufeng Shen; Samuel H. Payne; Richard D. Smith; Pacific Northwest National Laboratory, Richland, WA
- WOB pm 3:10 **Picked Protein FDR, a Scalable Approach for Protein False Discovery Rate Estimation in Large Proteomic Data Sets;** Mathias Wilhelm¹; Mikhail Savitski²; Hannes Hahne¹; Bernhard Kuster¹; Marcus Bantscheff²; ¹Technische Universität München, Freising, Germany; ²Cellzome GmbH a GSK company, Heidelberg, Germany

- WOB pm 3:30 **Protein Identification with Accurate Statistical Significance Assignment using Mass Spectrometry;** Gelio Alves; Aleksey Ogurtsov; Yi-Kuo Yu; National Center for Biotechnology Information, NLM, Bethesda, MD
- WOB pm 3:50 **Controlling False Discovery Rates (FDRs) in Genome-Wide Proteomics Datasets;** Stefka Tyanova; Pavel Sinitcyn; Matthias Mann; Juergen Cox; Max-Planck-Institute of Biochemistry, Martinsried, GERMANY
- WOB pm 4:10 **“How to Recover from a Bad Day” Data Processing Tolerant to Experimental Errors;** Amandine Boudreau; Gordana Ilosev; Vlad Savchenko; CJ Baker; Suya Liu; Stephen A Tate; Sciex, Concord, Canada

**2:30 – 4:30 PM, WEDNESDAY AFTERNOON
REACTIONS, DYNAMICS AND THEORY OF GAS PHASE IONS**
**Zhibo Yang (University of Oklahoma) presiding
Room 123/124**

- WOC pm 2:30 **Does Spin-Orbit Coupling Really Matter? The Interesting Case of Th⁺ + CH₄;** Peter Armentrout¹; Richard M. Cox¹; Wibe de Jong²; ¹University of Utah, Salt Lake City, UT; ²Lawrence Berkeley National Laboratory, Berkeley, CA
- WOC pm 2:50 **Binding of Xe and Perfluorinated Compounds Inside Cucurbit[n]uril Hosts: Computational and Experimental Results and Anomalous Dissociation;** Conner Harper; David V. Dearden; Brigham Young University, Provo, UT
- WOC pm 3:10 **Opposing Charges in ESI-MS of Noncovalent Complexes Explain Many Observations;** Rachel Loo; Huilin Li; Joseph A. Loo; UCLA, Los Angeles, CA
- WOC pm 3:30 **Using MS to Invent a New Metal Catalyzed “Molecular Switcheroo” Reaction;** Richard A. J. O’hair¹; George N. Khairallah²; Jiawei Li¹; Paul Donnelly¹; Asif Noor²; ¹University of Melbourne, Victoria, AUSTRALIA; ²Bio21 Inst, Uni of Melbourne, Melbourne, AUSTRALIA
- WOC pm 3:50 **Gas-Phase Conformations, Energetics, and Mechanisms for Glycosidic Bond Dissociation of Protonated 2'-Deoxycytidine and Cytidine;** Ranran Wu; Mary T. Rodgers; Wayne State University, Detroit, MI
- WOC pm 4:10 **New Insight into Ion/Molecule Chemistry with Isomeric Metal and Metal-Oxo Complexes using ESI-TWIMS-MS: C-F Bond-Activation, Active Species Structure and Mechanism;** Nicole Rijs; Maria Schlangen; Helmut Schwarz; TU Berlin, Berlin, Germany

**2:30 – 4:30 PM, WEDNESDAY AFTERNOON
NUCLEIC ACIDS**
**Valérie Gabelica (University of Bordeaux) presiding
Room 120/127**

- WOD pm 2:30 **A Proteomics-like Pipeline for the Epitranscriptome: Automated Analysis of Posttranscriptionally Modified RNAs;** Collin Wetzel; Patrick A. Limbach; University of Cincinnati, Cincinnati, OH
- WOD pm 2:50 **LC-MS/MS for Simultaneous Assessment of Oxidative DNA Adducts and a DNA Epigenetic Biomarker in an Animal Model of Wilson’s Disease;** Yang Yu; Candace R. Guerrero; Yinsheng Wang; University of California, Riverside, Riverside, CA

WEDNESDAY AFTERNOON ORAL SESSIONS

- WOD pm 3:10 **Using Negative Mode ESI/MSMS to Sequence miRNAs and Detect Modifications;** Samuel Wein; Simone Sidoli; Benjamin A. Garcia; *University of Pennsylvania, Philadelphia, PA*
- WOD pm 3:30 **Structural Elucidation and Antisense Properties of a Sugar-Modified DNA Analogue;** Yvonne Hari; Christian Leumann; Stefan Schürch; *Department of Chemistry and Biochemistry, Bern, Switzerland*
- WOD pm 3:50 **Ion Mobility and Tandem Mass Spectrometry Reveal the Effects of Solution on Gas-phase RNA Hairpin Structure;** Kevin Ilek; Jessica Rabuck-Gibbons; Brandon Ruotolo; Kristina Hakansson; *University of Michigan, Ann Arbor, MI*
- WOD pm 4:10 **Discriminating Local Versus Global Dynamics in Structured Biopolymers by Ion Mobility Spectrometry-Mass Spectrometry;** Jennifer Lippens¹; Rebecca D'Esposito¹; Srivathsan Ranganathan¹; Papa Nii Asare-Okai²; Daniele Fabris¹; ¹*The RNA Institute, University at Albany, Albany, NY*; ²*State University of New York at Albany, Albany, NY*

2:30 – 4:30 PM, WEDNESDAY AFTERNOON FOOD CHEMISTRY AND SAFETY Timothy Croley (FDA) presiding Theater

- WOE pm 2:30 **Beeromics: From QC to ID's of Differentially Expressed Compounds in Craft Beers;** Christine A. Hughey; Chelsey McMinn; Jenny Phung; *James Madison University, Harrisonburg, VA*
- WOE pm 2:50 **Evaluation of the Composition and Toxicity of Electronic Cigarette Liquids;** Sandra E. Spencer¹; Rachel A. Harris¹; Steven L. Reeber¹; Phillip Clapp²; Ilona Jaspers²; Gary L. Glish²; ¹*UNC Chapel Hill, Department of Chemistry, Chapel Hill, NC*; ²*UNC Chapel Hill, School of Medicine, Chapel Hill, NC*
- WOE pm 3:10 **Direct Identification of Prohibited Substances in Cosmetics Using a Miniature Mass Spectrometry System;** Qiang Ma^{1,2}; R. Graham Cooks²; Zheng Ouyang²; ¹*Chinese Academy of Inspection and Quarantine, Beijing, China*; ²*Purdue University, West Lafayette, IN*
- WOE pm 3:30 **Ambient Mass Spectrometry Imaging of Food Contaminants;** Michel W. Nielen^{1,2}; Wilco Duvivier²; Teris van Beek²; ¹*RIKILT-Institute of Food Safety, Wageningen, Netherlands*; ²*Wageningen University, Wageningen, NL*
- WOE pm 3:50 **Identification of Biological Species using Spectral Libraries;** Magnus Palmblad¹; Merel Nessen²; Tune Wulff³; Hans Dalebout¹; Rob Marissen¹; Dana Ohana¹; Suzanne van der Plas-Duivesteyn¹; Arzu Tugce Guler¹; Coen Mulders¹; Sander Grevers¹; Dennis van der Zwaan²; Alexandra Galitsyna¹; Anastasia Stolyarova¹; Martijn Staats²; Flemming Jessen³; Martha van der Beek¹; Jeroen de Keijzer¹; Peter van Veelen¹; Michael Engelbrecht Nielsen³; Esther Kok²; Ed Kuijper¹; Jonas Bergquist⁴; André Deelder¹; ¹*Leiden University Medical Center, Leiden, Netherlands*; ²*RIKILT Wageningen UR, Wageningen, Netherlands*; ³*National Food Institute, Technical University of Denmark, Lyngby, Denmark*; ⁴*Uppsala University, Uppsala, Sweden*
- WOE pm 4:10 **Tracking Gluten Hydrolysis Throughout the Brewing Process;** Katherine L. Fiedler; Rakhi Panda; Whitney L. Stutts; Chung Y. Cho; Eric A.E. Garber; Timothy R. Croley; *CFSAN, U.S. FDA, College Park, MD*

2:30 – 4:30 PM, WEDNESDAY AFTERNOON H/D EXCHANGE: TECHNOLOGIES AND APPLICATIONS Derek Wilson (York University) presiding Room 106

- WOF pm 2:30 **>95% Sequence Coverage within 10 Minutes for Structural Elucidation of Antibodies by Middle Down HDX/MS;** Jingxi Pan¹; Suping Zhang¹; Albert Chou¹; Christoph Borchers^{1,2}; ¹*University of Victoria-Genome BC Proteomics Centre, Victoria, BC, Canada*; ²*Dept. of Biochem. & Microbiol., Univ. of Victoria, Victoria, BC, Canada*
- WOF pm 2:50 **Temperature-dependent Conformational Dynamics in Whole Dengue Viral Particles by Hydrogen/Deuterium Exchange Mass Spectrometry;** Xin Xiang Lim; Arun Chandramohan; Ganesh S. Anand; *NUS Singapore, Singapore, Singapore*
- WOF pm 3:10 **Monte Carlo Simulations of Hydrogen Exchange Reveal Surprising Insights about the Isotopic Distribution;** David Weis; *University of Kansas, Lawrence, KS*
- WOF pm 3:30 **Exploring the Potential of Hydrogen-Deuterium Exchange Mass Spectrometry for Screening Protein/Ligand Interactions in Drug Discovery;** Haihong Zhou¹; Robin Rolser¹; Robert Myers¹; Judyann Wiltsie¹; Jose Castro-Perez¹; David McLaren¹; Stephen Previs¹; George Addona²; Michael Kavana¹; ¹*Merck & Co., Inc., Kenilworth, NJ*; ²*Merck Co. & Inc., Boston, MA*
- WOF pm 3:50 **Electrochemical Reduction of Large and Highly Disulfide-Bonded Proteins – Complete Sequence Coverage in HDX-MS Experiments;** Esben Trabjerg^{1,2}; Rasmus U. Jakobsen¹; Simon Myslind³; Søren Christensen²; Thomas J.D. Jørgensen⁴; Kasper D. Rand¹; ¹*Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark*; ²*Biologics, H. Lundbeck A/S, Valby, Denmark*; ³*Finsen Laboratory, Rigshospitalet and BRIC, Copenhagen, Denmark*; ⁴*Department of Biochemistry and Molecular Biology, University of Southern Denmark, Odense, Denmark*
- WOF pm 4:10 **Investigating the Importance of Protein Conformational Dynamics During Catalysis by HDX-MS: Focus on the F₁F₀-ATP Synthase Molecular Machine;** Siavash Vahidi; Yumin Bi; Stanley Dunn; Lars Konermann; *Univ. of Western Ontario, London, CANADA*

2:30 – 4:30 PM, WEDNESDAY AFTERNOON ENERGY, PETROLEUM, AND BIOFUELS: ADVANCES IN SAMPLE PREPARATION AND MS INTERFACE

Mark P. Barrow (University of Warwick) presiding
Ballroom 222/224

- WOG pm 2:30 **Modern Petroleomics;** Ryan P. Rodgers^{1,2}; Winston K. Robbins³; Jonathan Putman²; Vladislav Lobodin^{1,2}; Priscila Lalli^{1,2}; David Podgorski^{1,2}; Steven Rowland^{1,2}; Jie Lu²; Yuri Corilo^{1,2}; Alan Marshall^{1,4}; ¹*National High Magnetic Field Laboratory, Tallahassee, FL*; ²*Future Fuels Institute, Tallahassee, FL*; ³*Consultant, Brunswick, ME*; ⁴*FSU Department of Chemistry and Biochemistry, Tallahassee, FL*
- WOG pm 2:50 **Monitoring the Photo Transformation of Crude Oils using SAIMS-FT-ICR MS;** Paolo Benigni¹; Kathia Sandoval¹; Christopher Thompson²; Mark Ridgeway³; Melvin A. Park³; Piero Gardinali¹; Francisco Fernandez Lima¹; ¹*Florida International University, Miami, FL*; ²*Bruker Daltonics Inc., Billerica, MA*; ³*Bruker Daltonic, Billerica, MA*



- WOG pm 3:10 **Petrochemical Isomer Distribution Analysis Using Cold EI GC/MS**; Adam J. Patkin; Sharanya Reddy; Andrew N. Tyler; *PerkinElmer, Shelton, CT*
- WOG pm 3:30 **Lignomic Profiling of Extractives from Grasses using Electrospray Ionization and LC-TOFMS with Gamma-Valerolactone as a Renewable High-Boiling Mobile Phase**; Afrand Kamali Sarvestani¹; Leonardo Da Costa Sousa^{2,3}; Venkatesh Balan^{2,3}; Bruce E. Dale^{2,3}; A. Daniel Jones III^{1,3}; ¹*Department of Chemistry, Michigan State University, East Lansing, MI*; ²*Dept of Chemical Eng, Michigan State University, East Lansing, MI*; ³*Great Lakes Bioenergy Research Center, East Lansing, MI*
- WOG pm 3:50 **Determination of the Average Molecular Weight of Crude Oil by Using Gas and Liquid Chromatography and Tandem Mass Spectrometry**; Ravikiran Yerabolu; Raghavendhar Kotha; Xueming Dong; Hilka Kenttamaa; *Purdue University, West Lafayette, IN*
- WOG pm 4:10 **Selective Chromatographic Separation of Crude Oil Mixtures by Online Coupling with Ultrahigh Resolution Mass Spectrometry**; Wolfgang Schrader; Alessandro Vetere; Lilla Molnárme Guricza; *Max-Planck Inst für Kohlenforschung, Mülheim / Ruhr, GERMANY*

**2:30 – 4:30 PM, WEDNESDAY AFTERNOON
ANTIBODIES AND ANTI-BODY DRUG CONJUGATES**
Keyang Xu (Genentech, Inc.) presiding
Ballroom 220/221

- WOH pm 2:30 **Comprehensive Characterization of Three IgG Forms using CESI-MS**; Bryan Fonslow¹; Olga V. Friese²; K. Steven Cook²; ¹*SCIEX, Brea, CA*; ²*Pfizer, Chesterfield, MO*
- WOH pm 2:50 **In-depth Characterization of Lysine-Conjugated Antibody-Drug Conjugates (ADCs) by a Multiplexed MS/MS Data Acquisition Strategy Combined with Multi-Enzyme Digestion**; Liuxi Chen¹; Robert Birdsall¹; Henry Shion¹; Ying-Qing Yu¹; Frank Kotch²; April Xu³; Thomas Porter⁴; Weibin Chen¹; ¹*Waters Corporation, Milford, MA*; ²*Pfizer Bioprocess Research & Development, Pearl River, NY*; ³*Pfizer Analytical Research & Development, Pearl River, NY*; ⁴*Pfizer Analytical Research & Development, Andover, MA*
- WOH pm 3:10 **Antibody-Drug Conjugate (ADC) Bioanalysis by Immuno-capture LC-MS/MS Hybrid Assays: Challenges, Solutions and Complementarity with Ligand Binding Assays (LBA)**; Jian Wang; Ang Liu; Huidong Gu; Frank Zambito; Alexander Kozhich; Heather Myler; Mark Arnold; Anne-Françoise Aubry; *Bristol-Myers Squibb, Princeton, NJ*
- WOH pm 3:30 **Improved Top-Down and Middle-Down Characterization of Complex Biopharmaceuticals on a Modified Tribrid Mass Spectrometer**; Luca Fornelli¹; Philip D. Compton¹; Seema Sharma²; Jesse D. Canterbury²; Christopher Mullen²; Vlad Zabrouskov²; Michael W. Senko²; Andrew P. Mazar¹; Neil L. Kelleher¹; ¹*Northwestern University, Evanston, IL*; ²*Thermo Fisher Scientific, San Jose, CA*
- WOH pm 3:50 **Dissecting the FcRn Binding Mode of Antibodies with Different Pharmacokinetic Profiles by Hydrogen/Deuterium Exchange Mass Spectrometry**; Pernille Foged Jensen¹; Vincent Larraillet²; Angela Schoch²; Maximiliane Hilger²; Thomas Emrich²; Tilman Schlothauer²; Kasper D. Rand¹; ¹*Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark*; ²*pRED, Roche Innovation Center, Penzberg, Germany*

- WOH pm 4:10 **Novel Sample Treatment and LC/MS Strategies Achieved Highly Accurate and Sensitive Investigation of Tissue Distributions of Therapeutic Monoclonal Antibody**; Ming Zhang; Bo An; Haoying Yu; Jun Qu; *SUNY at Buffalo, Buffalo, NY*

**4:45 – 5:30 PM, WEDNESDAY AFTERNOON
ASMS MEETING**

Jenny Brodbelt, ASMS President, presiding
Enjoy a beverage and hear the latest ASMS news.
Ballroom 222/224, level 2

**5:45 – 7:00 PM, WEDNESDAY AFTERNOON
WORKSHOPS**

There are light refreshments in the common areas.

01. The role of High Resolution Mass Spectrometry in the Regulatory Environment, Room 130
02. Emerging Contaminants for Emerging Scientists, Room 131
03. Mass spectrometry instrumentation at the forefront of technology as miscible tools for forensic and security evidence, Room 132
04. Gas-phase ion chemistry: thermodynamics, kinetics, structures and spectroscopy, Room 123/124
05. Emerging Technologies Advancing Mass Spectrometry Research: 3D Printing, Room 120/127
06. CHORUS - A community solution for the Storage Visualization, Sharing, and Analysis of Mass Spectrometry Data on the Cloud, Room 260/267
07. The Big Fat Questions: Tthe future for lipidomics in cell biology and clinical diagnostics? Room 274
08. Characterization of Protein Therapeutics by Mass Spectrometry, Room 275
09. Getting the Most out of Undergraduate Research in Mass Spectrometry, Room 230
10. Working with Federal Agencies to Obtain Research Support: Mock NIH Study Section and Q&A with Agency Staff, Room 231
11. Room 232
12. Ligand Binding Assays (LBA) and LC-MS/MS Integrated Antibody-Drug Conjugate (ADC) Bioanalysis -Immuno-capture LC-MS/MS Hybrid Assays: Challenges, Solutions, and Complementarity with LBA, Ballroom 222/224
13. Hydrogen-Deuterium Exchange, Covalent Labeling and Crosslinking, Ballroom 220/221

**AFTER 8:00 PM
CORPORATE HOSPITALITY SUITES
RENAISSANCE GRAND HOTEL**



THURSDAY MORNING ORAL SESSIONS

8:30 – 10:30 AM, THURSDAY MORNING

MINI/OORTABLE/FIELDABLE MS

Zheng Ouyang (Purdue University) presiding
Hall 5

- ThOA am 08:30 **Investigation of NIR Diode Wavelength and Material Combinations for Increased Permeability in Portable Membrane Inlet Mass Spectrometry**; Phillip Mach¹; Kenneth Wright²; Guido Verbeck¹; ¹University of North Texas, Denton, TX; ²Inficon, Syracuse, NY
- ThOA am 08:50 **Chemical Ionization Mass Spectrometry Using Carbon Nanotube Field Emission Electron Sources**; Erich Radauscher¹; Adam Keil²; Mitch Wells²; Jason Amsden¹; Jeffrey Piascik³; Charles Parker¹; Brian Stoner³; Jeffrey Glass¹; ¹Duke University, Durham, NC; ²FLIR Systems, West Lafayette, IN; ³Engineering and Applied Physics Division, RTI Int, Research Triangle Park, NC
- ThOA am 09:10 **Rarefied Choked Flow in a Microscale Ion Trap Operated at High Pressure**; Bruno Couplier; Kevin Schultze; Sorin Mitran; J. Michael Ramsey; UNC Chapel Hill, Chapel Hill, NC
- ThOA am 09:30 **Old Dog, New Tricks: Enhanced Quadrupole Performance by Addition of a Magnetic Field**; Simon Maher^{1,2}; Sarfaraz U. A. Syed³; John R. Gibson²; Fred P. M. Jjunju²; Barry L. Smith⁴; David Taylor⁴; Iain S. Young¹; Ron M. A. Heeren³; Stephen Taylor²; ¹Institute of Integrative Biology, University of Liverpool, UK; ²Dept. of Electrical Engineering and Electronics, University of Liverpool, UK; ³FOM Institute for Atomic and Molecular Physics, Amsterdam, Netherlands; ⁴Q Technologies, Liverpool, UK
- ThOA am 09:50 **A Mini-Mass Spectrometer with Continuous Atmospheric Pressure Interface: Pushing the Limits of Ion Transfer Device, Vacuum System and Ion Trap**; Yanbing Zhai; Muye He; Yongzheng Wei; Wei Xu; Beijing Institute of Technology, Beijing, CHINA
- ThOA am 10:10 **Development of Portable Particle Mass Spectrometer with Ambient Aerodynamic Ion Source**; Caiqiao xiong¹; Yiming Zhang²; Suming Chen¹; Zongxiu Nie¹; ¹Institute of Chemistry Chinese Academy of Sciences, Beijing, China; ²Jiangsu Skyray Instrument Inc., Suzhou, Kunshan

8:30 – 10:30 AM, THURSDAY MORNING

INFORMATICS: PEPTIDE IDENTIFICATION AND QUANTIFICATION

William Noble (University of Washington) presiding
Room 130/132

- ThOB am 08:30 **Machine Learning Approach for Inferring Atomic Composition of Peptides from Peaks with Unresolved Isotopic Fine Structure**; Tikira Temu¹; Annette Michalski^{1,2}; Stefka Tyanova¹; Matthias Mann¹; Juergen Cox¹; ¹Max-Planck Institute of Biochemistry, Martinsried, DE; ²Bruker Daltonik GmbH, Bremen, DE
- ThOb am 08:50 **Fast and Accurate Unrestricted Spectrum Interpretation: You Don't Know What You're Missing**; Arun Devabhaktuni; Josh Elias; Stanford University, Stanford, CA
- ThOB am 09:10 **De novo Sequencing using MELD Proteolysis Coupled to a "Sequence Assembly" Algorithm**; Gabriel Mazzucchelli¹; Tyler A Zimmerman²; Nicolas Smargiasso¹; Dominique Baiwir³; Marie-Alice Meuwis⁴; Edwin De Pauw¹; ¹Univeristy of Liege, MS Lab - GIGA, Liege, Belgium; ²National Institute of Standards and Technology, Gaithersburg, MD; ³University of Liege, GIGA-Proteomics, Liege, Belgium; ⁴CHU, Gastroenterology unit, Liege, Belgium

- ThOB am 09:30 **Isobaric Labeling Assisted Proteome Identification and Quantification Based on Database Search and Denovo Sequencing**; Yichu Shan¹; Shen Zhang^{1,2}; Lihua Zhang¹; Yukui Zhang¹; ¹Dalian Institute of Chemical Physics, dalian, china; ²University of Chinese Academy of Sciences, Beijing, china
- ThOB am 09:50 **Increasing Depth of Proteomic Profiling in MS Data-Dependent Acquisition (DDA) Discovery Experiments Using Advanced Precursor Ion Selection Algorithms**; Simion Kreimer¹; William Danielson²; Mikhail Belov²; Barry Karger¹; Alexander R. Ivanov¹; ¹Barnett Inst., Northeastern University, Boston, MA; ²Spectrograph LLC, Kennewick, WA
- ThOB am 10:10 **Accurate and Rapid Quantification of Co-Eluting Deamidated and Non-Deamidated Peptides using a Novel Deconvolution Technique**; Yong Kil¹; Marshall W. Bern¹; Eric Carlson¹; Chris Becker¹; David Morgenstern²; Beatrix Ueberheide²; ¹Protein Metrics Inc., San Carlos, CA; ²NYU School of Medicine, New York City, NY

8:30 – 10:30 AM, THURSDAY MORNING NEW AND DEVELOPING ION ACTIVATION METHODS

Kaveh Jorabchi (Georgetown University) presiding
Room 123/124

- ThOC am 08:30 **Enhancement of Ion Activation and CID by Simultaneous Dual Dipolar Excitation in X and Y Directions in Linear Ion Trap**; Xiao Dong Xie¹; Qiankun Dang¹; Fuxing Xu¹; Xinhua Dai²; Xiang Fang²; Chuan-Fan Ding¹; ¹Fudan University, Shanghai, China; ²National Institute of Metrology, Beijing, China
- ThOC am 08:50 **Charge Transfer Dissociation (CTD) Mass Spectrometry**; Glen Jackson; William Hoffmann; West Virginia University, Morgantown, WV
- ThOc am 09:10 **High-Energy (> 50 eV) Electron-Induced Dissociation of Therapeutic Drugs in a QTOF Mass Spectrometer**; Yury V Vasil'ev; Valery G. Voinov; Samuel E. Bennett; Joseph S. Beckman; Douglas F. Barofsky; Oregon State University, Corvallis, OR
- ThOC am 09:30 **Ultraviolet Photodissociation for Analysis of Native Proteins, Protein Complexes, and Charge-Reduced Proteins in the Gas Phase**; Dustin Holden²; Jennifer Brodbelt¹; ¹The University of Texas, Austin, TX; ²University of Texas Chemistry, Austin, TX
- ThOC am 09:50 **Interrogation of Protein Structure using Conformer Selection, UVPD, and ETnoD**; Bruno Bellina¹; Jeff Brown²; Jakub Ujma¹; Kevin Giles²; Paul Murray²; Rebecca Beveridge¹; Eleanor Dickinson¹; Jonathan P. Williams²; Mike Morris²; Perdita Barran¹; ¹The University of Manchester, Manchester, UK; ²Waters Corporation, Wilmslow, UK
- ThOC am 10:10 **Efficient and Selective Covalent Bond Formation between Peptide Ion Dimers Using 355 nm Light**; Christopher Shaffer; Andy Dang; Emilie Viglino; Frantisek Turecek; University of Washington, Seattle, Washington

8:30 – 10:30 AM, THURSDAY MORNING

NEW NANO-SCALE AND MICROFLUIDIC SEPARATIONS AND MS

Liangliang Sun (University of Notre Dame) presiding
Room 120/127

- ThOD am 08:30 **A Handheld Ultrafast CE Interfaced to MS for the Analysis of Explosives, Illicit Drugs, Amino Acids and their Optical Isomers**; Mehdi Moini; Christopher Rollman; George Washington University, Washington, DC



- ThOD am 08:50 **Identification of Metabolites in Crustacean Hemolymph via *in vivo* Microdialysis by Capillary Electrophoresis-Matrix-Assisted Laser Desorption/Ionization Mass Spectrometric Imaging Platform**; Shan Jiang; Zhidan Liang; Lingjun Li; *UW-Madison, Madison, WI*
- ThOD am 09:10 **Development, Characterization and Application of Slug Flow Microextraction (SFME) for Direct MS Analysis of Biological Samples**; Yue Ren; Zheng Ouyang; *Purdue University, West Lafayette, IN*
- ThOD am 09:30 **Microchip Capillary Electrophoresis with Integrated Electrospray Ionization for Rapid and Efficient Analysis of Polar Metabolites in Biological Samples**; J. Scott Mellors¹; Michael Pacold³; Elizaveta Freinkman³; Erin Redman²; J. Michael Ramsey²; *1908 Devices Inc., Boston, MA*; ²*University of North Carolina, Chapel Hill, NC*; ³*Whitehead Institute for Biomedical Research, Cambridge, MA*
- ThOD am 09:50 **Development of High Sensitivity Intact Monoclonal Antibody (mAb) Analysis Using an Integrated Microfluidics MS System**; Gregory Roman; Henry Shion; Weibin Chen; James Murphy; *Waters Corporation, Milford, MA*
- ThOD am 10:10 **Analysis of Proteins, Protein Complexes and Proteomes under Non-Denaturing Conditions Using Sheathless Capillary Electrophoresis Coupled with Native Mass Spectrometry**; Alexander R. Ivanov¹; Rosa Viner²; Marcia R. Santos³; Arseniy M. Belov¹; Chitra K. Ratnayake³; David M. Horn⁴; Marshall W. Bern⁵; Barry L. Karger¹; *1*Barnett Inst., *Northwestern University, Boston, MA*; *2*ThermoFisher Scientific, *San Jose, CA*; *3*Sciex, *Brea, CA*; *4*Thermo Fisher Scientific, *San Jose, CA*; *5*Protein Metrics, *Palo Alto, CA*
- 8:30 – 10:30 AM, THURSDAY MORNING
STRUCTURE/REACTIVITY AND ENERGETICS OF
GAS-PHASE IONS AND COMPLEXES**
**Ken Ervin (University of Nevada, Reno) presiding
Theater**
- ThOE am 08:30 **Gas-Phase Reactivity of Phenoxy Radical Cations of Tyrosine and Related Model Compounds**; Michael Lesslie¹; Andrii Piatkivskiy¹; Sandra Osburn²; Richard A. J. O'Hair²; Victor Ryzhov¹; *1*Northern Illinois University, *DeKalb, IL*; *2*University of Melbourne, *Melburne, Australia*
- ThOE am 08:50 **The Effects of Protonation vs Noncovalent Interactions with Sodium Cations on the Structures and Stability of DNA and RNA Nucleosides**; Mary T. Rodgers¹; Ranran Wu¹; Yanlong Zhu¹; Chenchen He¹; Stephen Strobehn¹; Juehan Gao²; Jos Oomens²; *1*Wayne State University, *Detroit, MI*; *2*Radboud University Nijmegen, *Nijmegen, NETHERLANDS*
- ThOE am 09:10 **Gas-Phase Reactions of Ionic Liquid Anions**; Charles Nichols^{1,2}; W. Carl Lineberger^{1,2}; Veronica M. Bierbaum^{1,2}; *1*University of Colorado, *Boulder, CO*; *2*JILA, *Boulder, Colorado*
- ThOE am 09:30 **Pushing it to the Red: Probing the Influence of Ligands on the Antisymmetric Uranyl Stretching Frequency using IRMPD Spectroscopy**; Michael J. Van Stipdonk¹; John Gibson²; Bert De Jong²; Phuong Dau²; Giel Gerden³; Jos Oomens³; *1*Duquesne University, *Pittsburgh, PA*; *2*Lawrence Berkeley Nat'l Lab, *Berkeley, CA*; *3*Radboud University Nijmegen, *Nijmegen, Netherlands*
- ThOE am 09:50 **Water-Network Mediated, Electron Induced Proton Transfer in Anionic $[C_5H_5N(H_2O)_n]^-$ Clusters: Size-Dependent Formation of the Pyridinium Radical for $n \geq 3$** ; Andrew F. DeBlase^{1,4}; Gary H. Weddle^{2,4}; Kaye A. Archer³; Kenneth D. Jordan³; Mark A. Johnson⁴; *1*Purdue University, *West Lafayette, IN*; *2*Fairfield University, *Fairfield, CT*; *3*University of Pittsburgh, *Pittsburgh, PA*; *4*Yale University, *New Haven, CT*
- ThOE am 10:10 **Disentangling Reactive Isomers in Combustion Chemistry using Photoelectron Photoion Coincidence Spectroscopy**; Tina Kasper¹; Thomas Bierkandt¹; Patrick Oßwald²; Markus Köhler²; Patrick Hemberger³; *1*Thermodynamics, *University of Duisburg-Essen, Duisburg, Germany*; *2*DLR – *Institute of Combustion Technology, Stuttgart, Germany*; *3*Molecular Dynamics Group, *SLS, Paul Scherrer Inst., Villigen, Switzerland*
- 8:30 – 10:30 AM, THURSDAY MORNING
MS IN PROTEIN FOOTPRINTING:
MICHAEL GROSS 75TH BIRTHDAY**
**Ragu Ramanathan and
Christopher L. Hohlman (Pfizer, Inc.) presiding
Room 106**
- ThOF am 08:30 **Review of Fast PhotoChemical Oxidative Footprinting Development in the Gross Lab**; David Hambly; *Amgen Inc., Longmont, CO*
- ThOF am 08:50 **In Cell Protein Footprinting for the Analysis of Protein Structure**; Lisa M. Jones; *Indiana University-Purdue University Indianapolis, Indianapolis, IN*
- ThOF am 09:10 **Mass Spectrometry for Probing Protein Higher Order Structure: An Industry Perspective**; Guodong Chen; Richard Huang; Hui Wei; Ekaterina Deyanova; Bethanne Warrack; Adrienne Tymiak; *Bristol-Myers Squibb, Princeton, NJ*
- ThOF am 09:30 **Fast Photochemical Oxidation of Proteins (FPOP) Reveals the Binding Interface of an Antigen and Antibody**; Ying Zhang¹; Aaron Weckslers²; Patricia Molina²; Galahad Deperalta²; Michael L. Gross¹; *1*Washington University in St. Louis, *St. Louis, MO*; *2*Genentech Inc., *South San Francisco, CA*
- ThOF am 09:50 **Protein Footprinting for Quantitative Topography Analysis of Protein Structure**; Mark Chance; Janna Kiselar; Parminder Kaur; *Case Western Reserve University, Cleveland, OH*
- ThOF am 10:10 **HDX, FPOP, and Specific Amino-acid Labeling are Complementary Methods for MS-based Protein Footprinting**; Michael L. Gross; *Washington University, St Louis, MO*
- 8:30 – 10:30 AM, THURSDAY MORNING
TARGETED QUANTIFICATION OF PROTEINS AND
POST-TRANSLATIONAL MODIFICATIONS**
**Birgit Schilling (Buck Institute for Research on Aging) presiding
Ballroom 222/224**
- ThOG am 08:30 **Proteome Reaction Monitoring by Top-Down Proteomics: Moving from Discovery to Targeted Validation of Intact Protein Biomarkers**; Timothy K. Toby¹; Luca Fornelli¹; Kyunggon Kim¹; Michael M. Abecassis²; Daniel R. Salomon³; Neil L. Kelleher¹; *1*Northwestern University, *Evanston, IL*; *2*Northwestern Feinberg School of Medicine, *Chicago, IL*; *3*The Scripps Research Institute, *La Jolla, CA*

THURSDAY MORNING ORAL SESSIONS

- ThOG am 08:50 **Ubiquitin Ser65 Phosphorylation Affects Ubiquitin Structure, Chain Assembly and Hydrolysis;** Kirby Swatek; Tobias Wauer; Jane Wagstaff; Christina Gladkova; Jonathan Pruneda; Martin Michel; Malte Gersch; Christopher Johnson; Stefan Freund; David Komander; *MRC Laboratory of Molecular Biology, Cambridge, UK*
- ThOG am 09:10 **Refinement of Parallel Reaction Monitoring Methods to Improve Accuracy in Peptide Quantification;** Sebastien Gallien; Daniel Ayoub; Sang Yoon Kim; Antoine Lesur; Bruno Doman; *Luxembourg Clinical Proteomics Center, Strassen, LUXEMBOURG*
- ThOG am 09:30 **Optimized Protocol for MRM-based Protein Quantification in Archived Cancer Tissues;** Jacob Kennedy¹; Regine Schoenherr¹; Ping Yan¹; Jeff Whiteaker¹; Richard Ivey¹; Melissa Lerch²; Geoffrey Baird²; Andy Hoofnagle²; Amanda Paulovich¹; ¹*Fred Hutchinson Cancer Research Center, Seattle, WA*; ²*UW Dept of Laboratory Medicine, Seattle, WA*
- ThOG am 09:50 **Using Targeted Proteomics to Characterize the Relative Distribution of Apolipoprotein E Allele-Specific Isoforms in Clinically-Relevant Matrices;** James G. Bollinger¹; Han-Yin Yang¹; Clark Henderson¹; Nicole Kuderer¹; Christine Wu²; C. Anthony Blau¹; Andrew Hoofnagle¹; Michael MacCoss¹; ¹*University of Washington, Seattle, WA*; ²*Stratus Biosciences, Seattle, WA*
- ThOG am 10:10 **From Discovery Proteomics to Targeted Biomarker Assays: Identification of Tau Post-Translational Modifications that Track O-GlcNAcase inhibition by Thiamet G;** Nathan G. Hatcher¹; Ronald A. Miller¹; Zhenlian Ke¹; Julie Lee²; Helene L. Cardasis³; Giuseppe Terracina²; Lili Zhang⁴; Jacob Marcus¹; Xiaohai Wang¹; Dawn M. Toolan¹; Bonnie J. Howell¹; John J. Renger¹; Sean M. Smith¹; Daniel S. Spellman¹; ¹*Merck Research Labs, West Point, PA*; ²*Merck Research Labs, Kenilworth, NJ*; ³*Thermo Fisher Scientific, Cambridge, MA*; ⁴*Novartis Institute for Biomedical Research, Cambridge, MA*

8:30 – 10:30 AM, THURSDAY MORNING ION MOBILITY: SMALL MOLECULES, PHARMACEUTICALS AND DMPK

**Erkinjon Nazarov (University of South Florida) presiding
Ballroom 220-221**

- ThOH am 08:30 **Potential for Ion Mobility Spectrometry in Small Molecule Chiral Analysis;** Tawnya Flick; Iain D G Campuzano; Michael D Bartberger; *Amgen Inc., Thousand Oaks, CA*
- ThOH am 08:50 **Separation of Isomeric Steroids using Ion Mobility QTOF-LC/MS;** Christopher D. Chouinard¹; Christopher R. Beekman¹; Timothy J. Garrett²; Richard A. Yost¹; ¹*Department of Chemistry, University of Florida, Gainesville, FL*; ²*Department of Pathology, University of Florida, Gainesville, FL*
- ThOH am 09:10 **Collision Cross Section Calibration Strategies for Traveling-Wave Ion Mobility - Mass Spectrometry in Negative-Ion Mode;** Jay Forsythe^{1,2}; Chelsea Walker^{1,2}; Anton Petrov^{1,2}; Samuel Allen³; Matthew Bush³; Nicholas Hud^{1,2}; Facundo Fernandez^{1,2}; ¹*Georgia Tech, School of Chemistry and Biochemistry, Atlanta, GA*; ²*NSF/NASA Center for Chemical Evolution, Atlanta, GA*; ³*University of Washington, Department of Chemistry, Seattle, WA*

- ThOH am 09:30 **Comprehensive Screening and Characterisation of Metabolites and Biomolecules by Collisional Cross Section using a Novel Geometry Travelling-Wave IMS-QToF Mass Spectrometer;** Richard Gallagher¹; Christine Pattison¹; Kathryn Pickup¹; Nick Tomczyk²; Martin Palmer²; Jason Wildgoose²; Darren Hewitt²; Daniel Weston²; ¹*Astrazeneca, Macclesfield, UK*; ²*Waters, Wilmslow, UK*
- ThOH am 09:50 **Ultra-Fast Separation and Quantification of Isobaric Barbiturates in Serum using LDTD-MS/MS Combined with Differential Mobility Spectrometry;** Sylvain Letarte; Alex Birsan; Serge Auger; Jean Lacoursière; Pierre Picard; *Phytronix Technologies, Inc., Quebec, Canada*
- ThOH am 10:10 **Application of Differential Mobility Spectrometry Coupled with Multiple Ion Monitoring for Quantitation of Peptides Not Suited for MRM Analysis;** Yuan-Qing Xia¹; Eugene Ciccimaro, Jr²; Naiyu Zheng²; Mingshe Zhu²; ¹*Scienc, Framingham, MA*; ²*Bristol-Myers Squibb Company, Lawrenceville, NJ*

10:30 AM – 2:30 PM, THURSDAY
THURSDAY POSTER SESSION
Poster/Exhibit Hall
Lunch concessions are open 11:00 am – 2:00 pm





2:30 – 4:30 PM, THURSDAY AFTERNOON

MS IN SURGERY

Zoltan Takats (Imperial College London) presiding
Hall 5

- ThOA pm 2:30 **Development of a System for the Investigation of Near Real-Time Tissue Identification Using Rapid Evaporative Ionisation Time-of-Flight Mass Spectrometry.**; Steven Pringle¹; Julia balog²; Emrys A Jones¹; Tamas Karancsi²; Keith Richardson¹; Mike Morris¹; ¹Waters Corporation, Wilmslow, United Kingdom; ²Waters Research Center, Budapest, Hungary
- ThOA pm 2:50 **Ambient Ionization MS for Rapid Tissue Diagnosis During Surgical Intervention of Human Brain Cancer**; Alan Jarmusch¹; Valentina Piro¹; Zane Baird¹; Clint Alfaro¹; Eyas Hattab²; Aaron Cohen-Gadol³; R. Graham Cooks¹; ¹Purdue University-Department of Chemistry, West Lafayette, IN; ²Department of Pathology, IUSM, Indianapolis, IN; ³Department of Neurological Surgery, IUSM, Indianapolis, IN
- ThOA pm 3:10 **Chemical Biopsy based on SPME Approach: A New Medical Tool**; Janusz Pawliszyn¹; Barbara Bojko¹; German Augusto Gomez-Rios¹; Krzysztof Gorynski¹; Jan Matthias Knaak²; Tiago Machuca³; Erasmus Cudjoe¹; Vinzent Spetzler²; Michael Hsin³; Markus Selzner²; Mingyao Liu³; Marcelo Cypel³; Shaf Keshavjee³; ¹University of Waterloo, Waterloo, Canada; ²Department of Surgery, Toronto General Hospital, Toronto, Canada; ³University Health Network, University of Toronto, Toronto, Canada
- ThOA pm 3:30 **Endometriosis Foci Differentiation by Direct High Resolution Mass Spectrometry Methods.**; Alexey Kononikhin^{1,4}; Anna Bugrova^{1,3}; Natalia Starodubtseva^{1,2}; Anna Borisova¹; Denis Bormotov⁴; Yury Kostyukovich²; Vladimir Naumov¹; Igor Popov⁴; Vladimir Frankevich¹; A. V. Kozachenko¹; E. A. Kogan¹; Leila V. Adamyan¹; Gennady T. Sukhikh¹; Eugene Nikolaev^{2,4}; ¹Research Center for Obstetrics, Gynecology, Moscow, Russia; ²Institute for Energy Problems of Chemical Physics, Moscow, Russia; ³Emanuel Institute of Biochemical Physics, Moscow, Russia; ⁴Moscow Institute of Physics and Technology, Moscow, Russia
- ThOA pm 3:50 **Molecular Assessment of Gastric and Pancreatic Cancer Surgical Margins by Ambient Mass Spectrometry Imaging**; Livia S. Eberlin; Robert Tibshirani; Katy Margulis-Goshen; Ivette Planell-Mendez; Moe Jalali; Teri A. Longacre; George A. Poultsides; Richard N. Zare; Stanford University, Stanford, CA
- ThOA pm 4:10 **Development of a Novel Instrument for ex-vivo and in-vivo Real-Time Analysis**; Benoit Fatou¹; Maxence Wisztorski¹; Cristian Fosca²; Michael Ziskind²; Michel Salzet¹; Isabelle Fournier¹; ¹INSERM U1192 PRISM - University of Lille, Villeneuve d'Ascq, France; ²CNRS UMR 8523 PhLAM - University of Lille, Villeneuve d'Ascq, France

2:30 – 4:30 PM, THURSDAY AFTERNOON

MULTI-PTMS: COMPREHENSIVE ANALYSIS

Leslie M. Hicks (University of North Carolina, Chapel Hill) presiding
Room 130/132

- ThOB pm 2:30 **Comprehensive Discovery of Protein Post-translational Modifications in Proteomic Datasets**; Michael R. Shortreed¹; Qiyao Li¹; Brian L. Frey¹; Craig D. Wenger²; Mark Scalf¹; Lloyd M. Smith¹; ¹University of Wisconsin, Madison, WI; ²Unaffiliated, North Branford, CT

- ThOB pm 2:50 **Peptide Variant Discovery in Lens Tissue using Penalty-Based Spectral Alignment**; Laurence E. Bernstein; Nuno Bandeira; University of California, San Diego, La Jolla, CA
- ThOB pm 3:10 **Complete Characterization of the Protein Post-Translational Modification Profiles through Combination of Native and Bottom-Up Mass Spectrometry**; Fan Liu; Yang Yang; Albert J.R. Heck; Utrecht University, Utrecht, The Netherlands
- ThOB pm 3:30 **Tracing Protein Post-Translational Modifications at Different Growth Stages of the Archaeon *Sulfolobus islandicus* with Bottom-Up and Top-Down Proteomics**; Egor Vorontsov; Elena Rensen; David Prangishvili; Mart Krupovic; Julia Chamot-Rooke; Institut Pasteur, Paris, France
- ThOB pm 3:50 **A Bottom-Up Informed Top-Down Approach Provides Insights into the Ubiquitin Code of Immune Cell Signaling**; Giuseppe Infusini; Thomas Nebel; John Silke; Andrew Webb; The Walter & Eliza Hall Institute, Parkville, Australia
- ThOB pm 4:10 **Sirtuin 4 is a Lipoamidase Regulating Pyruvate Dehydrogenase Complex Activity**; Rommel Mathias; Todd M. Greco; Adam Oberstein; Hanna Budayeva; Rumela Chakrabarti; Elizabeth Rowland; Yibin Kang; Thomas Shenk; Ileana M. Cristea; Princeton University, Princeton, NJ

2:30 – 4:30 PM, THURSDAY AFTERNOON

PEPTIDE FRAGMENTATION AND PEPTIDOMICS

Carlito Lebrilla (University of California, Davis) presiding
Room 123/124

- ThOC pm 2:30 **Analytic Framework for Peptidomics Applied to Large-Scale Neuropeptide Identification**; Christian Kelstrup¹; Anna Secher²; Jesper V. Olsen¹; ¹NNF CPR, University of Copenhagen, Copenhagen, Denmark; ²Novo Nordisk, Måløv, Denmark
- ThOC pm 2:50 **Ion Mobility Peptidomic Analysis of Endogenous Peptides Reveals Functions through Conformations**; Andres Guerrero¹; Miguel Angel Garcia Mompean²; Cassandra Yee¹; David Wong³; Carlito Lebrilla¹; ¹UC Davis, Chemistry Department, Davis, CA; ²Institute of Physical Chemistry Rocasolano, CSIC, Madrid, Spain; ³Agilent Technologies, Inc., Santa Clara, CA
- ThOC pm 3:10 **Lymph-Carried Self-Antigens Derive from a Variety of Processing Enzymes and Contribute to the Dendritic Cells MHC II Peptidome**; Cristina Clement¹; Aniuska Becerra²; Liusong Yin²; Valerio Zolla¹; Scott Shafer²; Lawrence J. Stern²; Laura Santambrogio¹; ¹Albert Einstein College Medicine, Bronx, NY; ²University of Massachusetts. Medical School, Worcester, MA
- ThOC pm 3:30 **Incorporation of Ultra-Violet Photodissociation (UVPD) into a Phosphoproteomic Pipeline improves Phosphosite Assignments**; Kyle L. Fort; Clement M. Potel; Andrey Dyachenko; Albert J.R. Heck; Utrecht University, Utrecht, Netherlands
- ThOC pm 3:50 **Photodissociation Study of Hydrogen-Rich and Hydrogen-Deficient Cation Radicals in Tyrosine-Containing Peptides**; Emilie Viglino; Christopher Shaffer; Frantisek Turecek; University of Washington, Seattle, Washington
- ThOC pm 4:10 **Electron Deficient Radical B-Type Ions Undergo Sequence Scrambling and Dissociation by Different Mechanisms than Corresponding b-Ions**; Declan Williams¹; Justin Kai-Chi Lau^{1,2}; Stefanie Maedler¹; Yating Wang¹; Junfang Zhao¹; Irine Saminathan¹; K.W. Michael Siu^{1,2}; Alan C. Hopkinson¹; ¹York University, Toronto, Canada; ²University of Windsor, Windsor, Canada

THURSDAY AFTERNOON ORAL SESSIONS

2:30 – 4:30 PM, THURSDAY AFTERNOON FORENSIC APPLICATIONS

**Kenyon Evans-Nguyen (University of Tampa) presiding
Room 120/127**

- ThOD pm 2:30 **Identification of Plant-based Forensic Evidence by Direct Analysis in Real Time Mass Spectrometry (DART-MS), Chemotaxonomic Profiling and Chemometrics;** Ashton D. Lesiak¹; Justine E. Giffen¹; Robert B. Cody²; A. John Dane²; Rabi A. Musah¹; ¹University at Albany-SUNY, Albany, NY; ²JEOL USA, Inc., Peabody, MA
- ThOD pm 2:50 **Rapid Analysis of Synthetic Cannabinoids using a Miniature Mass Spectrometer with Ambient Ionization Capability;** Qiang Ma^{1,2}; R. Graham Cooks²; Zheng Ouyang²; ¹Chinese Academy of Inspection and Quarantine, Beijing, China; ²Purdue University, West Lafayette, IN
- ThOD pm 3:10 **A New Approach in Hair Forensics: Longitudinal Scanning of Drugs of Abuse in Hair using DART-MS;** Wilco F. Duvivier¹; Teris A. van Beek¹; Michel W.F. Nielen^{1,2}; ¹Wageningen University, Wageningen, The Netherlands; ²RIKILT-Institute of Food Safety, Wageningen, The Netherlands
- ThOD pm 3:30 **Isobaric Drug Analyses using Hydrogen/Deuterium Exchange and CID;** William D. Hoffmann; Glen P. Jackson; West Virginia University, Morgantown, WV
- ThOD pm 3:50 **CSI Sheffield Hallam University: Forensic Analysis of Fingermarks by MALDI MS and the Integration into Currently Employed Fingerprint Examination Workflows;** Robert Bradshaw¹; Neil Denison²; Stephen Bleay³; Malcolm Clench¹; Simona Francese¹; ¹BMRC, Sheffield Hallam University, Sheffield, United Kingdom; ²Head of Identification Services, Yorkshire and the Humber (YaTH) Regional Policing, United Kingdom; ³CAST, Home Office UK, St Albans, United Kingdom
- ThOD pm 4:10 **Forensic Serology Testing by Mass Spectrometry;** Heyi Yang¹; Samantha Monier²; Kaylee Hershfeld¹; Matthew Goldstein¹; Donald Siegel¹; ¹Office of Chief Med Exam, New York, NY; ²Columbia University, New York, NY

2:30 – 4:30 PM, THURSDAY AFTERNOON SYNTHETIC POLYMERS

**Wendy Zhong (Merck) presiding
Theater**

- ThOE pm 2:30 **Characterization of Atmospheric Pressure Polyolefin Pyrolysis Products by Fourier Transform Mass Spectrometry and Ion Mobility – Mass Spectrometry;** Carlos Afonso¹; Mathilde Farenc^{1,2}; Matthias Witt³; Kirsten Craven⁴; Caroline Barrère-Mangote²; Pierre Giusti²; ¹University of Rouen, Mont Saint Aignan, France; ²TOTAL Refining and Chemicals, Gonfreville l'Orcher, France; ³Bruker Daltonik GmbH, Bremen, Germany; ⁴Waters, Manchester, UK
- ThOE pm 2:50 **Analysis of Alkyl Polyglycosides (APGs) using Polarity vs. Shape Sensitive Multidimensional Mass Spectrometry;** Chrys Wesdemiotis; Ahlam Alalwiat; The University of Akron, Akron, OH
- ThOE pm 3:10 **Tandem Mass Spectrometry to Read Messages Encoded in Synthetic Copolymers;** Laurence Charles¹; Jean-François Lutz²; ¹Aix-Marseille University, Marseille Cedex 20, France; ²Institut Charles Sadron, Strasbourg, France
- ThOE pm 3:30 **Iron(III) Catalyzed Branching Reactions of Polymeric Methylene Diphenyl Diisocyanate;** Anthony P. Gies; Zdravko Stefanov; Debashis

Chakraborty; Paul Chauvel; Dow Chemical Company, Freeport, TX

- ThOE pm 3:50 **Shining New Light on Nitroxide-Mediated Photopolymerisation by Photodissociation Action Spectroscopy;** David L Marshall¹; Jason C Morris¹; Christopher S Hansen²; Adam J Trevitt²; Stephen J Blanksby¹; ¹Queensland University of Technology, Brisbane, Australia; ²University of Wollongong, Wollongong, Australia
- ThOE pm 4:10 **Application of Matrix-Assisted Ionization–Ion Mobility Spectrometry–Mass Spectrometry to Polymeric Surfaces Directly from Natural Environments;** Casey Foley¹; Barbara S. Larsen²; Sarah Trimpin¹; ¹Wayne State University, Detroit, MI; ²The DuPont Company, Wilmington, DE

2:30 – 4:30 PM, THURSDAY AFTERNOON CHEMICAL CROSS-LINKING AND COVALENT LABELING Lars Konermann (University of Western Ontario) presiding Room 106

- ThOF pm 2:30 **The Novel Isotopically-Coded Photo-Reactive Homo-Bifunctional Short-Range Crosslinker TATA for Studying Protein Structures.;** Nicholas Brodie¹; Evgeniy Petrotchenko¹; Christoph Borchers^{1,2}; ¹University of Victoria-Genome BC Proteomics Centre, Victoria, BC, Canada; ²Dept. of Biochem. & Microbiol., Univ. of Victoria, Victoria, BC, Canada
- ThOF pm 2:50 **A Highly Optimized Strategy for Dissecting the Architectures of Endogenous Macromolecular Assemblies;** Yi Shi¹; Riccardo Pellarin²; Peter Fridy¹; Javier Fernandez-Martinez¹; Mary Thompson¹; Yinyin Li¹; Qing Jun Wang³; Andrej Sali²; Michael Rout¹; Brian Chait¹; ¹The Rockefeller University, Nyc, NY; ²University of California, San Francisco, San Francisco, CA; ³University of Kentucky, Lexington, KY
- ThOF pm 3:10 **New Tools for Studying Molecular Architecture and Conformational Changes of Large Protein Complexes using Chemical Cross-Linking;** Alexander Leitner¹; Thomas Walzthoeni^{1,2}; Ruedi Aebersold^{1,3}; ¹ETH Zurich, Zurich, Switzerland; ²Gene Center, LMU Munich, Munich, Germany; ³University of Zurich, Zurich, Switzerland
- ThOF pm 3:30 **A New In Vivo Cross-linking Mass Spectrometry Platform to Define Protein-Protein Interactions in Living Cells;** Kaake Robyn¹; Xiaorong Wang¹; Anthony Burke¹; Clinton Yu¹; Wynne Kandur¹; yingying yang¹; Tonya Second²; Jicheng Duan¹; Athit Kao¹; Shenheng Guan³; Danielle Vellucci¹; Scott Rychnovsky¹; Lan Huang¹; ¹University of California, Irvine, CA; ²Thermo Fisher Scientific, San Jose, CA; ³University of California, San Francisco, CA
- ThOF pm 3:50 **Hydroxyl Radical Footprinting of Human SOD1 Reveals Solvent Accessibility of the Interior of SOD1 β -Barrel;** Yuwei Sheng^{1,2}; Puneet Souda¹; Joan Valentine^{1,3}; Julian Whitelegge¹; ¹University of California, Los Angeles, Los Angeles, CA; ²Boston University, Boston, MA; ³Ewha Womans University, Seoul, South Korea
- ThOF pm 4:10 **ETD-Based High Spatial Resolution Hydroxyl Radical Protein Footprinting Reveals an Extended Robo1-Heparin Binding Interface;** Zixuan Li¹; Heather Moniz¹; Shuo Wang¹; Annapoorani Ramiah¹; Fuming Zhang²; Kelley W. Moremen¹; Robert J. Linhardt²; Joshua S. Sharp¹; ¹University of Georgia, Athens, GA; ²Rensselaer Polytechnic Institute, Troy, NY



**2:30 – 4:30 PM, THURSDAY AFTERNOON
ECOLOGICAL AND HUMAN ENVIRONMENTAL
CHEMISTRY AND TOXICOLOGY**

**Dana Boyd Barr (Emory University) presiding
Ballroom 222/224**

- ThOG pm 2:30 **Identification of Unknown Hemoglobin Adducts Based on Adductome LC-MS Data;** Henrik Carlsson; Margareta Törnqvist; *Stockholm University, Stockholm, Sweden*
- ThOG pm 2:50 **Exploring the Mechanism of Neurodegeneration by using an *in vitro* 3D Dopaminergic Cell Model and Metabolomics;** Liang Zhao; Georgina Harris; Lena Smirnova; Thomas Hartung; *Johns Hopkins University, Baltimore, MD*
- ThOG pm 3:10 **LC-MS Method for Simultaneous Detection and Quantification of Common Toxicologically Important Mycotoxins in Human Plasma Samples for Exposure Studies;** Irina Slobodchikova; Cian Monnin; Samiur Rahman; Reajean Sivakumar; Dajana Vuckovic; *Concordia University, Montreal, Canada*
- ThOG pm 3:30 **Characterization of Petroleum Emerging Environmental Contaminants in Louisiana Salt Marsh Samples Four Years after the Deepwater Horizon Oil Spill;** Steven M. Rowland¹; Huan Chen²; Aixin Hou³; Yuri E. Corilo^{1,2}; Qianxin Lin⁴; Jie Lu¹; Irving A. Mendelsohn⁴; Rui Zhang³; Ryan P. Rodgers^{2,3}; Amy M. McKenna²; ¹*Future Fuels Institute, FSU, Tallahassee, FL*; ²*National High Magnetic Field Laboratory, Tallahassee, FL*; ³*Department of Environmental Sciences, LSU, Baton Rouge, LA*; ⁴*Department of Oceanography & Coastal Sciences, LSU, Baton Rouge, LA*
- ThOG pm 3:50 **Compositional Comparison of Weathering Trends for Four Different Oil Spills Determined by Ultrahigh Resolution FT-ICR Mass Spectrometry;** Logan C. Krajewski¹; Huan Chen²; Ryan P. Rodgers^{2,3}; Christopher M. Reddy⁴; Karin T. Lemkau⁵; Chistoph Aeppli⁶; Robert F. Swarthout⁴; Alan Marshall^{1,2}; Amy M. McKenna²; ¹*Department of Chemistry and Biochemistry, FSU, Tallahassee, FL*; ²*National High Magnetic Field Laboratory, FSU, Tallahassee, FL*; ³*Future Fuels Institute, FSU, Tallahassee, FL*; ⁴*Woods Hole Oceanographic Institute, Woods Hole, MA*; ⁵*University of California, Santa Barbara, CA*; ⁶*Bigelow Laboratory for Ocean Sciences, East Boothbay, ME*
- ThOG pm 4:10 **Non-Targeted Analysis to Assess Human Exposure to Semivolatile Organic Contaminants in the Indoor Environment;** Lee Ferguson; Bernadette Vogler; Heather Stapleton; *Duke University, Durham, NC*

**2:30 – 4:30 PM, THURSDAY AFTERNOON
APPLYING LC-MS TECHNIQUES TO SOLVE CHALLENGING
DRUG METABOLISM PROBLEMS**

**Natasha Penner (Biogen Idec) presiding
Ballroom 220/221**

- ThOH pm 2:30 **Changing the Paradigm of Metabolite Analysis in DMPK using UPLC Coupled with High Resolution Mass Spectrometry;** Hongying Gao¹; Shibo Deng²; R. Scott Obach¹; ¹*Pfizer Inc, Groton, CT*; ²*Pfizer Inc, San Diego, CA*
- ThOH pm 2:50 **High Resolution LC/MS-based Background Subtraction for Unambiguous Identification of Metabolites of Macrocyclic Peptides *in vivo*;** Haiying Zhang; Jennifer X. Qiao; Yue-Zhong Shu; Michael A. Poss; W. Griffith Humphreys; *Bristol-Myers Squibb R&D, Princeton, NJ*

- ThOH pm 3:10 **Characterization of a Selective Androgen Receptor Modulator Drug Candidate and Identification of *in vitro* Generated Metabolites for Sports Drug Testing;** Mario Thevis^{1,2}; Andreas Lagojda³; Andreas Thomas¹; Josef Dib¹; Annelie Hansson⁴; Mikael Hedeland^{4,5}; Ulf Bondesson⁴; Tina Wigger⁶; Uwe Karst⁶; Wilhelm Schänzer¹; ¹*German Sport University, Cologne, DE*; ²*Europ. Monitoring Ctr. for Emerging Doping Agents, Cologne/Bonn, DE*; ³*BayerCropScience, Monheim, DE*; ⁴*Uppsala University, Uppsala, SE*; ⁵*Nat'l Veterinary Institute, Uppsala, SE*; ⁶*University of Münster, Münster, DE*
- ThOH pm 3:30 **Detection and Quantitation of Insulin Analogues by Differential Mobility Coupled to Mass Spectrometry;** J.C. Yves Leblanc; Brad Schneider; J. Larry Campbell; *SCIEX, Concord, On, Canada*
- ThOH pm 3:50 **Therapeutic Protein Quantitation using Dried Blood Spot Sampling to Support Discovery Stage PK Studies;** Lisa O'Callaghan¹; Qian Zhang¹; Daniela Tomazela²; Daniel Spellman¹; Maribel Beaumont²; Bao-Jen Shyong¹; Jacqueline Kenny¹; Scott Fauty¹; Kerry Fillgrove¹; Jane Harrelson¹; Kevin Bateman¹; ¹*Merck & Co., West Point, PA*; ²*Merck & Co., Palo Alto, CA*
- ThOH pm 4:10 **Human *In vivo* Protein Turnover Measurements by Sequential Immunoaffinity and Targeted Mass Spectrometry;** Vahid Farrokhi¹; Xiaoying Chen²; Hendrik Neubert¹; ¹*Pfizer, PDM-NBE, Andover, MA*; ²*Pfizer, PDM-NBE, Cambridge, MA*

PLENARY LECTURE

**Vicki H. Wysocki (The Ohio State University) presiding
Hall 5**



The Evolution of Modern Neurosurgery: A History of Trial and Error, Success and Failure

G. Michael Lemole, Jr.
The University of Arizona College of Medicine

**6:30 – 9:00 PM, THURSDAY
CLOSING EVENT
CITY MUSEUM
Ticket is required.**

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

MALDI: Sample Preparation.....001-015
 Ambient Ionization: Application.....016-046
 Instrumentation: New Developments in Ionization
 and Sampling.....047-076
 Instrumentation: New Developments in Mass Analyzers.....077-093
 LC-MS: instrumentation and Software.....094-107
 FAIMS and DMS.....108-125
 Ion Mobility: Theory.....126-135
 Ion Mobility: Instrumental.....136-155
 Imaging MS: Instrumentation.....156-175
 Imaging MS: Software.....176-184
 H/D Exchange: Hardware, Software and Methodology.....185-199
 Top-Down Protein Analysis: Relatively Pure Sample.....200-219
 Natural Products.....220-246
 Small Molecules: Quantitative Analysis.....247-276

Drug Discovery/DMPK/ADME.....277-298
 Diagnostic Clinical Chemistry.....299-332
 Metabolomics: General.....333-360
 Metabolomics: Sample Preparation.....361-376
 Metabolomics: Quantitative Analysis.....377-405
 Informatics: Metabolomics.....406-418
 Informatics: Algorithms and Statistical Advances.....419-443
 Biomarkers: Discovery.....444-466
 Biomarkers: Quantitative Analysis (Protein).....467-488
 Plant-omics.....489-502
 Proteomics: Tissue.....503-515
 Proteomics: Quantitative - Label Free Quantification.....516-542
 Proteomics: Clinical Applications.....543-569
 Phosphopeptides: Enrichment Methods.....570-580
 Glycoproteins: Method Development.....581-605
 Systems Biology: Proteomics.....606-627
 Systems Biology: Other.....628-641
 Energy: Hydrocarbon and Petrochemical.....642-666
 Carbohydrates I.....667-692
 Special Posters displayed Monday through Thursday.

**MALDI: SAMPLE PREPARATION
 001 - 015**

- MP 001 **The Analyses of Fluorescently Labeled Biomolecules with Fluorophore-Assisted Laser Desorption/Ionization-Mass Spectrometry (FALDI-MS);** Raymond West; Justin Jacobs; Dragan Isailovic; *University of Toledo, Toledo, OH*
- MP 002 **Peptides Quantification: Improved Performance by the Binary Matrices System for MALDI-TOF-MS;** Milena Luizete; João Luiz Bronzel Junior; Humberto Milagre; *UNESP - Univ Estadual Paulista - Institute of Chem, Araraquara, Brazil*
- MP 003 **Rapid and Simple Fixed-Charge Derivatization of Alcohols for Analysis by MALDI and SALDI Mass Spectrometry;** Roman Borisov; Dmitry Zhilyaev; Nikolai Polovkov; Vladimir Zaikin; *Topchiev Institute of Petrochemical Synthesis, Moscow, Russian Federation*
- MP 004 **Ionic Liquids as Combined CE Additive and MALDI Matrix;** Leila Josefsson; Jessica Bernsteen; Saara Mikkonen; Åsa Emmer; *KTH Royal Institute of Technology, Stockholm, Sweden*
- MP 005 **Simple on-plate PNGase F Digestion Combined with LC/MALDI-MS for Site-Specific N-glycosylation Analysis;** Ritsuko Yoda; Yusaku Hioki; Takashi Nishikaze; Naoki Kaneko; Hideharu Shichi; Shinichi Iwamoto; Koichi Tanaka; *Shimadzu Corporation, Kyoto, Japan*
- MP 006 **A Bi-Functional Glass Membrane Designed to Interface SDS-PAGE Separations of Proteins with the Detection of Peptides by Mass Spectrometry;** Kenneth Parker; Stephen J. Hattan; Marvin Vestal; *SimulTOF/ VIC Instruments, Sudbury, MA*
- MP 007 **A Fully Automated, Bottom-up Approach for MALDI-TOF MS Based Discovery Workflows;** M. Nazim Boutaghou¹; David Colquhoun¹; Kevin W. Meyer²; Brian J. Feild¹; Scott Kuzdzal¹; ¹*Shimadzu Scientific Instruments, Columbia, MD*; ²*Perfinity Biosciences, West Lafayette, IN*
- MP 008 **Simple Fabrication of Superhydrophobic AKD Coated MALDI Concentration Plates for Increased Sensitivity;** Johan Jacksén; Joakim Romson; Charlotte Sidenbladh; Åsa Emmer; *KTH Royal Institute of Technology, Stockholm, Sweden*
- MP 009 **Optimization of Sample Preparation for Detection of Common Food-borne Pathogens by Matrix-Assisted Laser Desorption Ionization-Time of Flight Mass Spectrometry;** Lay Hoon Seah; Tze Horng Liew; Thye Ngak Mathew Lau; , *Singapore, Singapore*
- MP 010 **Evaluation of Microalgae Protein Profile by MALDI-**

- TOFMS with the Increase of TFA Concentration in the sDHB Matrix Solvent;** Lidiane Maria Andrade; Maria Anita Mendes; Claudio Augusto Oller do Nascimento; *Universidade de São Paulo - USP, Sao Paulo, Brazil*
- MP 011 **High-Throughput Screening MALDI-TOF Assays beyond 100,000 Samples per Day;** Sergei Dikler¹; Scott A. Busby²; W. Adam G. Hill²; Paul J. Kowalski¹; Anja Resemann³; Detlev Suckau³; ¹*Bruker Daltonics Inc., Billerica, MA*; ²*Novartis Institutes for BioMedical Research Inc., Cambridge, MA*; ³*Bruker Daltonik GmbH, Bremen, Germany*
- MP 012 **Cyano-phenylenevinylene Oligomer as a Novel Electron Transfer Ionization MALDI Matrix;** Laura Castellanos¹; Melissa Cely²; César A. Sierra²; Cristian Blanco-Tirado¹; Marianny Y. Combariza¹; ¹*UIS, Bucaramanga, Colombia*; ²*Universidad Nacional de Colombia, Bogotá, Colombia*
- MP 013 **Rational Design and Efficient Synthesis of cyano-Containing Phenylenevinylene Derivatives as Potential MALDI Matrixes for Electron Transfer Ionization;** Juan Ramirez; *Universidad Industrial de Santander, Floridablanca, Colombia*
- MP 014 **Charged Droplets: Physics and Applications;** Drew Sauter; *Nanoliter, LLC, Henderson, NV*
- MP 015 **Solvent-free Metal Nanoparticle Application and Comparison for Nanoparticle Assisted Laser Desorption Ionization Mass Spectrometry of Plant Metabolites;** Gargey Yagnik^{1,2}; Young-Jin Lee^{1,2}; ¹*Iowa State University, Ames, Iowa*; ²*Ames Laboratory-US DOE, Ames, Iowa*

**AMBIENT IONIZATION: APPLICATION
 016 - 046**

- MP 016 **Investigation of Aqueous Phase Electrochemical Reactions by Desorption Electrospray Ionization Mass Spectrometry;** Mei Lu¹; Yong Liu²; Roy Helmy²; Gary Martin²; Howard Dewald¹; Hao Chen¹; ¹*Ohio University, Athens, OH*; ²*Merck & Co., Rahway, NJ*
- MP 017 **Breath Analysis Using Direct Analysis in Real Time Mass Spectrometry - A Fun "Food is Chemistry" Student Demonstration;** Curtis Mowry; Adam Pimentel; *Sandia National Laboratories, Albuquerque, NM*
- MP 018 **Reproducibility and Quantitation using Matrix-Assisted Ionization (MAL) Mass Spectrometry;** Shubhashis Chakrabarty^{1,2}; Kevin Jooss³; Srinivas B. Narayan³; Sarah Trimpin^{2,4}; ¹*MSTM, LLC., Hockessin, DE*; ²*Department of Chemistry, Wayne State University, Detroit, MI*; ³*Detroit Medical Center: Detroit Hospital (DMC), Detroit, MI*; ⁴*Cardiovascular Research Institute, Wayne State University*

- MP 019 *School of Medicine, Detroit, MI*
Micro-area Analysis of Tooth Surface Using Surface Desorption Atmospheric Pressure Chemical Ionization Mass Spectrometry; Qian Li¹; Haiwei Gu²; Jiang Wang¹; Xiaotun Guo¹; Eric Handberg¹; ZhiHao Wang¹; Shuiping Yang³; Huanwen Chen¹; ¹*East China Institute of Tech., Nanchang, China;* ²*Northwest Metabolomics Research Center, Department, Seattle, WA;* ³*East China Institute of Technology, Fuzhou, China*
- MP 020 **Atmospheric Pressure Neutral Reionization Mass Spectrometry for Structural Analysis;** Pengyuan Liu; Hao Chen; *Ohio University, Athens, OH*
- MP 021 **The Multifunctional Single-Probe for Single Cell Mass Spectrometry Analysis;** Ning Pan; Zhibo Yang; Wei Rao; Anthony Burgett; Kothapalli Naga Rama; *University of Oklahoma, Norman, OK*
- MP 022 **In vivo Detection of Plant Molecules by Low-Temperature Plasma Mass Spectrometry (LTP-MS);** Sandra Martínez Jarquín; Robert Winkler; *CINVESTAV Unidad Irapuato, Irapuato, Mexico*
- MP 023 **Regulated Generation of Molecular Ions or Protonated Molecules under Atmospheric-Pressure Helium-Plasma-Ionization (HePI) Mass Spectrometric Conditions;** Athula B. Attygalle; Rekha Gangam; Julius Pavlov; *Stevens Institute of Technology, Hoboken, NJ*
- MP 024 **Different Materials Coated Paper Substrates for Paper Spray Mass Spectrometry;** Yajun Zheng¹; Xiaoling Zhang¹; Qian Wang¹; Xinrong Zhang²; Zhiping Zhang¹; ¹*Xi'an Shiyou University, Xi'an, China;* ²*Tsinghua University, Beijing, China*
- MP 025 **Characterization of Large Saturated Hydrocarbons by Automatic Raster Laser-Induced Acoustic Desorption/ Atmospheric Pressure Oxygen Chemical Ionization Mass Spectrometry;** Chunfen Jin¹; Hanyu Zhu¹; Alex Dow¹; Viidanoja Jyrki²; Hilikka Kenttämä¹; ¹*Purdue University, West Lafayette, IN;* ²*Neste Oil, Keilaranta, Finland*
- MP 026 **Touch Spray Mass Spectrometry with Medical Swabs for Direct Analysis of Bacteria and Drugs in Oral Fluid;** Valentina Pirro^{1,2}; Alan K. Jarmusch¹; Kevin S. Kerian¹; Marco Vincenti²; R. Graham Cooks¹; ¹*Chemistry Department, Purdue University, West Lafayette, IN;* ²*Antidoping and Toxicology Center A. Bertinaria, Orbassano, IT*
- MP 027 **Microbial Communication through the Air: Analyzing Volatile Bacterial Compounds by Comparative GC-MS and DART-MS Approaches;** Matthew Pavlovich; Violetta Medik; Slava Epstein; Adam Hall; *Northeastern University, Boston, MA*
- MP 028 **Improving Ionization Efficiency of Direct Analysis in Real Time-Mass Spectrometry (DART-MS) by using DC Corona Discharges;** Kanako Sekimoto¹; Motoshi Sakakura²; Hiroshi Hike²; Takatomo Kawamukai²; Teruhisa Shiota²; Mitsuo Takayama¹; ¹*Yokohama City Univ., Yokohama, Japan;* ²*AMR Inc., Tokyo, Japan*
- MP 029 **Thermal Degradation of β -Carotene and Flavonoids Studied Using Atmospheric Solid Analysis Probe Mass Spectrometry (ASAP-MS);** Xiaoyin Xiao; James Hochrein; Lance Miller; *Sandia National Laboratories, Albuquerque, NM*
- MP 030 **Investigation of Biological Fingerprints Using Atmospheric Solid Analysis Probe Mass Spectrometry (ASAP-MS);** James Hochrein; Xiaoyin Xiao; Lance Miller; Kylea Parchert; Ducle Hayes; *Sandia National Laboratories, Albuquerque, NM*
- MP 031 **A DESI MS Based Screening Method for Phthalates in Consumer Goods;** Sabine Schulz¹; Sebastian Wagner¹; Stefanie Gerbig¹; Herbert Waechter²; Detlef Sielaff³; Dieter Bohn⁴; Bernhard Spengler¹; ¹*Justus Liebig University Giessen, Giessen, Germany;* ²*Bavarian State Laboratory f. Health a. Food safety, Erlangen, Germany;* ³*State*
- MP 032 *Laboratory of Rhineland-Palatinate, Koblenz, Germany;* ⁴*Hessen State Laboratory, Giessen, Germany*
- MP 033 **Single Cell Mass Spectrometry Analysis of Marine Algae: Detection of Creatine;** Mei Sun; Ning Pan; Wawrik Boris; Zhibo Yang; *University of Oklahoma, Norman, OK*
- MP 034 **Comparison of Metabolites from Small Populations of Adherent and Detached Hepatocytes Analyzed by Transmission Geometry LAESI Mass Spectrometry;** Rachelle S. Jacobson; Richard L. Thurston; Akos Vertes; *George Washington University, Washington, DC*
- MP 035 **Profiling Unsaturated Lipids in Tissue Using Reactive Extraction Spray Mass Spectrometry;** Yuan Su; Xiaoxiao Ma; Yu Xia; Zheng Ouyang; *Purdue University, West Lafayette, IN*
- MP 036 **Tandem Mass Spectrum and Collision Cross Section Libraries for High-Throughput Identification of Metabolites in Adherent Hepatocytes by LAESI Mass Spectrometry;** Wei Yuan; Bindesh Shrestha; Akos Vertes; *George Washington University, Washington, DC*
- MP 037 **In situ Ink Analysis from Various Types of Documents by Nanospray Desorption Ionization (nano-DESI) Mass Spectrometry;** Sangwon Cha; Gwangbin Lee; Dongkun Lee; *Hankuk Univ. Foreign Studies, Yongin, South Korea*
- MP 038 **Improved Methods for the Analysis of Human Dried Blood Spot Samples by LESA Mass Spectrometry;** Rian Griffiths; Andrew Creese; Joscelyn Sarsby; Helen Cooper; *University of Birmingham, Birmingham, UK*
- MP 039 **Rapid Analysis of Extra Virgin Olive Oil Adulteration with Other Oils with No Sample Preparation using Ambient Ionization Mass Spectrometry;** Avinash Dalmia^{1,2}; Craig M. Whitehouse²; ¹*PerkinElmer, Shelton, CT;* ²*PerkinElmer, Branford, CT*
- MP 040 **Graphene Oxide-Assisted Paper Spray For Analysis of Malachite Green;** Fen Shen; Pang-Hung Hsu; *NTOU, New Taipei City, Taiwan (R.O.C.)*
- MP 041 **Increased Disulfide Peptide Sequence Coverage via "Cleavage ON/OFF" Switch during Nanoelectrospray;** Guangming Huang; *University of Science and Technology of China/USTC, Hefei, P.R. China*
- MP 042 **Real-time Breath Monitoring of Valproic Acid by Mass Spectrometry with Low Temperature Plasma Ionization Source;** Xiaoxia Gong; Songyue Shi; Gerardo Gamez; *Texas Tech University, Lubbock, TX*
- MP 043 **Reaction Acceleration using Paper Spray Ionization and the Haloform Reaction;** Ryan Bain; Shannon Raab; Christopher Pulliam; R. Graham Cooks; *Purdue University, West Lafayette, IN*
- MP 044 **How to Electro-clean APCI Sources between Injections;** Joseph Di Bussolo; *Thermo Fisher Scientific, West Chester, PA*
- MP 045 **Comparative Depth Resolution of Extractive Analysis Techniques;** Mariam S Elnaggar; *Prosolia, Inc., Indianapolis, IN*
- MP 046 **Depth Profiling of Solid Sample by Dielectric Barrier Discharge Plasma Jet Coupled with Ion Trap Mass Spectrometry;** Songyue Shi; Xiaoxia Gong; Gerardo Gamez; *Texas Tech University, Lubbock, TX*

INSTRUMENTATION: NEW DEVELOPMENTS IN IONIZATION AND SAMPLING

047 - 076

- MP 047 **Spectroscopic Characterization of a Windowless, Electron-Beam-Pumped Excimer Lamp (EBEL) in the VUV Spectral Region of 50 – 200 nm**; Hendrik Kersten; Sebastian Klopotoski; Sebastian Winkelmann; Thorsten Benter; *Bergische Universität Wuppertal, Wuppertal, Germany*
- MP 048 **Advancements in Atmospheric-Vacuum Interfaces of Mass Spectrometers with Increased Gas Throughput and Enhanced Sensitivity**; Eloy R. Wouters; Satendra Prasad; Jean-Jacques Dunyach; *Thermo Fisher Scientific, San Jose, CA*
- MP 049 **A Method for Performing In-trap Photoionization in a Miniature Ion Trap Mass Spectrometer**; Corey Stedwell; Daniel Debord; Conor Mullens; Michael Spencer; David Rafferty; *1st Detect Corporation, Webster, TX*
- MP 050 **Direct Real-Time Monitoring and Assessment of Single Leaf Carbon Fixation and Respiration Rates for *Arabidopsis thaliana* by Mass Spectrometry**; Karl K. Weitz¹; Kim K. Hixson¹; Mary S. Lipton¹; Ronald J. Moore¹; Therese RW. Clauss¹; Norman G. Lewis²; Laurence B. Davin²; Richard D. Smith¹; *¹Battelle Pacific Northwest National Laboratories, Richland, WA; ²Washington State University, Pullman, WA*
- MP 051 **New Development of Low Pressure Electrospray Ionization Source**; Rui Wang; Xiaoqiang Zhang; Qiao Jin; Jiaqi Shen; Wenjian Sun; *Shimadzu Research Laboratory (Shanghai) Co. Ltd., Shanghai, China*
- MP 052 **Optimized Conditions for the Analysis of Oligonucleotides by Inductive Based Fluidics Mass Spectrometry**; Robert Ross¹; Drew Sauter²; Patrick A. Limbach¹; *¹University of Cincinnati, Cincinnati, OH; ²Nanoliter, LLC, Henderson, NV*
- MP 053 **Development of a Dual-Mode Laminar Flow Ion Source for APPI- and APLI-GC-MS**; Kai Kroll; Walter Wissdorf; Hendrik Kersten; Thorsten Benter; *University of Wuppertal, Wuppertal, Germany*
- MP 054 **Concept Study for a Sensitive and Versatile Chemical Ionization TOF Flight Instrument**; Sascha Albrecht¹; Armin Afchine¹; Jochen Barthel¹; Markus Dick¹; Heinz Rongen¹; Fred Stroth¹; Thorsten Benter²; *¹Forschungszentrum Jülich GmbH, Jülich, Germany; ²University of Wuppertal, Wuppertal, Germany*
- MP 055 **Evaluation of Sonic Spray Ionization Mass Spectrometry for Proteomics Analysis**; Spiros Pergantis; Manos Maurakis; *University of Crete, Heraklion, Greece*
- MP 056 **Investigating Compatibility of Electrospray for LC-MS *in situ* Analysis of Icy Bodies in the Solar System**; Adrian Southard¹; Stephanie Getty²; Jerome Ferrance³; Manuel Balvin²; Jamie E. Elsila²; Ana Mellina Espiritu²; Carl Kotecki²; Paul Mahaffy²; *¹University Space Research Agency, Greenbelt, Maryland; ²NASA GSFC, Greenbelt, MD; ³J2f engineering, Charlottesville, VA*
- MP 057 **Golf-ball Assisted Electrospray Ionization of Mass Spectrometry for Determination of Trace Amino Acids in Complex Samples**; Yen-Hsien Li; Maw-Rong Lee; *National Chung-Hsing University, Taichung, Taiwan*
- MP 058 **Optimization of a Vacuum Ultraviolet Photoionization source for Gas Chromatography used with a High Resolution Time of Flight Mass Spectrometer**; Lloyd Allen; Viatcheslav Artaev; *LECO Corp., Saint Joseph, MI*
- MP 059 **Direct Sampling, Extraction and Ionization Probe with Screening-Printed Electrode (SPE) Based Paper Spray**; Che-I Liao; Kuo-Lung Ku; *National Chiayi University, Chiayi City, Taiwan*
- MP 060 **A Helium Metastable Seeded Secondary Plasma in the Low MBAR Pressure Regime – Characterization and Evaluation for Mass Spectrometric Applications**; Klaus Brockmann¹; David Mueller¹; Yessica Brachthäuser¹; Hendrik Kersten¹; Thorsten Benter¹; Achim von Keudell²; Thomas Kuschel²; Marc Boeke²; Joerg Winter²; Michel Aliman³; Gennady Fedosenko³; Ruediger Reuter³; Alexander Laue³; Hin Yiu Chung³; *¹University of Wuppertal, Wuppertal, Germany; ²University of Bochum, Bochum, Germany; ³Carl Zeiss SMT, Oberkochen, Germany*
- MP 061 **Micro-plasma Based Pulsed Direct Charge Transfer Stage Coupled to a FT-IT Mass Spectrometer**; Yessica Brachthäuser¹; David Mueller¹; Hendrik Kersten¹; Klaus Brockmann¹; Thorsten Benter¹; Michel Aliman²; Gennady Fedosenko²; Ruediger Reuter²; Alexander Laue²; Hin Yiu Chung²; *¹University of Wuppertal, Wuppertal, Germany; ²Carl Zeiss SMT, Oberkochen, Germany*
- MP 062 **Coupling a Visible-Wavelength Laser to a MALDI TOF/TOF Mass Spectrometer for the Analyses of Biomolecules**; Raymond West¹; Eric Findsen¹; Jens Hoehndorf²; Dragan Isailovic¹; *¹The University of Toledo, Toledo, OH; ²Bruker Daltonics, Bremen, Germany*
- MP 063 **Proton Transfer Mass Spectrometry (PT-MS) with H₃⁺ as Reagent Ions**; David Mueller¹; Yessica Brachthäuser¹; Hendrik Kersten¹; Klaus Brockmann¹; Thorsten Benter¹; Michel Aliman²; Gennady Fedosenko²; Ruediger Reuter²; Alexander Laue²; Hin Yiu Chung²; *¹University of Wuppertal, Wuppertal, Germany; ²Carl Zeiss SMT, Oberkochen, Germany*
- MP 064 **Investigation of Space Distribution of Elements in Solid Samples using Dielectric Barrier Discharge Probe Coupled with ICP-MS**; Yi Zheng¹; Zhi Xing²; Lipeng Liu¹; Xiaofeng Yu¹; Gangqiang Li¹; *¹Focused Photonics(Hangzhou), Inc., Hangzhou, China; ²Department of Chemistry, Tsinghua University, Beijing, China*
- MP 065 **A Cryofocuser/Quadrupole Mass Spectrometer Coupled to a Catalysis Unit for Detection of Nitrogen Oxide Catalysis Products**; Weigang Lu¹; Behrooz Zekavat¹; Abayomi D. Olaitan¹; Matthew R. Brantley¹; Deniz A. Erdogan²; Emrah Ozensoy²; Touradj Solouki¹; *¹Chemistry and Biochemistry Department, Baylor University, Waco, TX; ²Department of Chemistry, Bilkent University, Bilkent, Ankara, Turkey*
- MP 066 **Performance Characterization of a Unique Radio-Frequency Ionization Source**; Abayomi D. Olaitan; Behrooz Zekavat; Matthew R. Brantley; Touradj Solouki; *Department of Chemistry and Biochemistry, Baylor University, Waco, TX*
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- MP 074 **Slurry FIA/APCI-MS for Quantitative Real-Time Monitoring of Batch Slurry Reactions: An Alternative Setup**; Zhenqian Zhu¹; David Cho²; John Bartmess¹; Mary Ellen McNally³; Ron Hoffman³; Kelsey D. Cook¹; Ligu Song¹; ¹Department of Chemistry, University of Tennessee, Knoxville, TN; ²FBI Laboratory, Quantico, VA; ³DuPont Crop Protection, Newark, Delaware
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- MP 081 **Frequency-Multiple Detection Compatible with Optimized Ion Trap Geometry for Enhanced Fourier Transform Ion Cyclotron Resonance Mass Spectral Resolution**; Tong Chen^{1,2}; Steven C. Beu³; Nathan K. Kaiser¹; Donald F. Smith¹; Greg T. Blakney¹; John P. Quinn¹; Daniel G. McIntosh¹; Vaughan Williams¹; Alan G. Marshall^{1,2}; Christopher L. Hendrickson¹; ¹National High Magnetic Field Laboratory, Tallahassee, FL; ²Florida State University, Tallahassee, FL; ³S C Beu Consulting, Austin, TX
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- MP 248 **A Case Study for Oxcarbazepine Variation in Sample Extracts Due To Adsorption in 96-well Plates by LC-MS/MS;** Richard Lavallée; Georges Koudssi; Milton Furtado; Fabio Garofolo; *Algorithme Pharma Inc., Laval, Canada*
- MP 249 **Development and Validation of a High Throughput LC-MS/MS Method for Determination of Clobazam and N-Desmethyclobazam in Human Plasma;** Jasper X. Chu; Yuzhu Xue; Mary Hillegas; Yuan-Shek Chen; *QPS LLC, Newark, DE*
- MP 250 **Quantitative Measurement of Lovastatin and Lovastatin Acid in Human Plasma using Column Switching and Tandem Mass Spectrometry;** Jingduan Chi; Erika Helgerson; Lisa McIntosh; Fumin Li; *PPD Inc, Madison, WI*
- MP 251 **Simultaneous Quantitation of Delamanid (OPC-67683) and its Eight Metabolites in Human Plasma using UHPLC-MS/MS;** Min Meng¹; Bradley Bessette¹; Benjamin Smith¹; Brad Johnston¹; Spencer Carter¹; *Jerry Brisson²; Sharin E. Roth²; ¹Tandem Labs, Salt Lake City, UT; ²Otsuka Pharmaceutical Development, Rockville, MD*
- MP 252 **Increase Selectivity in Quantitative LC-MS/MS Analysis using On-line Extraction via an Analyte Interaction Exclusion Process ;** Mathieu Lahaie; Milton Furtado; Fabio Garofolo; *Algorithme Pharma Inc., Laval, Canada*
- MP 253 **Determination of Methamphetamine in Human Hair by Ultra High Performance Liquid Chromatography/Tandem Mass Spectrometry;** Chao Ma¹; Kai Zhang²; Yumin Di²; Yueqi Li¹; Guixiang Yang¹; Taohong Huang¹; Shin-ichi Kawano¹; Yuki Hashi¹; *¹Shimadzu Global COE, Shimadzu (China) Co., Ltd, Beijing, China; ²Tianjin Public Security Bureau, Tianjin, China*
- MP 254 **Identification of a Contaminant Interfering with 6-Hydroxymorphine Quantification by using TOF-MS;** Eugénie-Raphaëlle Bérubé; Milton Furtado; Fabio Garofolo; *Algorithme Pharma Inc., Laval, Canada*
- MP 255 **Quantification of Thiazolidine-4-carboxylic Acid in Toxicant-Exposed Cells by Liquid Chromatography-Mass Spectrometry Reveals an Intrinsic Antagonistic Response to Oxidative Stress-Induced Toxicity;** Jingjing Liu; *Hong Kong, China*
- MP 256 **Quantitative Analysis of Antipsychotics in Urine by Liquid Chromatography-Triple Quadrupole Mass Spectrometry;** Flaubert Mbeunkui; Carla Lyon; R. Brent Dixon; *Physicians Choice Laboratory Services, Rock Hill, SC*
- MP 257 **Development of the Separation of Three Tyrosine Isomers in Protein Hydrolysate Samples;** Huseyin Kayadibi^{1,2}; Tammy Bullwinkle³; Noah Reynolds³; Medha Raina³; Adil Moghal³; Eleftheria Matsa³; Andrei Rajkovic³; Farbod Fazlollahi¹; Christopher Ryan¹; Kym Faul¹; Michael Ibba³; *¹UCLA, Los Angeles, CA; ²Adana Military Hospital, Adana, Turkey; ³Ohio State University, Columbus, OH*
- MP 258 **Development and Validation of LC-MS/MS Method for Determination of N-Tetracosanoylsphinganine in Human Plasma;** Hui Jiang; Jean Schaffer; Daniel Ory; *Xuntian Jiang; Diabetic Cardiovascular Disease Center, Washington, St. Louis, MO*
- MP 259 **Matrix Effect, Sensitivity and Throughput of Microflow Liquid Chromatography vs. HPLC: A Case Study With Buprenorphine and Norbuprenorphine;** Laurence Mayrand-Provencher; Milton Furtado; Fabio Garofolo; *Algorithme Pharma Inc., Laval, Canada*
- MP 260 **Event Investigation of Sample Inhomogeneity in Acidified Human Plasma Samples in a First-in-Human Study;** Philip S. Wong; Jian jiang; Christopher James; *Amgen, Thousand Oaks, CA*
- MP 261 **Quantification of Nicotine and Its Metabolite Cotinine in Human Tooth Using Triple Quad 6500 LC-MS/MS;** HongKun Wu¹; Junyu Lee²; Joshua Froning²; *Yong-Xi Li²; ¹West China Hospital of Stomatology, Chengdu, China; ²Medpace Bioanalytical Laboratories, Cincinnati, OH*
- MP 262 **Improved Sensitivity and Selectivity by using LC-HRMS for the Quantification of Latanoprost Acid in Dog Plasma at 5.00 pg/mL;** Richard Lavallée¹; Milton Furtado¹; Deepank Utkhede^{2,3}; Fabio Garofolo¹; *¹Algorithme Pharma Inc., Laval, Canada; ²Mati Therapeutics (Canada) Inc., Burnaby, Canada; ³Mati Therapeutics Inc., Austin, Texas*
- MP 263 **Simultaneous Determination of 12 Volatile Organic Compounds in Human Blood by SPME-GC/MS/MS;** Zhiyun Jin¹; Rocío Aranda-Rodríguez¹; Ashley Cabecinha¹; Jeromy Harvie¹; Axelle Marchand²; Robert Tardif²; Andy Nong¹; Sami Haddad²; *¹Health Canada, Ottawa, Canada; ²Université de Montréal, Montréal, Canada*
- MP 264 **Effective Carryover Reduction by Derivatization of Residual Analyte in HPLC System during LC-MS/MS Quantification;** Vinicio Vasquez; Sylvain Latour; Milton Furtado; Fabio Garofolo; *Algorithme Pharma Inc., Laval, Canada*
- MP 265 **Validation of a Liquid Chromatography-Tandem Mass Spectrometric Assay for Tacrolimus in Peripheral Blood Mononuclear Cells;** Min Chang Kim; Jun Hwa Shim; Hwa-Suk Kim; Seo Hyun Yoon; Kyung-Sang Yu; In Jin Jang; Joo Youn Cho; *Seoul National University, Seoul, South Korea*
- MP 266 **Overcoming Hematocrit Impact Using Homogenization Beads for Dried Blood Spots (DBS) by LC-MS/MS Analysis;** Nikolay Youhnovski; Julien Nantel; Milton Furtado; Fabio Garofolo; *Algorithme Pharma Inc., Laval, Canada*
- MP 267 **A Rapid LC-MRM/MS Assay for Simultaneous Quantification of Choline, Betaine, Trimethylamine, Trimethylamine N-oxide and Creatinine;** Xueqing Zhao¹; Steven Zeisel¹; Shucha Zhang²; *¹Nutrition Research Institute, UNC Chapel Hill, Kannapolis, NC; ²Brigham and Women's Hospital, Boston, MA*
- MP 268 **A Validated Method for the Quantitation of Evogliptin in Human Plasma using Liquid Chromatography-Tandem Mass Spectrometry;** Jun Hwa Shim; Hwa-Suk Kim; Min Chang Kim; Seo Hyun Yoon; Kyung-Sang Yu; In-Jin Jang; Joo-Youn Cho; *Seoul National University College of Medicine, Seoul, South Korea*
- MP 269 **Evaluation of Bench-top Quadrupole Orbitrap Ultra High Resolution Mass Spectrometer for Rapid Quantitative Analysis of Immunosuppressant Drugs in Blood Samples;** Mindy Gao; Marta Kozak; *ThermoFisher Scientific, San Jose, CA*
- MP 270 **Simultaneous Quantification of Loxapine and its Four Metabolites in Human Plasma using LC-MS/MS;** Min Meng¹; Benjamin Smith¹; Laixin Wang¹; Brad Johnston¹; Scott Reuschel¹; Charisse Green²; Steven H Gorman²; *¹Tandem Labs, Salt Lake City, UT; ²Teva Branded Pharmaceutical Products R & D, Inc, West Chester, PA*
- MP 271 **Quantitative Analysis of Cotinine in Human Plasma and Urine Utilizing a Simple Liquid/Liquid Extraction and GC-MS/MS;** Chad Christianson¹; Ekong Basse²; Keith Miller¹; *¹Alturas Analytics, Moscow, ID; ²ThermoFisher Scientific, San Jose, CA*
- MP 272 **Novel HILIC-LC-MS/MS Quantitative Method for the Bio-Analysis of Gemini Surfactants Designed as Nanomaterial Drug Carriers;** McDonald Donkuru; George Katselis; Anas El-Aneed; *University of Saskatchewan, Saskatoon, Canada*

- MP 273 **Method Validation of Quantitative Analysis of [¹⁴C] YH4808 in Human Plasma by Accelerator Mass Spectrometry**; Hwa Suk Kim¹; Jun Hwa Shim¹; Min Chang Kim¹; Byung-Yong Yu²; Howard Lee¹; In-Jin Jang¹; Joo-Youn Cho¹; ¹Seoul National University Hospital, Seoul, South Korea; ²Korea Institute of Science and Technology, Seoul, South Korea
- MP 274 **Rapid Determination of Multiple Non-Steroidal Anti-Inflammatory Drugs (NSAIDs) in Microliter Quantities of Human Plasma using LC-MS/MS**; Chen Zhang; A. Daniel Jones; Michigan State University, East Lansing, MI
- MP 275 **Increase of Sensitivity and Precision at Low Concentration for LC-MS/MS Quantification of 11-Hydroxy- Δ^9 -tetrahydrocannabinol by Summation of the MRM Transitions**; Romain Beauvois; Vinicio Vasquez; Milton Furtado; Fabio Garofolo; *Algorithme Pharma Inc.*, Laval, Canada
- MP 276 **Robust LCMSMS Determination of Intact Conjugated Dextrorphan when Hydrolysis is Inefficient**; Genevieve Emond; Philippe Bélanger; Luc Bouchard; Louis-Charles Boisvert; Marie-Josée Marcoux; Nancy Lampron; Nadine Boudreau; Ann Lévesque; *InVentiv Health Clinical*, Québec, Canada
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- MP 277 **Automated *in vitro* ADME Screening Analysis in a Small Footprint, using TQ-S Micro Triple Quadrupole Mass Spectrometer**; Yun Alelyunas; Kelly Doering; Stephen McDonald; Mark Wrona; *Waters Corporation, Milford, MA*
- MP 278 **Software-Assisted Structural Characterization of Disulphide-Rich Macromolecular Peptides in Drug Discovery Research**; Asoka Ranasinghe; Eugene F. Ciccimaro; Serhiy Hnatyshyn; Celia D'Arienzo; Timothy Olah; *Bristol-Myers Squibb Company, Princeton, NJ*
- MP 279 **Comparison of Blood Microsampling Techniques for Discovery PK Studies in Rats: Capillary Microsampling (CMS) and a Dried Matrix Microsampling Device**; Walter Korfmacher¹; Yongyi Luo²; Stacy Ho¹; Jie Wang²; Gregory Snow³; Thomas O'Shea¹; ¹Genzyme, Waltham, MA; ²Sanofi, Waltham, MA; ³Agilux Labs, Worcester, MA
- MP 280 **Expression of Drug-Adme-Associated Proteins in Human Small Intestine, Liver, and Kidney Microsomes: Swath-MS-Based Absolute Protein Quantification**; Shingo Ito^{1,3}; Kenji Nakamura²; Mio Hirayama^{1,3}; Sumio Ohtsuki^{1,3}; ¹Fac. of Life Sci., Kumamoto Univ., Kumamoto, Japan; ²Grad. Sch. of Pharma. Sci., Kumamoto Univ., Kumamoto, Japan; ³CREST, JST, Kawaguchi, Japan
- MP 281 **A Mass Spectrometry Based Assay to Identify New Lead Compounds against Drug Resistant Bacterial Infections**; Daniel Todd¹; David Zich¹; Martha Leyte-Lugo¹; Alexander Horswill²; Nadja Cech¹; ¹Univ. of N. Carolina Greensboro, Greensboro, NC; ²University of Iowa, Iowa City, IA
- MP 282 **Novel Approach for Pharmacokinetics and Protein Binding Analysis of Tenepliptin using LC-ESI-QTOF Accurate Mass Spectrometer and Ultra-filtration: *in-vitro*, *in-vivo* Correlation**; Shanti Kumar Saladi¹; Prasanth B¹; Veerhadra Swamy C¹; Srinivas R²; Satheesh Kumar N¹; ¹NIPER-Hyderabad, Hyderabad, India; ²National Center for Mass Spectrometry, IICT, Hyderabad, India
- MP 283 **Assessing Hemolysis Failures for LC-MS/MS Assays Using LC-HRAM on a Q-Exactive Mass Spectrometer**; Laixin Wang¹; Alicia Pietrasiewicz¹; Chad Moore¹; Carrie Pederson¹; Scott Reuschel¹; Min Meng¹; Hongxia Wang²; David Horn²; Jonathan Josephs²; ¹Tandem Labs, Salt Lake City, UT; ²Thermo Fisher Scientific, San Jose, CA
- MP 284 **Quantitation of Thioether-Prodrug NS1040 and Its Metabolites in Rat Plasma Using Ultra-Performance Liquid Chromatography-Tandem Mass Spectrometry**; Emma Hughes¹; Daniel Appella²; Matthew Hassink²; Nathaniel Shank²; Kara George-Rosenker²; Xin Xu¹; Amy Wang¹; ¹NCATS NIH, Rockville, MD; ²NIDDK NIH, Bethesda, MD
- MP 285 **Differential Mobility Spectrometry as a Measure of Physicochemical Properties Related to *in vitro* Absorption (permeability, solubility and lipophilicity)**; Jeffrey Shields¹; Chang Liu²; John Janiszewski¹; Hui Zhang¹; J. Larry Campbell²; J.C. Yves Leblanc²; ¹Pfizer Inc., Groton, CT; ²AB SCIEX, Concord, ON
- MP 286 **An Ion-Pairing Strategy to Overcome PEG-400 Caused Matrix Effect in Routine Drug Discovery Blood Sample Analysis**; Linlin Dong; Michael Johnson; Mark Qian; Shaoxia Yu; *Takeda Pharmaceuticals International Co.*, Cambridge, MA
- MP 287 **Evaluation of Supercritical Fluid Chromatography/Mass Spectrometry for Use in PK/PD Studies**; Fangbiao Li¹; Bernard Choi¹; Cynthia M. Chavez-Eng¹; Christopher Kochansky¹; Eric Streakfuss¹; Joan Ellis¹; Bang-lin Wan¹; Emily Adarayan¹; Brad Coopersmith²; Richard Depinto²; Isabelle Vutrieu²; Eva Gallea²; Lucinda Cohen¹; Rena Zhang¹; Kevin Bateman¹; ¹Merck Research Laboratories, West Point, PA; ²Waters, Richboro, PA
- MP 288 **Radio-Labeled Compound Detection Using Fine Isotopic Structures From Very High Resolution Mass Spectrometry**; Xiaojie C. Ding¹; Tim Stratton²; Ji Ma³; ¹Thermo Scientific, San Jose, CA; ²Thermo Fisher Scientific, San Jose, CA; ³Amgen Inc., South San Francisco, CA
- MP 289 **Segmentation of the Tumour Microenvironment using Multimodal Molecular Imaging to Refine PK/PD Modelling**; Jo Cappell¹; Richard Goodwin²; Peter Webb²; Ron M.A. Heeren¹; ¹University of Maastricht, Maastricht, Netherlands; ²AstraZeneca, Macclesfield, UK
- MP 290 **A Sample Preparation and Detection Strategy for Quantifying Proteolytically Unstable Therapeutic Peptides for Early-ADME Tissue Distribution Studies**; Yasmin Boukhedimi¹; Aristidis Gritsas¹; Garnet McRae²; Roger Leger¹; Paul Drogaris¹; ¹Thrasos therapeutics, Montreal, Canada; ²G McRae Consulting, Ottawa, Canada
- MP 291 **A Sensitive Liquid Chromatography-Tandem Mass Spectrometric Method for Determination of Octreotide in Human Plasma**; Yuling Song; Jinting Yao; Hongyuan Hao; Taohong Huang; Shin-ichi Kawano; Yuki Hashi; *Shimadzu (China) Co., LTD, Shanghai, China*
- MP 292 **Antibody-Free Mass Spectrometry Workflow For Protein Expression Analysis of Intestinal Efflux Transporters in Knock Out Cell Lines**; Yongsheng Xiao; James J Walters; Maureen Bourner; David C. Thompson; Kevin Ray; *Sigma-Aldrich, St. Louis, MO*
- MP 293 **Evaluation of High Resolution Mass Spectrometry for Bioanalytical Quantitation and Simultaneous Metabolite Identification**; Matthew Zimmerman; Firat Kaya; Veronique Dartois; Brendan Prideaux; *Rutgers University, Newark, NJ*
- MP 294 **Comparison of a 4-N-hydroxycytidine Ribonucleoside Phosphoramidate Prodrug with Sofosbuvir: Interspecies Hepatocytes and Human Cardiomyocytes Metabolic Profiles**; Sijia Tao¹; Franck Amblard¹; Yong Jiang¹; Sheida Amiralaie¹; Hao Li¹; Steven Coats²; Raymond Schinazi¹; ¹Emory University School of Medicine, Atlanta, GA; ²CoCrystal Pharma, Inc., Tucker, GA
- MP 295 **MS Transporter Assay for d9-ergothioneine on Carnitine/Organic Cation Transporter (OCTN1/SLC22A4)**; Chien-Ming Li; Xuexiang Zhang; Wenjie Jiang; Yong Huang; *Optivia Biotechnology, Menlo Park, CA*
- MP 296 **A UHPLC-MS/MS Method for the Direct Analysis of Thymoquinone in Mouse Plasma and its Application to Pharmacokinetics**; Jinghua Zhu; Qishan Lin; *University at Albany, Rensselaer, NY*

- MP 297 **Robust and Sensitive Quantitation of Midazolam and Hydroxylmidazolam in Plasma using High Capacity UHPLC and a New Triple Quadrupole Instrument;** Craig Love¹; Laura Pollum¹; Smiti Khera¹; Lester Taylor¹; Anabel Fandino¹; Martin Greiner²; Na Pi Parra¹; ¹Agilent Technologies, Inc., Santa Clara, CA; ²Agilent Technologies, Waldbronn, Germany
- MP 298 **Evaluation of a High Resolution Accurate Mass Instrument for Discovery Microsomal Clearance and Metabolite ID Analysis;** Mustafa Varoglu¹; Lieu Nguyen¹; Xiaowei He¹; Keith Goodman²; ¹Cubist Pharmaceuticals, Lexington, MA; ²AB Sciex, Framingham, MA
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- MP 299 **Quantitative Measurement of Vitamin D Metabolic Distributions in Human Serum after Chemical Derivatization;** Miriam Müller; Dietrich Volmer; Saarland University, Saarbrücken, Germany
- MP 300 **Development of a Multi-Method Approach for Determining Biomarkers of Sarin Exposure using a Single Blood Sample;** Ronald Evans¹; Richard Lawrence¹; Michael Busch²; Ashley Fancher²; ¹U.S. Army ECBC, Aberdeen Proving Ground, MD; ²Excet Corporation, Aberdeen Proving Ground, MD
- MP 301 **Determining the Binding Ratio of Protein-Ketamine Conjugates with Nanodiamond Mass Spectrometry and Immunizing Mice with the Conjugates;** Hsi-An Chen¹; Tsong-Yung Chou²; Shun-Hsing Tuan²; Wen-Ping Peng¹; ¹National Dong Hwa University, Shoufeng, Hualien, Taiwan; ²Tzu Chi University, Hualien, Taiwan
- MP 302 **A Rapid Multi-Analyte Screening of Amino Acids and Acylcarnitines in Newborns, using Dried Blood Spots [DOCUMENT NO: IVD-MKT-012057-A];** Prem K. Gupta¹; Sanjeev Pandey¹; Praveen K. Sharma²; Manoj Pillai²; ¹Innovative Life Discovery, IMT, Manesar, Haryana, India; ²Sciex, 121 Udyog Vihar, Phase IV, Gurgaon, Haryana, India
- MP 303 **Quantification of Micafungin in Human Plasma by Liquid Chromatography-Tandem Mass Spectrometry;** Sebastiano Barco; , Genoa, Italy
- MP 304 **Clinical Diagnostics of Neuronal Ceroid Lipofuscinoses on Dry Blood Spots: Development of New Cathepsin Substrates for MRM-MS Determination;** Laura Ion¹; Brindusa-Alina Petre²; Thomas Braulke³; Angela Schulz³; Michael Przybylski¹; ¹Steinbeis Centre Biopolymer Analysis and Biomedica, Ruesselsheim, Germany; ²A.I. Cuza University, Iasi, Romania; ³University Hospital Eppendorf, Hamburg, Germany
- MP 305 **Detection of Aldosterone in Serum by a Liquid Chromatography and Tandem Mass Spectrometry on the Shimadzu LCMS-8050 System;** Robin Karras; Danni Li; University of Minnesota, Minneapolis, MN
- MP 306 **Diagnostic Protein Quantitation of 26 Actionable Targets in Patient Biopsies using Clinical Mass Spectrometry;** Wei-Li Liao; Fabiola Cecchi; Adele Blackler; Sheeno Thyparambil; Eunkyung An; Zhichang Yang; Kathleen Bengali; Alexi Drilea; Joseph Reilly; Marlene Darfler; David Krizman; Jon Burrows; Todd Hembrough; *OncoPlex Diagnostics, Rockville, MD*
- MP 307 **Development of an SPLC/MS/MS Method for Paclitaxel and Other Compounds in Whole Blood;** Kerry Hassell¹; Scott Citrowske²; Keith Waddell¹; ¹ThermoFisher Scientific, Somerset, NJ; ²Boston Scientific - MTAC, Maple Grove, MN
- MP 308 **Evaluation and Comparison of Nonderivatization and Derivatization Tandem Mass Spectrometry Methods for Multianalyte Analysis in Dried Blood Spot;** Xiaolei Xie; Marta Kozak; Thermo Fisher Scientific, San Jose, CA
- MP 309 **Quantitative 'Immuno-MS/MS' of Clinically Relevant Heterogeneous Post Translational Protein Modifications: Oxidized and Truncated Parathyroid Hormone;** Li Cui¹; John Wall²; Angela Podgorski²; Fabrizio Bonelli²; Marie Philipneri³; Amy Kreig³; Mustafaa Mahmood³; Kevin Martin³; Gavin Reid^{1, 4}; ¹Michigan State University, East Lansing, MI; ²DiaSorin Inc., Stillwater, MN; ³Saint Louis University, Saint Louis, MO; ⁴University of Melbourne, Parkville, Australia
- MP 310 **Rapid and Accurate LC-MS/MS Method for the Analysis of Nicotine, Nicotine Metabolites, and Minor Tobacco Alkaloid in Urine;** Rob Freeman; Shun-Hsin Liang; Frances Carroll; Sharon Lupo; Ty Kahler; Paul Connolly; Rick Lake; Carrie Sprout; Restek, Bellefonte, PA
- MP 311 **Applications of Parylene-Matrix Chips on MALDI-TOF MS for Highly Sensitive Bacterial Antibiotic Susceptibility Test and new-Born Screening Test;** Jo-Il Kim; Jong-Min Park; Joo-Yoon Noh; Jae-Chul Pyun; Yonsei University, Seoul, South Korea
- MP 312 **Selextion Ion Mobility Enhances Assay Performance for the Determination of F₂ Isoprostane in Urine by LC-MS/MS;** Joseph Greenwood; Jim Bruton; Jennie Ward; Daniel Hoefner; Joseph McConnell; Health Diagnostic Laboratory, Richmond, VA
- MP 313 **Optimization of Automated Online SPE-LC-MS/MS Used in Pain Management Drug Monitoring;** Mark J. Hayward¹; Rick Youngblood¹; Kim Gamble¹; Martin Johnson²; Matthew Hardison²; ¹ITSP Solutions, Hartwell, GA; ²Assurance Scientific Laboratories, Bessemer, AL
- MP 314 **Next Generation Sample Preparation for MS Analysis Of Targeted Plasma Metabolites;** Fred Regnier^{1, 2, 3}; Timothy Schlabach^{1, 2}; Jinhee Kim^{1, 2}; Tim Woenker^{1, 2}; Jiri Adamec⁴; ¹Novilytic, West Lafayette, IN; ²Novilytic, West Lafayette, IN; ³Purdue University, Carmel, IN; ⁴University of Nebraska, Lincoln, NE
- MP 315 **Multi-site Comparison of a High-Throughput Immuno-MALDI Plasma Renin Activity Assay with Methods Currently Used in Clinical Laboratories;** Michael Chen¹; Robert Popp²; Andrew Chambers²; Shaun Eintracht¹; Elizabeth McNamara¹; Christoph Borchers^{2, 3}; ¹Dept. of Diagnostic Medicine, Jewish Gen. Hospital, Montreal, Quebec, Canada; ²University of Victoria-Genome BC Proteomics Centre, Victoria, BC, Canada; ³Dept. of Biochem. & Microbiol., Univ. of Victoria, Victoria, BC, Canada
- MP 316 **A Direct LC/MS/MS Method for Quantitative Determination of 25-Hydroxyvitamin D2 and D3 in Human Plasma;** Zhi Wei Edwin Ting¹; Jun Xiang Lee²; Jie Xing¹; Zhaoqi Zhan¹; ¹Customer Support Centre, Shimadzu (Asia Pacific) Pte Ltd, Singapore; ²School of Physical & Mathematical Science, Nanyang Technological University, Singapore
- MP 317 **A Rapid and Sensitive LC-MS/MS Method for the Analysis of Free Thyroid Hormones;** Frances Carroll; Shun-Hsin Liang; Sharon Lupo; Ty Kahler; Paul Connolly; Rick Lake; Rob Freeman; Carrie Sprout; Restek, Bellefonte, PA
- MP 318 **Coupling of in-vivo Ultrasonic Neuronavigational System and Rapid Evaporative Ionization Mass Spectrometry for the Identification of Brain Tumors during Neurosurgery;** Babar Vaqas¹; Julia Balog^{1, 2}; Federico Roncaroli¹; Steven Pringle²; Kevin O'Neill¹; Zoltan Takats¹; ¹Imperial College London, London, UK; ²Waters Corporation, Wilmslow, UK
- MP 319 **Clinical Enzymology by Paper Spray Mass Spectrometry;** Xin Yan; Xin Li; Chengsen Zhang; Cassandra Moore; Yang Xu; R. Graham Cooks; Purdue University, West Lafayette, IN

- MP 320 **Mass Spectrometric Profiling of Intact Proteins Desorbed from Dried Serum Spots. A Novel Approach for Clinical Diagnostics of Pregnancy Complications;** Manja Wölter¹; Manuela Ruß¹; Werner Rath²; Ulrich Pecks²; Michael O. Glocker¹; ¹Proteome Center Rostock, Rostock, Germany; ²Department of Obstetrics and Gynecology, Aachen, Germany
- MP 321 **Isotope-Dilution Liquid Chromatography-Tandem Mass Spectrometry Candidate Reference Measurement Procedure for 24R,25-Dihydroxyvitamin D3 in Human Serum;** Susan Tai; Michael Nelson; NIST, Gaithersburg, MD
- MP 322 **Validation of An Automated SISCAPA-MALDI-TOF-MS Workflow for Quantification of Serum Apolipoproteins A-I and B-100 in Clinical Sera;** Irene Van Den Broek¹; Jan Nouta¹; Morteza Razavi²; Richard Yip²; Marco Bladergroen¹; Fred Romijn¹; Nico Smit¹; Oliver Drews³; Rainer Paape³; Detlev Suckau³; Andre Deelder¹; Yuri van der Burg¹; Terry Pearson²; Leigh Anderson²; Christa Cobbaert¹; ¹LUMC, Leiden, The Netherlands; ²SISCAPA Assay Technologies, Washington, DC; ³Bruker Daltonics GmbH, Bremen, Germany
- MP 323 **Improved Method for the Analysis of Drugs in Oral Fluids and Urine using the Thomson eXtreme Filter Vials® by LC-MS/MS;** Lisa Wanders; Sam Ellis; Thomson Instrument Company, Oceanside, CA
- MP 324 **Influence of Isobaric Interferences on the Accuracy of Results from LC-MS/MS Analysis of Vitamin D in Human Serum;** Dietrich Volmer; Yulin Qi; Timon Geib; Pascal Schorr; Meier Florian; Saarland University, Saarbrücken, Germany
- MP 325 **Polyvinyl Fluoride Bags for Exhaled Breath by Extractive Electrospray Ionization Mass Spectrometry;** Jiuyan Zhao¹; Lanlan Zhu¹; Eric Handberg²; Zhiqiang Zhu²; Xiaowei Fang²; Huanwen Chen²; Wei Zhang¹; ¹Jiangxi Key Department of Respiratory Medicine, Nanchang, China; ²East China Institute of Tech., Nanchang, China
- MP 326 **Design of Optimization: How to Improve Performance of High-Volume Clinical LC/MS/MS Assays;** Andrew Lickteig; Matthew Salske; Brian Rappold; Essential Testing, LLC, Collinsville, IL
- MP 327 **Intraoperative Tissue Identification using Rapid Evaporative Ionization: Principles of Real-time MS-guided Surgery;** Julia Balog^{1,2}; Edward R St. John²; Babar Vaqas²; James L Alexander²; David Phelps²; Mike Morris¹; Steven Pringle¹; Zoltan Takats²; ¹Waters Corporation, Wilmslow, UK; ²Imperial College London, London, UK
- MP 328 **Separation and Low Level Determination Of Thyroid Hormones From Human Serum By UHPLC-MS/MS Using A Novel C18-Based Stationary Phase;** Alan P. Mckeown¹; Geoffrey Faden²; ¹Advanced Chromatography Technologies Ltd, Aberdeen, UK; ²MACMOD Analytical Inc., Chadds Ford, PA
- MP 329 **Total Cholesterol and HDL Cross Validation between High Throughput LDTD-MS/MS Method and Reference Enzymatic Technique Used in Clinical Laboratory;** Jean Lacoursière¹; Annie-Claude Bolduc²; Gregory Blachon³; Serge Auger¹; Alex Birsan¹; Pierre Picard¹; ¹Phytronix Technologies Inc., Quebec, Canada; ²Université Laval, Québec, QC; ³Phytronix Technologies, Québec, QC
- MP 330 **The Analysis of Fentanyl and Its Analogues in Human Urine by LC-MS/MS;** Paul Connolly; Shun-Hsin Liang; Frances Carroll; Sharon Lupo; Ty Kahler; Rick Lake; Rob Freeman; Carrie Sprout; Restek, Bellefonte, PA
- MP 331 **Direct Metabolic Phenotyping of Newborns at the Molecular Level by High Resolution Mass Spectrometry Analysis of Exhaled Breath;** Vladimir Frankevich¹; Nataliia Starodubtceva¹; Igor Popov¹; Alexey Kononikhin¹; Anna Bugrova¹; Stanislav Pekov¹; Eugene Nikolaev²; ¹Federal State Budget Institution "Research Center, Moscow, RU; ²Institute for Energy Problems of Chemical Physics, Moscow, RU
- MP 332 **A Dilute and Shoot FI-MS/MS Method for Quantification of Glycocholic Acid and Bilirubin in Bile;** Ramakrishna Reddy Vogguru¹; Raghavi Kakarla¹; Janet R Donaldson²; Baochuan Guo¹; ¹Cleveland State University, Cleveland, Ohio; ²Mississippi State University, Starkville, MS
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- MP 333 **The Use of Variable Windows LC-SWATH-MS for Improved Detection and Quantification of Human Urine Metabolites;** Gerard Hopfgartner¹; Aivett Bilbao^{1,2}; Tobias Bruderer¹; Sandra Jahn¹; Emmanuel Varesio¹; ¹University of Geneva, Geneva, Switzerland; ²Swiss Institute of Bioinformatics, Geneva, Switzerland
- MP 334 **Metabolite Profiling can be Used for the Classification and Understanding of the Taxonomic Relationships within Chinese Native Citrus Species;** Li Jing¹; Zhentian Lei¹; Guiwei Zhang²; Alan Cesar Pilon³; David V. Huhman¹; Rangjin Xie²; Wanpeng Xi²; Zhiqin Zhou²; Lloyd W. Sumner¹; ¹Samuel Roberts Noble Foundation, Ardmore, OK; ²Southwest University, Chongqing, China; ³São Paulo State University, São Paulo, Brazil
- MP 335 **Metabolomics Studies Paradigm Shift with Quantification: Integrating Untargeted Profiling, Targeted and Pseudo-Targeted Analysis on One Platform;** Zeming Wu¹; Huichang Bi²; ¹Thermo Fisher Scientific (China), Shanghai, China; ²School of Pharmaceutical, Sun Yat-Sen University, Guangzhou, China
- MP 336 **MRManalyzer: An Integrated Targeted Metabolomic Platform for High-Throughput Metabolite Profiling and Automated Data Processing;** Yuping Cai; Kai Weng; Yuan Guo; Zhengjiang Zhu; Chinese Academy of Sciences, Shanghai, China
- MP 337 **Effects of Senescence and Water-Stress on Soybean Metabolomics: A High-Resolution Mass Spectrometry Investigation;** William Friesen¹; Ali Yilmaz²; Raymond Mutava³; Silvas Prince³; Babu Valliyodan³; Henry Nguyen³; Troy Wood¹; ¹SUNY at Buffalo, Buffalo, NY; ²University of Southampton, Southampton, UK; ³University of Missouri, Columbia, MO
- MP 338 **Intact Metabolome Analysis of Mice Liver by Probe Electrospray Ionization-Tandem Mass Spectrometry (PESI-MS/MS);** Yumi Hayashi^{1,2}; Kei Zaitsumi^{1,2}; Tasuku Murata³; Hiroki Nakajima³; Tamie Nakajima⁴; Hitoshi Tsuchihashi¹; Akira Ishii¹; Tetsuya Ishikawa¹; ¹Nagoya University Graduate School of Medicine, Nagoya, Japan; ²Institute for Advanced Research, Nagoya University, Nagoya, Japan; ³Shimadzu Corporation, Kyoto, Japan; ⁴Chubu University, Kasugai, Japan
- MP 339 **Quantification of Oxidative Stress Metabolites in Human Serum by Liquid Chromatography Tandem Mass Spectrometry Reveals Beneficial Effects of Mediterranean Diet;** Maria G. Kakkoura^{1,2}; Kleitos Sokratos¹; Christiana Demetriou¹; Maria A. Loizidou¹; Andreas Hadjisavvas^{1,2}; Kyriacos Kyriacou^{1,2}; ¹Cyprus Institute of Neurology and Genetics, Nicosia, Cyprus; ²Cyprus School of Molecular Medicine, Nicosia, Cyprus
- MP 340 **Can 2-deoxyglucose be metabolized? An Isotope-Based Metabolomic Analysis;** Susan Gelman; Ying-Jr Amanda Chen; Jacob Schaefer; Gary J. Patti; Washington University in St. Louis, St. Louis, MO
- MP 341 **Targeted Metabolic Profiling using High-Resolution Accurate Mass Database to Identify and Confirm Potential Biomarkers in Rose and Sunflower Plant Extracts;** Jeffrey D. Miller¹; Cyrus Papan²; Jens Pfannstiel³; Iris Klaiber³; Baljit K. Ubhi⁴; Fadi Abdi¹; Tobias Bruderer⁵; Emmanuel Varesio⁵; Gerard Hopfgartner⁵; ¹SCIEX, Framingham, MA; ²SCIEX, Darmstadt, Germany; ³Universität Hohenheim, Stuttgart, Germany; ⁴SCIEX, Redwood City, CA; ⁵University of Geneva, Geneva, Switzerland

- MP 342 **Comparison of Orthogonal Column Chemistries and Ionization Polarity for Increased High Resolution Metabolome (HRM) Coverage;** Vilinh Tran; Douglas Walker; Karan Uppal; Shuzhao Li; Sophia Banton; Dean Jones; *Clinical Biomarker, Emory School of Medicine, Atlanta, GA*
- MP 343 **Expanding the Coverage of Metabolome Using Multiple Liquid Chromatography Modes;** Junhua Wang¹; Gina Tan¹; Xiaodong Liu²; Yingying Huang¹; ¹*Thermo Fisher Scientific Inc, San Jose, CA*; ²*Thermo Fisher Scientific, Sunnyvale, CA*
- MP 344 **LC-MS/MS Monitoring of the Knockout of Lysine Dehydrogenase and Amino adipic Semialdehyde Dehydrogenase in *Ruegeria pomeroyi*;** Izabella A. Pena Neshich¹; Lygia Marques²; Marcos Eberlin²; Paulo Arruda^{1,3}; ¹*Centro de Biologia Molecular e Engenharia Genética, Campinas, Brazil*; ²*Laboratório ThOMSon de Espectrometria de Massas, Campinas, Brazil*; ³*Departamento de Genética e Evolução, Campinas, Brazil*
- MP 345 **Validation of a Retention Time Accurate Mass Library for Semi-Polar Metabolites using Open Source MS-DIAL Software and NIST MS PepSearch;** Stephanie Samra; Ingrid Gennity; Megan Showalter; Oliver Fiehn; *UC Davis, Davis, CA*
- MP 346 **Determination of Intracellular Metabolites by Ion-Paring Liquid Chromatography-Mass Spectrometry;** Lili Guo; Andrew Worth; Clementina Mesaros; Ian A. Blair; *University of Pennsylvania, Philadelphia, PA*
- MP 347 **Metabolomics Method to Comprehensively Analyze Amino Acids in Different Domains;** Haiwei Gu^{1,2}; Jianhai Du¹; Fausto Carnevale Neto^{1,3}; Patrick Carroll⁴; Sally Turner¹; Gabriela Chiorean^{1,5}; Robert Eisenman⁴; Daniel Raftery^{1,4}; ¹*University of Washington, Seattle, WA*; ²*East China Institute of Technology, Nanchang, China*; ³*Sao Paulo State University, Araraquara, Brazil*; ⁴*Fred Hutchinson Cancer Research Center, Seattle, WA*; ⁵*Indiana University Melvin and Bren Simon Cancer Ce, Indianapolis, IN*
- MP 348 **Application of Metabolic Transistor Strategy to Control Electron Transfer Chain Function in *Escherichia coli* by Manipulating Quinone Synthesis Pathway;** Leepika Tuli²; Hui Wu¹; George Bennett²; Ka-Yiu San²; ¹*State Key Laboratory of Bioreactor Engineering, Shanghai, China*; ²*Rice University, Houston, TX*
- MP 349 **A Metabolomic Comparison of Primary and Immortalized Cells of the Same Lineage;** Jessica Lloyd Genenbacher; Gary J. Patti; *Washington University, Saint Louis, MO*
- MP 350 **Quantitative Profiling of Specialized Metabolites from Transgenic Lines of *Camptotheca acuminata* using Liquid Chromatography, Multiplexed CID and Time-of-Flight Mass Spectrometry;** Sujana Pradhan; Radin Sadre; Maria Magallanes-Lundback; Vonny Salim; Dean DellaPenna; A. Daniel Jones; *Michigan State University, East Lansing, MI*
- MP 351 **Construction of a Metabolite MS/MS Library for Laser Desorption Ionization Mass Spectrometry from Silicon Nanopost Arrays;** Andrew Korte¹; Nicholas Morris²; Trust Razunguzwa²; Akos Vertes¹; ¹*George Washington University, Washington, DC*; ²*Protea Biosciences Inc., Morgantown, WV*
- MP 352 **Understanding the Contribution of Glutamine in Fatty Acid Biosynthesis using ¹³C-stable Labelled Metabolites in Conjunction with an Integrated High-Throughput Methodology;** Darren Dumlao¹; Mary Piotrowski¹; Jefry Shields¹; Richard Kibbey²; John Janiszewski¹; Russell Miller³; Min Wan³; ¹*Pfizer, Inc, Groton, CT*; ²*Yale School of Medicine, New Haven, CT*; ³*Pfizer, Inc, Cambridge, MA*
- MP 353 **Investigation of Imidacloprid toxicity on the central nervous system of the snail *Lymnaea Stagnalis* by targeted Metabolomics;** Sara Tufi¹; Marja H. Lamoree¹; Christian Ravensborg²; Aiko Barsch²; Pim E.G. Leonards¹; ¹*Institute for Environmental Studies, VU University, Amsterdam, Netherlands*; ²*Bruker Daltonics, Bremen, Germany*
- MP 354 **High-Performance Chemical Isotope Labeling Liquid Chromatography Mass Spectrometry for Investigating the Effect of Drinking Red Wine on Urine Metabolome;** Yunong Li; Liang Li; *UAlberta, Edmonton, Canada*
- MP 355 **¹³Glucose Infusion in Human Subjects: Metabolomic analysis in the Q Exactive;** Stephen B. Harvey; *University of Minnesota, Minneapolis, MN*
- MP 356 **An Interactive Digital Pathway Map: A Resource for Interpreting Metabolomic Data;** Nick Spittler^{1,2}; Fuad Naser^{1,2}; Gary J Patti¹; ¹*Washington University in St. Louis, St. Louis, MO*; ²*Connex, St. Louis, MO*
- MP 357 **Uncovering Metabolic Changes in Single *Drosophila melanogaster* infected by Nematode Parasites using Capillary Electrophoresis Mass Spectrometry;** Sam Choi; Rosemary Onjiko; Shruti Yadav; Ioannis Eleftherianos; Peter Nemes; *George Washington University, Washington, DC*
- MP 358 **Development of a Chromatographic Screening Approach for Metabolomic Profiling;** Thomas Horvath; Michael Pontikos; David Hawke; Phil Lorenzi; John Weinstein; *University of Texas MD Anderson Cancer Center, Houston, TX*
- MP 359 **Detection and Annotation of the Small Molecule Fraction of Soil Organic Matter;** Stefan Jenkins; Peter Andeer; Tami Swenson; Trent Northen; *Lawrence Berkeley National Laboratory, Berkeley, CA*
- MP 360 **Determining Nutrient Utilization Rates Without Isotopes in Early Zebrafish Development;** Jonathan Spalding^{1,2}; Anna Chen^{1,2}; Nathaniel Mahieu¹; Stephen Johnson²; Gary Patti^{1,3}; ¹*Department of Chemistry, Washington University, St. Louis, MO*; ²*Department of Genetics, Washington University, St. Louis, MO*; ³*Department of Medicine, Washington University, St. Louis, MO*
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- MP 361 **Coupling Liquid-Phase Microextraction with Paper Spray for Rapid Analysis of Malachite Green, Crystal Violet, and Their Metabolites Using Mass Spectrometry;** Jiewei Deng¹; Yuan Yu¹; Yunyun Yang²; Xiaowei Wang¹; Tiangang Luan¹; ¹*Sun Yat-Sen University, Guangzhou, China*; ²*China National Analytical Center Guangzhou, Guangzhou, China*
- MP 362 **Tissue Sample Preparation Optimization for Global Lipidomics by LC-MS;** Danielle McDougall; Rainey Patterson; Yu-Hsuan Tsai; Timothy J Garrett; Richard A Yost; *University of Florida, Gainesville, FL*
- MP 363 **Separating the Separation; Evaluation of μ -solid-phase extraction for On-Column Derivatization and Direct Injection Mass Spectrometry Sample Preparation;** Jessica Pandohee¹; Andrew Minett²; Oliver A.H Jones¹; ¹*ACROSS, School of Applied Sciences, RMIT University, Melbourne, Australia*; ²*EPREP Pty Ltd, Mulgrave, Australia*
- MP 364 **Desalting of Underivatized Small Metabolites on Fluorocarbon Coated Nanoporous Silicon for Solid Matrix-Free LDI-MS (SMALDI-MS);** Ya Zhou¹; Peng Chen¹; D. Jed Harrison^{1,2}; ¹*Department of Chemistry, University of Alberta, Edmonton, Canada*; ²*National Institute for Nanotechnology, Edmonton, Canada*
- MP 365 **Quantitative Targeted Metabolomics using Dried Plasma Spots Cards;** Kristaps Klavins; Guido Dallmann; Therese Koal; *Biocrates Life Sciences AG, Innsbruck, Austria*

- MP 366 **Variations of Human Blood Metabolome Depending on the Employed Sampling Techniques;** Kristaps Klavins; Guido Dallmann; Therese Koal; *Biocrates Life Sciences AG, Innsbruck, Austria*
- MP 367 **Influence of Sample Preparation and Extraction Steps on Metabolomics Analysis of *Elaeis guineensis* Leaves using LC-MS;** Luiz Henrique Vargas¹; José Ribeiro²; Daniel Sifuentes²; Anselmo Oliveira³; Manoel Souza Junior²; Clenilson Rodrigues²; Patrícia Verardi Abdelnur²; ¹University of Lavras, Lavras, Brazil; ²Embrapa Agroenergy, Brasília, Brazil; ³University of Goiás, Goiânia, Brazil
- MP 368 **The Non-Target Metabolomics of Rice Profiling Analysis by ultra-High Performance Liquid Chromatography / High-Resolution Mass Spectrometry;** Yue Song¹; Chaoyang Hu²; Jianxin Shi²; Sifan Li²; Dabing Zhang²; Lei Wang³; Shan-An Chan⁴; ¹Agilent, Shanghai, China; ²Shanghai Nature Standard R&D and Biotech Co., Ltd., Shanghai, China; ³Agilent, Beijing, China; ⁴Agilent, Taipei, Taiwan
- MP 369 **Derivatization of Amino Acids for Solid Matrix Laser Desorption/Ionization (SMALDI) Mass Spectrometry Analysis;** Jing Ji¹; D. Jed Harrison^{1,2}; ¹Department of Chemistry, University of Alberta, Edmonton, Canada; ²National Institute of Nanotechnology, Edmonton, Canada
- MP 370 **Automated Metabolite Profiling in Urine by GC-MS with EI, PICI and APCI Ionization;** Martin Moos¹; Kamil Petrus²; Jan Fesl¹; Petr Hušek^{1,3}; Iva Opekarová¹; Helena Zahradníčková¹; Ladislav Náměstek²; Petr Simek¹; ¹Biology Centre AS CR, Ceske Budejovice, Czech Republic, Europe; ²Pragolab s.r.o., Prague, Czech Republic; ³Faculty Hospital Ostrava, Ostrava, Czech Republic
- MP 371 **High Throughput Analysis of Secondary Metabolites Excreted by Actinobacillus Isolates using Robotics and LC-MS/MS;** Leslie Silva¹; Trent Northen²; ¹Lawrence Berkeley National Lab, Walnut Creek, CA; ²Lawrence Berkeley National Lab, Berkeley, CA
- MP 372 **Systematic Comparison of Recovery and Selectivity of Liquid-Based, Solid-Phase and Size-Exclusion Extraction Methods for Global LC-MS Metabolomics of Human Plasma;** Dmitri Sitnikov; Cian Monnin; Dajana Vuckovic; *Concordia University, Montreal, Canada*
- MP 373 **An Optimized Method for Extraction of Red Blood Cell Metabolites;** Mike Williams¹; Ann Guggisberg²; Christopher Beecher¹; Audrey Odom²; Timothy Garrett¹; ¹University of Florida, Gainesville, Florida; ²Washington University School of Medicine, St. Louis, MO
- MP 374 **Matrix Effect on Chemical Isotope Labeling and Its Implication in Metabolomic Sample Preparation for Quantitative Metabolomics;** Wei Han; Liang Li; *University of Alberta, Edmonton, Canada*
- MP 375 **Comprehensive Human Fecal Metabolome Analysis Using Chemical Isotope Labeling LC-MS;** Nan Wang¹; Wei Xu¹; Deying Chen¹; Xiaoling Su¹; Tao Huan²; Yingfeng Lu¹; Liang Li²; Lanjuan Li¹; ¹the First Affiliated Hospital, Zhejiang University, Hangzhou, China; ²Department of Chemistry, University of Alberta, Edmonton, AB
- MP 376 **Development of a Robotic Platform for Automated GCMS and LCMS Sample Preparation and Large-scale Plant Metabolomics;** David V. Huhman¹; Nicky Eastham²; Graham Ellison²; Robert Talintyre²; Mike Parnell²; Li Jing¹; Shelagh Henson¹; Andrew Whitwell²; Lloyd Sumner¹; ¹The Samuel Roberts Noble Foundation, Ardmore, OK; ²Labman Automation LTD, Seamer Hill, Stokesley, Middlesbrough, UK
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- MP 377 **Simultaneous Quantitation of Low-Molecular Weight Sugars and Carboxylates in Wine by 3-nitrophenylhydrazine Chemical Derivatization - LC-MS/MS;** Jun Han¹; Karen Lin¹; Christoph Borchers^{1,2}; ¹University of Victoria-Genome BC Proteomics Centre, Victoria, BC, Canada; ²Dept. of Biochem. & Microbiol., Univ. of Victoria, Victoria, BC, Canada
- MP 378 **Detection of Urinary Corticosteroids Metabolites by Gas Chromatography-Isotope Ratio Mass Spectrometry in Doping Control Analyses;** Xavier De La Torre¹; Marta Cilia¹; Davide Curcio¹; Cristiana Colamonic¹; Francesco Molaioni¹; Daniel Jardines¹; Francesco Botrè^{1,2}; ¹Laboratorio Antidoping FMSI, Rome, Italy; ²Dipartimento di Medicina Sperimentale, "Sapienza", Rome, Italy
- MP 379 **Identification and Characterization of Changes in Free Amino Acid and Dipeptide Concentrations in Body Fluids in Early Alzheimer's Disease;** Katherine Castor; Alfred Fonteh; Michael Harrington; *HMRI, Pasadena, CA*
- MP 380 **Combining DiLeu Isobaric Labeling and Label-free Approaches for Metabolite Quantification and Biomarker Discovery of Lower Urinary Tract Symptoms (LUTS);** Ling Hao¹; Tyler Greer²; Xuefei Zhong¹; David Page³; Sanghee Lee⁴; Chad Vezina⁵; Will Ricke⁵; Paul Marker¹; Dale Bjorling⁵; Wade Bushman⁴; Lingjun Li^{1,2}; ¹School of Pharmacy, University of Wisconsin-Madison, WI; ²Department of Chemistry, UW-Madison, WI; ³Department of Biostatistics & Medical Informatics, UW-Madison, WI; ⁴Department of Urology, UW-Madison, WI; ⁵School of Veterinary Medicine, UW-Madison, WI
- MP 381 **Ensuring Quantitative Data Reproducibility Within and Across Metabolomics Projects: Evaluation and Implementation of a Standard Quality Control for Serum/Plasma Metabolomics;** Lisa St John Williams; J Will Thompson; Laura Dubois; M Arthur Moseley; *Duke University, Durham, NC*
- MP 382 **¹²C/¹³C-labeled 3-nitrophenylhydrazine for Chemical Derivatization – UPLC-MS/MS Quantitation of Aldehyde Biomarkers of Oxidative Stress in Human Plasma;** Constance Sobsey¹; Jun Han¹; Karen Lin¹; Christoph Borchers^{1,2}; ¹University of Victoria-Genome BC Proteomics Centre, Victoria, BC, Canada; ²Dept. of Biochem. and Microbiol., Univ. of Victoria, Victoria, BC, Canada
- MP 383 **Quantitative and Targeted MRM-based Metabolomics Applications to Characterize Toxicity and AOP in a Zebrafish Larvae Exposure Model;** Bharat Chandramouli¹; Jonathan P. Benskin²; Susie SY Huang¹; John R. Cosgrove¹; ¹Axys Analytical Services, Ltd., Sidney, CA; ²Stockholm University, Stockholm, Sweden
- MP 384 **Comprehensive Analysis of Primary Metabolites by using Both Ion Pairing Chromatography and Non-Ion Pairing Chromatography;** Tsuyoshi Nakanishi¹; Takako Hlshiki²; Makoto Suematsu^{2,3}; ¹Shimadzu Corporation, Kyoto, Japan; ²Keio University, Tokyo, Japan; ³JST ERATO Suematsu Gas Biology Project, Tokyo, Japan
- MP 385 **An Approach to Overcome Ion Suppression for Small Molecule Profiling with LC-TOF MS using Post-Column Addition;** Oskar González^{1,4}; Frans Van der Kloet^{1,3}; Carola Damen^{1,5}; Rob J. Vreeken^{1,2}; Amy Harms¹; Thomas Hankemeier¹; ¹Leiden University, Leiden, Netherlands; ²Janssen Pharmaceutical, Beerse, BELGIUM; ³University of Amsterdam, Amsterdam, NL; ⁴University of the Basque Country, Leioa, SP; ⁵Waters, Manchester, UK
- MP 386 **Utilization of Alkyl Maleimide Tags for Quantitation Thiol Metabolite;** Xiaofeng Zhao; *Saint Louis, MO*



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- MP 387 **Quantitative LC-MS/MS Analysis of Polyamines and Their Metabolic Precursors in Lung Tissue;** Karolina M. Krasinska¹; Yue Xu²; Chuong Hoang²; Allis S. Chien¹; ¹SUMS, Stanford University, Stanford, CA; ²Dept. of Thoracic Surgery, School of Medicine, Stanford, CA
- MP 388 **Development of LC-MS/MS Methods for the Targeted Analysis of Urine Metabolites Associated with Respiratory Illnesses;** Mona Khamis^{1,2}; Hanan Awad¹; Kevin Allen¹; Darryl Adamko¹; Anas El-Aneel¹; ¹University of Saskatchewan, Saskatoon, Canada; ²Alexandria University, Alexandria, Egypt
- MP 389 **Quantitative and Qualitative Metabolomics for the Investigation of Intracellular Metabolism;** Brigitte Simons¹; Baljit Ubhi²; Douglas McCloskey³; ¹SCIEX, Concord, Canada; ²SCIEX, Redwood City, CA; ³University of California San Diego, La Jolla, CA
- MP 390 **Metabolic Effect of Drought Stress during the Grain Filling Growth Stage in Wheat Measured by Isotopic Ratio Outlier Analysis (IROA);** Felice De Jong¹; Chris Beecher²; ¹IROA Technologies LLC, Bolton, MA; ²University of Florida, Gainesville, FL
- MP 391 **Reproducible and Standardized Quantitative Bile Acids Phenotyping using UHPLC-ESI-MS/MS – International Ring Trial and Applications in Other Biologically Relevant Matrices;** Hai Pham Tuan; Doreen Kirchberg; Ines Zitturi; Therese Koal; *BIOCRATES Life Sciences AG, Innsbruck, Austria*
- MP 392 **Quantification of Genitourinary Cancer Metabolites using Liquid Chromatography Triple Quadrupole Mass Spectrometry;** Sumankalai Ramachandran; Xin-Qiao Zhang; Sankar Maity; Zhen Cai; Hui-Kuan Lin; Zahi Mitri; Jianjun Gao; Timothy Thompson; Christopher Logothetics; Eleni Efsthathiou; Mark Titus; *University of Texas MD Anderson Cancer Center, Houston, TX*
- MP 393 **Automated LC/MS/MS Methods Development for Targeted Bioanalysis of Metabolic Intermediates;** John Janiszewski¹; Mary Piotrowski¹; Brendon Kapinos¹; Hui Zhang¹; Darren Dumlaio¹; Wayne Lootsma²; Joseph Janiszewski²; Steven Ainley²; ¹Pfizer Inc., Groton, CT; ²Sound Analytics, East Lyme, CT
- MP 394 **A Kit for Mass-Spectrometry Based Absolute Quantification of Metabolic Enzymes;** Guido Mastrobuoni¹; Fabian Bindell¹; Karsten Schnatbaum²; Paul Ensle²; Julia Avramova-Nehmer²; Holger Wenschuh²; Ulf Reimer²; Stefan Kempa¹; ¹Berlin Institute for Medical Systems Biology, Berlin, Germany; ²JPT Peptide Technologies GmbH, Berlin, Germany
- MP 395 **Quantitative Analysis of Intracellular Metabolites of Microorganisms using Hyphenated Hydrophilic Interaction Liquid Chromatography Tandem Mass Spectrometry;** Reza Maleki Seifar; Cor Ras; Joseph J. Heijnen; *Delft University of Technology, Dept. Biotechnology, Delft, The Netherlands*
- MP 396 **Using Open Source MZmine Software for Targeted GC-MS Data Analysis in Plasma Samples;** Martha Zuluaga¹; Mimi Doll²; Luis Valdiviez²; Lana Amerie²; Nutan Kaushik³; Oliver Fiehn²; ¹University of Caldas, Manizales, Colombia; ²NIH West Coast Metabolomics Center UC Davis, Davis, CA; ³The Energy and Resource Institute (TERI), New Delhi, India
- MP 397 **Comprehensive Analysis of Primary & Secondary Metabolites in Citrus using an Automated Method Changeover UHPLC System Coupled to LC/MS/MS;** Yuka Fujito; Kiyomi Arakawa; Yoshihiro Hayakawa; *Shimadzu Corporation, Kyoto, Japan*
- MP 398 **Quantitative Metabolomics: Way to Understand the Planarian Regeneration;** Kannan Rangiah¹; Nivedita Natarajan¹; Padma Ramakrishnan¹; Vairavan Lakshmanan²; Dasaradhi Palakodeti²; ¹Metabolomics Facility, C-CAMP, NCBS, Bangalore, India; ²inSTEM, NCBS, Bangalore, India
- MP 399 **Combined Targeted Quantitation of Keto- and Amino Acids in GC-MS Analysis using MTBSTFA Derivatization;** Mimi Doll; Benjamin Wancewicz; Carol Tran; Mine Palazoglu; Oliver Fiehn; *NIH West Coast Metabolomics Center, UC Davis, Davis, CA*
- MP 400 **Liquid Chromatography Mass Spectrometric Quantification of Immunomodulatory Histidine Metabolites of Probiotic *Lactobacillus reuteri* Strains;** Daniel Roeth¹; Christina N. Morra²; James Versalovic²; Gabriel Gugiu¹; Markus Kalkum¹; ¹Department of Immunology, City of Hope, Duarte, CA; ²Texas Children's Hospital, Baylor College, Houston, TX
- MP 401 **Improved Performance of Targeted Metabolome Analysis with Waters Xevo® TQ-S and Xevo® TQ-S Micro Instruments;** Ines Zitturi¹; Christian Wachsmuth¹; Harold Zott¹; Michael Daxböck¹; Cornelia Röhring¹; Therese Koal¹; Andrew Peck²; ¹Biocrates Life Science AG, Innsbruck, Austria; ²Waters Corporation, Milford, MA
- MP 402 **Rapid Measurement of 8-oxo-7,8-dihydro-2'-deoxyguanosine in Urine of Colorectal Cancer Patients using Ultraperformance Liquid Chromatography–Tandem Mass Spectrometry;** Cheng Guo; Shu Zheng; *Zhejiang University, Hangzhou, China*
- MP 403 **Determination of Metabolites in Plasma or Blood Using Parallel Ion-Exchange Column-Switching and Reversed-Phase UHPLC-MS/MS with Fast Polarity Switching;** Kyoko Watanabe^{1,2}; Emmanuel Varesio¹; Neil J Loftus³; Gérard Hopfgartner¹; ¹University of Geneva, Geneva, Switzerland; ²Shimadzu Corporation, Kyoto, Japan; ³Shimadzu MS/BU, Manchester, UK
- MP 404 **Simultaneous Stable Isotope Dilution Targeted and Untargeted Steroid Analysis with Girard P Derivatization on a QExactive High Resolution Mass Spectrometer;** Alexander Frey; Nathaniel Snyder; *AJ Drexel Autism Institute, Philadelphia, PA*
- MP 405 **The Use of Capillary Electrophoresis Coupled to Mass Spectrometry (CESI-MS) for Quantitation of Nucleotides and Nucleosides with Minimal Sample Preparation;** Jose-Luis Gallegos-Perez; *Sciex, Framingham, MA*

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- MP 406 **MET-COFEA + MET-XAlign: Tools that Enable LC/MS-based Comparative Metabolomics;** Wenchao Zhang; Patrick Xuechun Zhao; *Samuel Roberts Noble Foundation, Ardmore, OK*
- MP 407 **Software for High-Throughput, Accurate Quantification of Mass Isotopomer Distributions from LC-MS Data for Metabolic Flux Analysis;** Yaroslav Lyutvinskiy¹; Mohit Jain²; Roland Nilsson¹; ¹Karolinska Institutet, Dept. of Medicine, Stockholm, Sweden; ²UCSD, Dept. of Pharmacology, La Jolla, CA
- MP 408 **GNPS: Charting Molecular Families and Structure over Tens of Thousands of Mass Spectrometry Runs;** Mingxun Wang¹; Haixu Tang²; Pieter Dorrestein³; Nuno Bandeira⁴; ¹UCSD, La Jolla, CA; ²Indiana University, Bloomington, IN; ³University of California, San Diego, Skaggs school, La Jolla, CA; ⁴University of California, San Diego, La Jolla, CA
- MP 409 **METASPACE: A New European Project on Bioinformatics for Spatial Metabolomics;** Theodore Alexandrov¹; Pieter Dorrestein²; Lennart Martens³; Oliver Panzer⁴; Charles Pineau⁵; Christoph Steinbeck⁶; Zoltan Takats⁷; Dennis Trede⁸; Kirill Veselkov⁷; ¹EMBL, Heidelberg, Germany; ²University of California, San Diego, Skaggs school, La Jolla, CA; ³VIB, Ghent, Belgium; ⁴European Research Services GmbH, Muenster, Germany; ⁵University of Rennes 1, Rennes, France; ⁶EMBL-EBI, Hinxton, UK; ⁷Imperial College London, London, NA; ⁸SciLS GmbH, Bremen, Germany

- MP 410 **Investigation of Complex Isotope Patterns of ¹³C-labeled Plant Metabolites by Mass Spectral Deconvolution;** Zhenzhen Wang¹; A. Daniel Jones¹; Yongdong Wang²; Ming Gu²; ¹Michigan State University, East Lansing, MI; ²Cerno Bioscience, Norwalk, CT
- MP 411 **Maximizing GC-MS Metabolic Profiling Power using Both Targeted and Non-Targeted Analyses;** Jinshu Qiu; Matt Jerums; Pik Kay Chan; Pavel Bondarenko; Amgen, Thousand Oaks, CA
- MP 412 **Metabolomics Analysis Operations Available for the BioCyc Pathway Database and Website;** Peter Karp; Sri International, Menlo Park, CA
- MP 413 **Development of Spectral Libraries for Use in Identification and Confirmation of Bourbon Authenticity;** William Long¹; Luke Adams²; Sue D'Antonio¹; ¹Agilent, Technologies, Little Falls, DE; ²Beam Suntory, Louisville, KY
- MP 414 **Recent Advances in Skyline: Small Molecule Targets and Ion Mobility Filtering;** Brian Pratt¹; Max Horowitz-Gelb¹; J. Will Thompson²; Erin Baker³; Michael J. Maccoss¹; Brendan Maclean¹; ¹University of Washington, Seattle, WA; ²Duke University School of Medicine, Durham, NC; ³Pacific Northwest National Laboratory, Richland, WA
- MP 415 **New approach for Metabolomics Pathway Analysis;** Takehiro Oshida¹; Teppei Ogawa¹; Yasuto Yokoi¹; Yukihiro Fukamachi¹; Michihiro Araki²; Hiroki Makiguchi¹; ¹Mitsui Knowledge Industry Co., Ltd., Minato-Ku, Japan; ²Kobe University, Hyogo, Japan
- MP 416 **Disparate Metabolomics Data Reassembler: A Novel Algorithm for Agglomerating Incongruent LC-MS Metabolomics Datasets;** Tytus Mak; Stephen Stein; NIST, Gaithersburg, MD
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- MP 418 **A Novel Method for Theoretically Determining the Success Rate of Identification by MS¹ Using a Human Metabolome Database;** Scott Walmsley; Nichole Reisdorph; National Jewish Health, Denver, CO
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- MP 419 **Masses and Expected Compounds: Automatic Creation of Context-Specific Databases and Tripartite Identification of Substances using SpiderMass;** Robert Winkler; CINVESTAV Unidad Irapuato, Irapuato, Mexico
- MP 420 **Stochastic Modeling of Proteome Turnover from Stable Isotope Labeling and LC-MS;** Ling Li²; Belinda Willard²; Tahir Kasumov²; Rovshan Sadygov¹; ¹University of Texas, Galveston, TX; ²Cleveland Clinic, Cleveland, OH
- MP 421 **A Logical Bayesian Framework to Dynamically Compose a Modular Inductive Model of a Proteomics Experiment;** Kurt De Grave; Jan Ramon; KU Leuven, Leuven, Belgium
- MP 422 **Assigning Confidence to Peptide Spectrum Matches Based on Permutation Analysis;** Brian Mitchell; Anoop Mayampurath; Stephen Kron; Samuel Volchenbom; University of Chicago, Chicago, IL
- MP 423 **Ranking Chemical Formulas by Isotopic Pattern Recognition;** Stephen E. Reichenbach¹; Mehrdad Zaker Shahrak¹; Qingping Tao²; ¹University of Nebraska - Lincoln, Lincoln, NE; ²GC Image, LLC, Lincoln, NE
- MP 424 **Towards the Development of a Factor Analysis Based Alignment Algorithm for Raw GC-TOFMS Data;** Peter Willis; Elizabeth Humston-Fulmer; Jihong Wang; Sandy Liu; LECO Corp, St. Joseph, MI
- MP 425 **Mathematical Qualimetry for Mass Spectrometry: Optimization and Harmonization of Sample Preparation, Data Processing and Data Mining;** Alexander Bolkhovitinov; IMS, New York, NY
- MP 426 **Analysis of Unexplained Peaks and Corresponding Relationship Patterns in MS/MS Spectra;** Aida Mrzic¹; Wout Bittremieux¹; Trung Nghia Vu³; Dirk Valkenburg²; Kris Laukens¹; ¹University of Antwerp, Antwerpen, Belgium; ²VITO Mol, Antwerpen, Belgium; ³Karolinska Institutet, Stockholm, Sweden
- MP 427 **Advancing Computer-Assisted Structure Elucidation Methods: A Large-Scale Fragment Assignment Project using Heuristic and Molecular Modeling Methods;** Michal Raab; Juraj Lutisan; Robert Mistrík; HighChem, Bratislava, Slovakia
- MP 428 **A Method for Automated Data Extraction and Peak Identification from Large GC-MS Data Sets Using Multivariate Analysis;** Joshua Coon; Mark Van Benthem; James Hochrein; Curtis Mowry; Sandia National Laboratories, Albuquerque, NM
- MP 429 **Targeted and Untargeted Feature Extraction for GC/MS Spectral Data Profiling;** Norton Kitagawa; Anthony Gray; Jennifer Gushue; Stephen Madden; Yinghang Yang; Agilent Technologies, Inc., Santa Clara, CA
- MP 430 **A Probabilistic Iterative Algorithm for Unrestrictive Protein Modification Localization;** Zhiwu An¹; Yan Fu¹; Wantao Ying²; Xiaohong Qian²; Fuzhou Gong¹; ¹Academy of Mathematics and Systems Science, CAS, Beijing, China; ²Beijing Proteome Research Center, Beijing, China
- MP 431 **An Algorithm for Generating a Representative Protein Sequence Database to Facilitate Proteomic Analysis of Unsequenced Organisms;** Marlon Dias Mariano Dos Santos¹; Juliana de Saldanha da Gama Fischer¹; Felipe da Veiga Leprvost¹; Valmir C. Barbosa²; Paulo Costa Carvalho¹; ¹Laboratory for Proteomics and Protein Engineering, Curitiba, Brazil; ²Systems Engineering and Computer Science Program, Rio de Janeiro, Brazil
- MP 432 **Computational Platform for the Comprehensive Analysis of Clinical Proteomic Data;** Stefka Tyanova¹; Tikira Temu¹; Arthur Carlson¹; Pavel Sinitcyn¹; Sally Deeb¹; Tamar Geiger²; Matthias Mann¹; Juergen Cox¹; ¹Max Planck Institute of Biochemistry, Martinsried, Germany; ²Sackler Faculty of Medicine, Tel Aviv University, Tel Aviv, Israel
- MP 433 **Concordance of Peptide Assignments between Different Search Engines;** Fatemeh Ghavidel³; Wout Bittremieux²; Kris Laukens²; Tomasz Burzykowski³; Dirk Valkenburg¹; ¹VITO, Mol, Belgium; ²University of Antwerp, Antwerp, Belgium; ³Hasselt University, Hasselt, Belgium
- MP 434 **Processing of 3D Imaging Hyperspectral Datasets for Explorative Analysis of Tumour Heterogeneity;** James McKenzie; Nicole Strittmatter; Anna Mróz; Zoltan Takats; Kirill Veselkov; Imperial College, London, UK
- MP 435 **Identifying Targeted Compounds in Un-Supervised Ion Clusters Using Advance Proteome Modeling;** Keith Fadden; Steve Ciavarini; Scott Geromanos; Waters Corporation, Milford, MA
- MP 436 **The Problem of Polydispersity: Tackling Complex Spectra with a Bayesian Approach;** Michael Marty; Carol Robinson; University of Oxford, Oxford, Oxfordshire
- MP 437 **Signature of Life in terrestrial mass distribution of C, H, N and O;** Roman Zubarev²; Alexander Zubarev¹; ¹EXNA AB, Stockholm, Sweden; ²Karolinska Institute, Stockholm, Sweden
- MP 438 **Proteoform Characterization by top-Down Tandem Mass Spectra;** Qiang Kou¹; Binhai Zhu²; Xiaowen Liu^{1,3}; ¹Indiana University Purdue University Indianapolis, Indianapolis, IN; ²Montana State University, Bozeman, MT; ³Indiana University School of Medicine, Indianapolis, IN
- MP 439 **Novor: Real-Time Peptide de Novo Sequencing;** Bin Ma; University of Waterloo, Waterloo, Canada

- MP 440 **Nonconvex Quasi-Norm-Based Normalization of MALDI MSI Data**; Luis Mancera¹; Philippa Hart¹; Fiona Henderson²; Hervé Boutin²; Adam McMahon²; Omar Belgacem¹; ¹Shimadzu, Kratos, Manchester, UK; ²Wolfson Molecular Imaging Centre, Manchester, UK
- MP 441 **De novo Identification of Small Molecules Using an Excel Add In**; Daniel L. Sweeney; MathSpec, Inc., Arlington Heights, IL
- MP 442 **Bioinformatics for Mass Spectrometry Imaging in Augmented Systems Histology**; Kirill Veselkov; James McKenzie; Ottmar Golf; Nicole Strittmatter; Reza Mirnezami; James Kinross; Ara Darzi; Elaine Holmes; Jeremy Nicholson; Zoltan Takats; Imperial College, London, London
- MP 443 **Validating and Comparing Component Detection Algorithms for LC-MS data**; Jane Razumovskaya; Joseph Brown; David Wright; Richard Baran; Iman Mohtashemi; Thermo Fisher Scientific, San Jose, CA
- BIOMARKERS: DISCOVERY
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- MP 444 **Combined Rat Serum Lipidomics and Brain Multimodal MS Imaging for the Detection of Mild Traumatic Brain Injury**; Scott Hogan; Rachel Bennett; Christina Jones; David Gaul; Melissa Alvarado-Valez; Michelle LaPlaca; Facundo Fernandez; Georgia Institute of Technology, Atlanta, GA
- MP 445 **A Mass Spectrometry Proteomics Based Approach for Differentiating Thoracic Tumor Subtypes**; Linan Wang^{1,2}; Konstantin Shilo^{1,3}; Charles Hitchcock^{1,3}; Michael A. Freitas^{1,2}; ¹Ohio State University, Columbus, OH; ²Department of Molecular Virology, Immunology and M, Columbus, OH; ³Department of Pathology, Columbus, OH
- MP 446 **Detection of FGF15 in Plasma by Stable Isotope Standard Capture with Anti-Peptide Antibodies and Targeted Mass Spectrometry**; Hamid Mirzaei¹; David Mangelsdorf¹; Steven Kliewer¹; Andrew Lemoff¹; Takeshi Katafuchi¹; Daria Esterhazy²; Xunshan Ding³; ¹University of Texas Southwestern, Dallas, TX; ²Rockefeller University, New York, NY; ³NGM Biopharmaceuticals, Inc., San Francisco, CA
- MP 447 **Receiver Operating Characteristic Analysis of Identified and Un-Identified Peptides using Label-Free Quantification in MaxQuant**; Jana M. Rucker; Lindsay Schambeau; Lewis K. Pannell; Mitchell Cancer Institute, Mobile, AL
- MP 448 **Application of TMTcalibrator+ for Detection of Markers of Microglia Activation in CSF of Alzheimer's Disease Patients**; Claire Russell¹; Vikram Mitra¹; Amanda Heslegrave²; Jennifer Pocock²; Henrik Zetterberg³; Ian Pike¹; Malcolm Ward¹; ¹Proteome Sciences plc, London, UK; ²Institute of Neurology, University College London, London, UK; ³University of Gothenburg, Gothenburg, Sweden
- MP 449 **N- and O-glycomics from Formalin-Fixed Paraffin-Embedded (FFPE) Clinical Specimens using Porous Graphitized Carbon LC-ESI IT-MS/MS**; Hannes Hinneburg^{1,2}; Petra Korac³; Slavko Gasparov^{4,5}; Peter H. Seeberger^{1,2}; Vlatka Zoldos³; Daniel Kolarich¹; ¹MPI of Colloids and Interfaces, Potsdam, Germany; ²Free University Berlin, Berlin, Germany; ³Dept. of Biology, University of Zagreb, Zagreb, Croatia; ⁴Inst. for Path. and Cytology, Uni Hospital Merkur, Zagreb, Croatia; ⁵Department of Pathology, Medical School Zagreb, Zagreb, Croatia
- MP 450 **High Resolution Shotgun Proteomic Analysis for Biomarker Discovery of Occupational and Environmental Nanoparticles Exposure**; Neserin Ali¹; Stefan Ljunggren²; Helen M Karlsson²; Jörn Nielsen¹; Anders Gudmundsson¹; Christian H Lindh¹; Bo AG Jönsson¹; Monica Kåredal¹; ¹Lund University, Lund, Sweden; ²Linköping University, Linköping, Sweden
- MP 451 **The Differentiation of Orexin Receptor Antagonists and GABA Agonists on Brain Acetylcholine and Histamine Using In Vivo Microdialysis and LC/MS**; Lihang Yao; Andres Ramirez; Anthony Gotter; Anthony Roecker; Steven Fox; Jason Uslander; Paul Coleman; Christopher Winrow; Sean Smith; John Renger; Merck, Co, Inc, West Point, PA
- MP 452 **Characterization and Quantitative Comparison of the Adult and Pediatric Urinary Glycomes by LC-MS To Develop a Baseline Standard**; Patricia Cho; Hui Zhou; Stephen Kostel; John Froehlich; Richard Lee; Boston Children's Hospital, Harvard Medical School, Boston, MA
- MP 453 **Genome-Scale Proteomic Profiling Identifies Breast Cancer Progression Markers**; Yair Pozniak¹; Iris Barshack²; Tamar Geiger¹; ¹Tel Aviv University, Tel Aviv, Israel; ²Sheba Medical Center, Ramat Gan, IL
- MP 454 **Identification of a Protein Substrate Specific for Histone Deacetylase 11 (HDAC11)**; Uwe Warnken¹; Marie Catherine Schier¹; Ramona Mayer¹; Hedwig Deubzer²; Olaf Witt³; Martina Schnölzer¹; ¹German Cancer Research Center, Heidelberg, Germany; ²Charité, Dept. of Pediatric Oncology, Berlin, Germany; ³University Hospital, Dept. of Pediatric Oncology, Heidelberg, Germany
- MP 455 **Development of PEP Technology for Biomarker Discoveries and Functional Proteomics Studies**; Xing Wang; Michael Davies; Array Bridge Inc., St. Louis, Missouri
- MP 456 **Proteomic Imaging for Brain and Spinal Cord from Experimental Allergic Encephalomyelitis (EAE) Mouse Model**; Takashi Nirasawa¹; Noriyuki Iwasaki¹; Takayuki Kondo²; Akimitsu Miyake³; Hiroki Yamashita³; Masaya Ikegawa³; ¹Bruker Daltonics K.K., Yokohama, Japan; ²Kyoto University, Kyoto, Japan; ³Doshisha University, Kyoto, Japan
- MP 457 **Identification of Biomarkers of Dermal Exposure to Toluene Diisocyanate**; Justin M. Hettick; Ajay P. Nayak; Paul D. Siegel; NIOSH, Morgantown, WV
- MP 458 **GC-MS Based Metabolomic Analysis of Plasma for Biomarker Discovery**; Cristina Di Poto; Alessia Ferrarini; Yue Luo; Mohammad R. Nezami Ranjbar; Rency Varghese; Chi Zhang; Habtom Resson; Georgetown University, Lombardi Cancer Center, Washington, DC
- MP 459 **Application of TMTcalibrator+ and Phosphopeptide Enrichment for Global Phosphoproteomic Analysis of CSF from Alzheimer's Disease Patients**; Claire Russell; Vikram Mitra; Ian Pike; Malcolm Ward; Proteome Sciences plc, London, UK
- MP 460 **The Use of Exhaled Breath for the Identification of Hypoxia Biomarkers**; Sean Harshman¹; Brian Geier¹; Maomian Fan¹; Sage Rinehardt¹; Brandy Watts¹; Leslie Drummond²; George Preti³; Jeffrey Phillips²; Darrin Ott¹; Claude Grigsby¹; ¹Air Force Research Laboratory, WPAFB, OH; ²Naval Medical Research Unit-Dayton, WPAFB, OH; ³Monell Chemical Senses Center, Philadelphia, PA
- MP 461 **IgG Glycosylation as a Biomarker for Pancreatic Diseases**; Hsi-Chang Shih^{1,3}; Ming-Chu Chang²; Chein-Hung Chen³; Ya-Po Kuo³; Chung-Hsuan Chen^{1,3}; Yu-Ting Chang²; ¹Dept. of Chemistry, National Taiwan University, Taipei, Taiwan; ²Dept. of Internal Medicine, NTU Hospital, Taipei, Taiwan; ³The Genomics Research Center, Academia Sinica, Taipei, Taiwan
- MP 462 **A Sensitive and Versatile Analytical Method for Quantification of Cyclic Nucleotide Monophosphates (cNMPs) in Biological Systems: Application to Novel Biomarkers**; Xin Jia; Emily Weinert; Emory University, Decatur, Georgia

- MP 463 **Detection and Confirmation of Novel Serum Lipid Biomarkers Predicting Preeclampsia using a Shotgun Lipidomics Approach;** Swati Anand¹; Sydney Young¹; Sean Esplin²; Bruce Jackson¹; Dennis H. Tolley¹; Steven W. Graves¹; ¹BYU, Provo, UT; ²University of Utah School of Medicine, Salt Lake City, UT
- MP 464 **Cross-Site Identification of Ovarian Cancer Proteomic Biomarkers from Cervicovaginal Fluid;** Lindsay Schambeau¹; Brian Hood²; Thomas Conrads²; Michael Finan¹; Rodney Rocconi¹; Laurie Owen¹; Michael Chambers³; Jana Rocker¹; Lewis Pannell¹; ¹Mitchell Cancer Institute, Mobile, AL; ²Women's Health Integrated Research Center, Annandale, VA; ³Swift Biotechnology LLC, Mobile, AL
- MP 465 **Radiation Exposure Induces Alterations Typical of Oxidative Stress Modifications Underlying Cardiovascular Disease;** Mark E. Mccomb¹; Markus M. Bachschmid¹; Chunxiang Yao¹; Maggie Kuo²; Stephen Whelan¹; Jean Spencer¹; Christian Heckendorf¹; Catherine E. Costello¹; Dan Berkowitz²; ¹Boston University School of Medicine, Boston, MA; ²Johns Hopkins University, Baltimore, MD
- MP 466 **The Investigation of Extraction Efficiency of Proteins from Brain Tissues Related to Alzheimer's Disease;** Siddhita Aparaj-Shirsat; Rachel Marvin; Kenneth Hensley; Dragan Isailovic; *University of Toledo, Toledo, OH*
- BIOMARKERS: QUANTITATIVE ANALYSIS (PROTEIN)**
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- MP 467 **SI-Traceable Quantification of 1-32 Brain Natriuretic Peptide in Plasma at Clinically Relevant Concentration Levels;** Frank Attila Torma^{1,2}; Kate Groves¹; Sabine Biesenbruch¹; Christopher Mussell¹; Rainer Cramer²; Milena Quaglia¹; ¹LGC LTD, Teddington, UK; ²University of Reading, Reading, UK
- MP 468 **Multiplexed Protein Quantification of Salivary Proteins by MRM-MS for Evaluation of Cancer Biomarkers;** Yi-Ting Chen¹; Hsiao-Wei Chen¹; Wei-Fan Chiang²; Jau-Song Yu¹; Yu-Sun Chang¹; Chun-Feng Wu¹; ¹Chang Gung University, Taoyuan, Taiwan; ²Chi-Mei Medical Center, Liouying, Taiwan
- MP 469 **Detection and Quantification of Relevant Proteins in GBM FPPE Tumor Tissue Using Selective Reaction Monitoring Mass Spectrometry;** Xiaolin Li¹; Jill Barnholtz-Sloan^{1,2}; Daniela M Schlatter¹; Mark Chance¹; ¹Case Western Reserve University, Cleveland, OH; ²Comprehensive Cancer Center University Hospitals, Cleveland, OH
- MP 470 **Development of the Workflow for targeted Proteomic Quantification of Osteopontin in Healthy and Cancerous Human Breast Tissues;** Katarzyna Macur¹; Lars Hagen²; Tomasz Ciesielski²; ¹Intercollegiate Faculty of Biotechnology UG-MUG, Gdansk, Poland; ²Norwegian University of Science and Technology, Trondheim, Norway
- MP 471 **First Quantification of Human CSF Tau Protein without Immunocapture using Triple Quadrupole Mass Spectrometer;** Christophe Hirtz¹; Pauline Bros¹; Nicolas Barthelemy¹; Vincent Delatour³; Jérôme Vialaret¹; Audrey Gabelle²; Sylvain Lehmann¹; ¹LBPC-IRB, CHU de Montpellier, Montpellier, France; ²Centre Mémoire Ressources Recherche, Montpellier, France; ³Laboratoire National de Métrologie et d'Essais, Paris, France
- MP 472 **Core-fucosylated Glycopeptides in Hepatocellular Carcinoma;** Haidi Yin¹; Zhijing Tan¹; Jing Wu¹; Jianhui Zhu¹; Jorge Marrero²; David Lubman¹; ¹University of Michigan, Ann Arbor, MI; ²University of Texas, Dallas, TX
- MP 473 **PTM Profiling of Cancer Cells by Sequential Enrichment for Methylation, Acetylation and Phosphorylation to Monitor Cellular Signaling Upon Adenosine-2',3'-Dialdehyde Treatment;** Ghaith Hamza²; Charles Farnsworth¹; Hongbo Gu¹; Xiaoying Jia¹; Jeffrey Silva¹; ¹Cell Signaling Technology, Danvers, MA; ²Endicott College, Beverly, MA
- MP 474 **Target Analysis of Prostate-Specific Antigen Glycopeptide Abundance in Prostate Cancer and Benign Hyperplasia from Urinary Samples;** Chun-Jen Hsiao^{1,2}; Tzong-Shin Tzai³; Chein-Hung Chen¹; Wen-Hong Yang³; Chung-Hsuan Chen¹; ¹Academia Sinica, Taipei, Taiwan; ²National Yang-Ming University, Taipei, Taiwan; ³National Chen Kung University Hospital, Tainan, Taiwan
- MP 475 **Quantification of Human IL-6 in Serum with an Automated Online Sample Preparation System Coupled with LC-MS;** Li Li¹; Nishi Rochelle²; Hirralben Patel¹; Kevin Schug¹; Joe Barrera¹; ¹University of Texas at Arlington, Arlington, TX; ²Shimadzu Scientific Instruments, Inc, Addison, IL
- MP 476 **Protein-based Biomarker Predicts Conversion from Clinically Isolated Syndrome to Multiple Sclerosis;** Eva Borràs^{1,2}; Ester Cantó³; Meena Choi⁴; Luisa María Villar⁵; Jose Carlos Álvarez-Cermeño⁵; Cristina Chiva²; Xavier Montalbán³; Olga Vitek⁴; Manuel Comabella³; Eduard Sabidó^{1,2}; ¹Proteomics Unit (CRG), Barcelona, Spain; ²University Pompeu Fabra (UPF), Barcelona, Spain; ³Cemcat. Institut de Recerca Vall Hebrón, Barcelona, Spain; ⁴Department of Statistics, Purdue University, West Lafayette, IN; ⁵Hospital Ramón y Cajal, Madrid, Spain
- MP 477 **Validation of LRG1 as a Potential Biomarker for Detection of Epithelial Ovarian Cancer by a Blinded Study;** Jing Wu; Haidi Yin; Jianhui Zhu; Ronald Buckanovich; David Lubman; *University of Michigan, Ann Arbor, MI*
- MP 478 **Human Cerebrospinal Fluid and Surrogate Matrix-Based Quantification of Alzheimer's Biomarker Amyloid Beta Protein by Liquid Chromatography-Tandem Mass Spectrometry;** Mei Chen¹; Weiming Xia²; ¹Harvard School of Public Health, Boston, MA; ²ENR Memorial VA Hospital, Bedford, MA
- MP 479 **Comparative Two Dimensional Polyacrylamide Gel Electrophoresis (2D-PAGE) of the Salivary Proteome of Children with Autism Spectrum Disorder (ASD);** Armand Ngounou¹; Kelly L. Wormwood¹; Laci Charette²; Jeanne P. Ryan³; Alisa G. Woods¹; Costel C. Darie¹; ¹Clarkson University, Potsdam, NY; ²SUNY Plattsburgh Neuropsychology Clinic, Plattsburgh, NY; ³Department of Psychology, SUNY Plattsburgh, Plattsburgh, NY
- MP 480 **LC-MS/MS Quantification of Factor P (Properdin), an Endogenous Protein, in Monkey Serum;** Xinliu Gao; Hui Lin; Wenkui Li; Jimmy Flarakos; Francis Tse; *Novartis Institutes for Biomedical Research, East Hanover, NJ*
- MP 481 **Quantitation of N-terminal Formaldehyde Adducts to Hemoglobin using UPLC-MS/MS;** Min Yang¹; Chui Tse²; Maria Ospina²; Hubert Vesper²; ¹Battelle Memorial Institute, Atlanta, GA; ²Centers for Disease Control and Prevention, Atlanta, GA
- MP 482 **Quantitation of Calcyclin and Heat Shock Protein 90 in Serum from Preeclampsia Patients by 2D Nano LC-MS/MS;** Coşkun Güzel¹; Caroline B. van den Berg¹; Régine P.M. Steegers-Theunissen¹; Lennard Dekker¹; Johannes P.C. Vissers²; Eric A.M. Steegers¹; Theo M. Luider¹; ¹Erasmus Medical Center, Rotterdam, Netherlands; ²Waters Corporation, Manchester, UK
- MP 483 **Measuring Acute Traumatic Brain Injury Biomarkers by Targeted Mass Spectrometry;** Sean Shen¹; Ina-Beate Wanner²; Joseph A. Loo¹; ¹Chemistry & Biochemistry, University of California, Los Angeles, CA; ²Semel Institute for Neuroscience & Human Behavior, University of California, Los Angeles, CA

- MP 484 **Detection and Relative Quantitation of Potential Salivary Antimicrobial Biomarkers (HNP 1-4) by LC-ESI-MS in Young Athletes;** N. Ashrafi; F.S. Pullen; B.V. Nielsen; *University of Greenwich, Chatham Maritime, UK*
- MP 485 **Western Diet Alters O-GlcNAcylation and Phosphorylation in Mouse Heart Metabolic Disorder;** Stephen A. Whelan¹; Jean Spencer¹; Christian Heckendorf¹; Junfeng Ma²; Chunxiang Yao¹; Jessica Behring¹; Deborah Siwick¹; Wilson Colucci¹; Richard Cohen¹; Markus Bachschmid¹; Gerald W. Hart²; Catherine E. Costello¹; Mark E. Mccomb¹; ¹*Boston University School of Medicine, Boston, MA*; ²*Johns Hopkins University School of Medicine, Baltimore, MD*
- MP 486 **Application of nanoLC-MS/MS to Measure Glycated N-terminal Beta Hemoglobin in Bottlenose Dolphins;** Michael Janech¹; Alison Bland¹; Stephanie Venn-Watson²; ¹*Medical University of South Carolina, Charleston, SC*; ²*The National Marine Mammal Foundation, San Diego, CA*
- MP 487 **Evaluation of Candidate Biomarkers for FGF-associated Breast Cancer by Selected Reaction Monitoring Mass Spectrometry;** Hongyan Zhao; Andrew Creese; Debbie Cunningham; John Heath; Helen Cooper; *School of Biosciences, University of Birmingham, Birmingham, UK*
- MP 488 **Quantitation of Bradykinin and Bradykinin 1-5 in Human Plasma Using a 2D-LC-MS/MS Assay with a Surrogate Analyte Approach;** Moucun Yuan¹; Hongmei Cao²; Eric Ma¹; William R. Mylott¹; Bruce Hidy¹; Rand Jenkins¹; Jiang Wu²; Ann Gooding²; Yongchang Qiu²; ¹*PPD, Richmond, VA*; ²*Shire, Lexington, MA*
- PLANT-OMICS
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- MP 489 **Investigation of Polyphenols in White and Coloured Flower Petals of Faba Bean Plants;** Yurdagul Ferhatoglu; Mahla Mirali; Randy W. Purves; Kirstin E. Bett; Albert Vandenberg; *University of Saskatchewan, Saskatoon, Canada*
- MP 490 **Identification of Cold-induced MAP Kinase Substrates in *Arabidopsis Thaliana* through Protein Kinase Assay Linked-Phosphoproteomics;** Chuan-Chih Hsu¹; Chunzhao Zhao²; Pengcheng Wang²; Jian-Kang Zhu²; Weiguo Andy Tao¹; ¹*Department of Biochemistry, Purdue University, West Lafayette, IN*; ²*Department of Horticulture, Purdue University, West Lafayette, IN*
- MP 491 **Label-free Quantitative Analysis by WiSIM-DIA with an Orbitrap Fusion to Identify Proteins Involved in the Cuticle Formation of Tomato Fruit;** Laetitia Martin¹; Joshua Nicklay²; Tara Schroeder²; Tahmid Hassan²; Elizabeth Anderson³; Jocelyn Rose¹; Sheng Zhang³; ¹*School of Integrative Plant Science, Cornell Univ, Ithaca, NY*; ²*Thermo Fisher Scientific, Somerset, NJ*; ³*Proteomics & Mass Spec Facility, Cornell Univ, Ithaca, NY*
- MP 492 **Acetyloyme Analysis Reveals Lysine Acetylation is in Regulation of Photosynthesis and Carbon Metabolism in Cyanobacterium *Synechocystis*;** Ran Mo²; Mingkun Yang²; Zhongyi Cheng¹; Xingling Yi¹; Feng Ge²; ¹*PTM Biolabs, Inc, Hangzhou, China*; ²*Chinese Academy of Sciences, Wuhan, CN*
- MP 493 **The Application of Capillary Electrospray Ionization with Negative Ion Electrospray Ionization to the Analysis of Plant Metabolites;** Stephen J. Lock¹; Edna Betgovargez²; ¹*ABSCIEX, Warrington, UK*; ²*Sciex Separations, Brea, CA*
- MP 494 **Determination of *in situ* Plant Root Metabolomes by Ambient Ionization Mass Spectrometry;** Rabi A. Musah¹; Robert B. Cody²; Ashton D. Lesiak¹; Max J. Maron¹; David Edwards²; A. John Dane²; Michael C. Long¹; ¹*University at Albany-SUNY, Albany, NY*; ²*JEOL USA, Inc., Peabody, MA*
- MP 495 **Elucidation of Cellulosic Transcription Factors in Stem Differentiating Xylem Tissue of *Populus trichocarpa*;** Philip Loziuk; Jennifer Parker; Wei Li; Chien-Yuan Lin; Jack Wang; Quanzi Li; Ronald Sederoff; Vincent Chiang; David Muddiman; *North Carolina State University, Raleigh, NC*
- MP 496 **Pathogen-triggered Protein-Protein Interactions Mediating Nonclassical Secretion of Mannitol Dehydrogenase in Plants;** Tricia Ho; Kevin Blackburn; John Williamson; Michael Goshe; *North Carolina State University, Raleigh, NC*
- MP 497 **Analysis of Gape Xylem Tissue and Sap Proteome;** Ramesh Katam; Varshini Sridhar; Sydney Lyda; *Department of Biological Sciences, Florida A&M Univ, Tallahassee, FL*
- MP 498 **¹³C-amino Acid Labeling Investigation of Acylsugar Related Aliphatic Acid Elongation via UHPLC-QTOF-MS/MS Analysis;** Xiaoxiao Liu¹; Banibrata Ghosh²; A. Daniel Jones^{1,2}; ¹*Department of Chemistry, Michigan State University, East Lansing, MI*; ²*Department of Biochemistry and Molecular Biology, Michigan State University, East Lansing, MI*
- MP 499 **Response of *Chlamydomonas reinhardtii* Proteome to Wastewater Culturing: A Comparative Label-Free Proteomic Analysis;** Anil K. Patel; Mark G. Lefsrud; *McGill University, Ste. Anne De Bellevue, Canada*
- MP 500 **Identification and Classification of *Salvia* Species using Ambient Ionization Mass Spectrometry;** Justine E. Giffen²; Ashton D. Lesiak²; Robert B. Cody¹; Rabi Musah²; ¹*JEOL USA, Inc., Peabody, MA*; ²*University at Albany-SUNY, Albany, NY*
- MP 501 **Mapping Phenolic Glycosides in *Populus deltoides* and *Populus grandidentata* by Leaf Spray Mass Spectrometry;** Dalton Snyder; Christina Schilling; Cris Hochwender; Arlen Kaufman; *University of Evansville, Evansville, IN*
- MP 502 **Comparative Proteomic Analysis of Two Rice Genotypes with Contrasting Drought Tolerance;** Mehdi Mirzaei¹; Yunqi Wu¹; Dana Pascovici²; Joel Chick³; Brian Atwell¹; Paul Haynes¹; ¹*Macquarie University, Sydney, Australia*; ²*Australian Proteome Analysis Facility, Sydney, Australia*; ³*Harvard Medical School, Boston, MA*
- PROTEOMICS: TISSUE
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- MP 503 **Differential Proteomics of *Pteropus* Wing Bones;** Timothy Cleland; Deepak Vashishth; *Rensselaer Polytechnic Inst, Troy, NY*
- MP 504 **Matching Therapies by Comparison of Kinase ATP Uptake in Lung Tumors and Drug Responses in Lung Cancer Cell Lines;** Bin Fang; Melissa Hoffman; Jiannong Li; Y. Ann Chen; Fumi Kinose; Katherine Fellows; Steven A. Eschrich; Uwe Rix; Eric B. Haura; John Koomen; *H. Lee Moffitt Cancer Center, Tampa, FL*
- MP 505 **Comparison of ATP Affinity Probe-based Kinome Enrichment at the Protein and Peptide Levels;** Yue Qi¹; Abdullah Mallisho²; Danjun Ma¹; Xiangmin Zhang¹; Michael Caruso¹; Divyasri Damacharla¹; Nishit Shah¹; Majed Abdullah Alharbi¹; Berhane Seyoum²; Zhengping Yi¹; ¹*Wayne State University, Detroit, MI*; ²*University Health Center, Detroit, MI*
- MP 506 **Spatial and Temporal MSI and Proteomic Studies of Rat Spinal Cord Injury: Evidence of Caudal Segment for Possible Therapy Target;** Stéphanie Devaux^{1,2}; Dasa Cizkova^{1,2}; Maxence Wisztorski¹; Lucia Slovinska²; Juraj Blasko²; Isabelle Fournier¹; Michel Salzet¹; ¹*INSERM U1192 - University of Lille 1, Villeneuve D'ascq Cedex, France*; ²*Slovak Academy of Sciences, Kosice, Slovakia*
- MP 507 **Cell-type Specific Proteomics from Formalin-Fixed Paraffin Embedded (FFPE) Tissue: A Challenge?;** Shruti Nayak; Eleanor Drummond; Thomas Wisniewski; Beatrix Ueberheide; *NYULMC, New York, NY*

- MP 508 **Proteomic and Bioinformatics Profile of Paired Human Alveolar Macrophages and Peripheral Blood Monocytes**; [Kathleen C Lundberg](#); Sara Tomechko; Jessica Walrath; Mark Chance; Richard Silver; *Case Western Reserve University, Cleveland, OH*
- MP 509 **Developing and Assessing Polyacrylamide Hydrogel Technologies for Improved Protein Extraction from Targeted Regions of Biological Tissues**; [David G. Rizzo](#)^{1,3}; Jessica L. Moore^{1,3}; Boone M. Prentice^{2,3}; Jeremy L. Norris^{2,3}; Richard M. Caprioli^{1,3}; ¹*Vanderbilt Dept. of Chemistry, Nashville, TN*; ²*Vanderbilt Dept. of Biochemistry, Nashville, TN*; ³*Vanderbilt University MSRC, Nashville, TN*
- MP 510 **Proteomic and Glycomic Analysis of the Mediodorsal Nucleus of Subjects with Schizophrenia**; [Lilla Turiak](#)¹; Harry Pantazopoulos^{2,3}; Nancy Leymarie¹; Sabina Berretta^{2,3}; Oliver D. King⁴; Joseph Zaia¹; ¹*Boston University, Boston, MA*; ²*Translational Neuroscience Laboratory, Mclean Hosp, Belmont, MA*; ³*Department of Psychiatry, Harvard Medical School, Boston, MA*; ⁴*Department of Cell and Developmental Biology UMass, Worcester, MA*
- MP 511 **Global Protein Profiling of Visceral Fat and Subcutaneous Fat from Obese Non-Diabetic and Obese T2D Subjects**; [Danjun Ma](#); Alemu Fite; Xiangmin Zhang; Yue Qi; Michael Howard Wood; Rebecca Tagett; Sorin Draghici; Berhane Seyoum; Zhengping Yi; *Wayne State University, Detroit, MI*
- MP 512 **Evaluation of Sample Preparation Methods for Label-Free Quantitative Proteomics of Human Brain Tissue**; [Kristin J. Boggio](#)¹; Marvin R. Natowicz²; John D. Leszyk¹; Scott A. Shaffer¹; ¹*University of Massachusetts Medical School, Worcester, MA*; ²*Pathology & Laboratory Medicine, Cleveland Clinic, Cleveland, OH*
- MP 513 **Genotype-Tissue-Protein: Quantitative Proteomic Analysis of Human Tissue Proteome**; [Lulu Cao](#); Michael Snyder; *Stanford University, Stanford, CA*
- MP 514 **MALDI Imaging-driven Microproteomics Workflow to Study Intra-Tumor Heterogeneity**; Deborah Alberts¹; Charles Pottier²; Nicolas Smargiasso¹; Gabriel Mazzucchelli¹; Dominique Baiwir³; Philippe Delvenne²; [Edwin De Pauw](#)¹; Rémi Longuespée¹; ¹*Mass Spectrometry Laboratory, University Of Liège, Liège, Belgium*; ²*Department of pathology, University of Liège, Liège, Belgium*; ³*GIGA Proteomics Facility, University of Liège, Liège, Belgium*
- MP 515 **SWATH-MS Profiling of FFPE Tissue Sections**; Sean McMillan; Kristin Reinsvold; [Jayme Wiederin](#); Melinda Wojtkiewicz; Weizhe Li; Howard E. Gendelman; Larisa Poluektova; Pawel Ciborowski; *University of Nebraska Medical Center, Omaha, NE*
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- MP 516 **Quantitative Analysis of Membrane-Enriched and Soluble Proteome of Cortex from Mice Exposed to Psychotropic Medication**; [Cátia Santa](#)^{1,2}; Susana C. Saraiva^{1,3}; Sandra Anjo^{1,4}; Vera M. Mendes^{1,5}; Graça Baltazar⁶; Michael J. Dunn⁷; David Cotter⁸; Bruno Manadas^{1,5}; ¹*Center for Neurosciences and Cell Biology, Coimbra, Portugal*; ²*Institute for Interdisciplinary Research, Coimbra, Portugal*; ³*Faculty of Pharmacy, University of Coimbra, Coimbra, Portugal*; ⁴*Faculty of Sciences and Technology, Coimbra, Portugal*; ⁵*Biocant - Biotechnology Innovation Center, Cantanhede, Portugal*; ⁶*CICS-UBI - Health Sciences Research Center, Covilhã, Portugal*; ⁷*Proteome Research Centre, University College, Dublin, Ireland*; ⁸*Department Psychiatry, Royal College of Surgeons, Dublin, Ireland*
- MP 517 **Proteomic Analysis of Superior Frontal Gyrus from Brains of Humans with Mild Cognitive Impairment and Alzheimer's Disease**; [Dale Chaput](#); Lisa Kirouac; Jaya Padmanabhan; Stanley M. Stevens, Jr; *University of South Florida, Tampa, Florida*
- MP 518 **How Many Proteins can be Measured and Quantified from 1000 and 5000 Cells?**; Beom-Jun Kim; [Sung Yun Jung](#); Jong Min Choi; Jun Qin; *Baylor College of Medicine, Houston, Texas*
- MP 519 **Osteoblast-released Matrix Vesicle Activity and Composition are Regulated by Sulfated Glycosaminoglycans**; [Johannes Schmidt](#)^{1,2}; Stefanie Kliemt^{1,3}; Carolin Preissler⁴; Stephanie Möller⁶; Martin von Bergen^{1,6}; Ute Hempel⁴; Stefan Kalkhof¹; ¹*Helmholtz Centre for Environmental Research - UFZ, Leipzig, Germany*; ²*Institute of Biochemistry, Leipzig University, Leipzig, Germany*; ³*B CUBE Center for Molecular Bioengineering, Dresden, Germany*; ⁴*Institute of Physiological Chemistry, TU Dresden, Dresden, Germany*; ⁵*Biomaterials Department, INNOVENT e.V., Jena, Germany*; ⁶*Department of Biotechnology, Aalborg University, Aalborg, Denmark*
- MP 520 **Label-free Quantitative Hippocampal Proteomics Reveals Pathways Linking Gamma Radiation Damage to Pathways Associated with Mitochondrial Function, Synaptic Activity and Memory**; [Lin Huang](#)¹; Samantha Wickramasekara¹; Jacob Raber²; Claudia Maier¹; ¹*Department of Chemistry, Oregon State University, Corvallis, OR*; ²*Behav Neurosci, Neurol, Radiat Med, OHSU, Portland, OR*
- MP 521 **Proteomics Analysis of Altered Cellular Metabolism Induced by Insufficient Copper Level**; Sohye Kang; Gang Xiao; Da Ren; Zhongqi Zhang; Nicole Le; Michael Trentalange; Shivani Gupta; Henry Lin; [Pavel Bondarenko](#); *Amgen, Inc., Thousand Oaks, CA*
- MP 522 **Identification of LRRK2 Substrates in a Drosophila Melanogaster Model of Parkinson's Disease**; [William Edelman](#); Leo Pallanck; Judit Villen; *University of Washington, Seattle, WA*
- MP 523 **Protein Quantitation False Discovery Rates and Environmental Proteomics**; [Paul A. Haynes](#); David Handler; Iniga Seraphina George; Samantha Emery; YunQi Wu; Vineet Vaibhav; Mehdi Mirzaei; *Macquarie University, North Ryde, Sydney, Australia*
- MP 524 **Proteomics-driven Exploration of Hypoxia-responsive Cellular Pathways associated to Metastasis in Osteosarcoma**; Zifeng Song¹; Liping Yang¹; Jeffrey Morre¹; Milan Milovancev²; Siva Kolluri³; Claudia Maier¹; ¹*Department of Chemistry, Oregon State University, Corvallis, Oregon*; ²*College of Veterinary, Oregon State University, Corvallis, OR*; ³*Department of Env.&Mol. Tox., Oregon State University, Corvallis, OR*
- MP 525 **Peptide Selection for Targeted Proteomics Quantitation: The Wisdom of the Crowds**; [Cristina Chiva](#)^{1,2}; Eduard Sabidó^{1,2}; ¹*Proteomics Unit (CRG), Barcelona, Spain*; ²*University Pompeu Fabra (UPF), Barcelona, Spain*
- MP 526 **Protein Profiling (HDMS[®]) for Monitoring of Chondrocyte Differentiation of Mesenchymal Stem Cells in 3D Pellet Culture in a Multi-Omic Approach**; [Shujuan Tao](#); Andrea R. Tan; David Chen; Clark T. Hung; Lewis M. Brown; *Columbia University, New York, NY*
- MP 527 **Use of High Resolution Accurate Mass (HRAM) MS1 to Test RNA – Interference Mediated Protein Suppression in Western Corn Rootworm**; [David Mccaskill](#)¹; Tao Xu¹; Sek Yee Tan¹; Murugesan Rangasamy¹; James Hasler¹; Haichuan Wang²; Ana Maria Velez Arango²; Hong Chen²; Jessica Jurzenski²; Narva Kenneth¹; Blair Siegfried²; ¹*Dow AgroSciences, Indianapolis, IN*; ²*University of Nebraska, Lincoln, NE*
- MP 528 **Measuring Time-Dependent Effects of Ionizing Radiation on Mammalian Tissue Using Quantitative Proteomics**; [Dyna L. Shirasaki](#); William McBride; Joseph Capri; Elizabeth Singer; Julian Whitelegge; Joseph A. Loo; *UCLA, Los Angeles, CA*

- MP 529 **Very Deep Coverage of the Human Proteome using a Very High Resolution Quadrupole Time-Of-Flight Instrument;** Scarlet Beck¹; Florian Meier¹; Annette Michalski²; Oliver R  ther²; Markus Lubeck²; Stephanie Kaspar²; Igor Paron¹; J  rgen Cox¹; Matthias Mann¹; ¹Max-Planck-Institute of Biochemistry, Martinsried (near Munich), Germany; ²Bruker Daltonik GmbH, Bremen, Germany
- MP 530 **Brain Organelle Proteomics: DDA and SWATH Based Quantifications of Biochemically Isolated Mouse Brain Synapse Sub-Fractions;** Nikhil J. Pandya¹; Frank Koopmans²; August B. Smit¹; Ka wan Li¹; ¹Dept. of Molecular Cellular Neurobiology, CNCR, VU, Amsterdam, The Netherlands; ²Dept. of Functional Genomics, CNCR, VU, Amsterdam, The Netherlands
- MP 531 **Knockdown and Overexpression of Phosphohistidine Phosphatase 1 Leads to Alterations in the Proteome of a Mouse Hepatocyte Cell Line;** Ashley Culver-Cochran; Stanley M. Stevens, Jr; *University of South Florida, Tampa, FL*
- MP 532 **MS1-based Label-Free Proteomics using a Quadrupole Orbitrap Mass Spectrometer;** Tali Shalit; Dalia Elinger; Alon Savidor; Alexandra Gabashvili; Yishai Levin; *Weizmann Institute of Science, Rehovot, Israel*
- MP 533 **Mapping the DNA Damage Response to the Temporal Occurrence of Histone Modifications;** Kevin Leahy; *Durham, NH*
- MP 534 **Comprehensive Relative Quantification of the Cytochromes P450 using SWATH™ Acquisition;** Rosalind E. Jenkins¹; Sibylle Heideberger²; Thomas Knapman²; Francesco L. Brancia²; Neil R Kitteringham¹; B. Kevin Park¹; ¹University of Liverpool, Liverpool, UK; ²Sciex, Warrington, UK
- MP 535 **In-depth Proteomic Analysis of Sorafenib-induced Resistance in Human Hepatocellular Carcinoma with Subcellular Fractionation;** Joon-Ho Park¹; Dohyun Han^{1,3}; Su Jong Yu²; Jung-Hwan Yoon²; Youngsoo Kim^{1,4}; ¹Department of Biomedical Engineering, SNUH, Seoul, Korea; ²Department of Internal Medicine, SNUH, Seoul, Korea; ³Biomedical Research Institute, SNUH, Seoul, Korea; ⁴Institute of Medical & Bioengineering MRC, SNU, Seoul, Korea
- MP 536 **Absolute Protein Quantification of Starved *Bacillus subtilis* during Adaptation to Oxidative Stress;** Sandra Maa  ; Sarah Wettst  dt; Florian Bonn; Michael Hecker; D  rte Becher; *Institute for Microbiology, Ernst Moritz Arndt University Greifswald, Greifswald, Germany*
- MP 537 **Annotation of the Domestic Pig Genome by Quantitative Proteomics;** Harald Marx^{1,2}; Hannes Hahne¹; Susanne Ulbrich³; Angelika Schnieke¹; Oswald Rottmann¹; Dmitriy Frishman¹; Bernhard Kuster¹; ¹TU Muenchen, Freising, Germany; ²University of Wisconsin, Madison, WI; ³ETH Zurich, Zurich, Switzerland
- MP 538 **Investigating the Effect of Estrogen on Renal Cell Carcinoma with Different VHL Genetic Backgrounds using Quantitative Proteomics;** Wei-Chi Ku¹; Chi-Jung Huang^{1,2}; Shao-Kuan Chen²; ¹Fu Jen Catholic University, New Taipei, Taiwan; ²Cathay General Hospital, Taipei, Taiwan
- MP 539 **IFIX is a Viral DNA Sensor Acting in Defense against Human DNA Viruses;** Marni Crow; Tuo Li; Benjamin Diner; Ileana M. Cristea; *Princeton University, Princeton, NJ*
- MP 540 **Drug-inducing Cell Death Mechanics is Rigid: A Proteomics Study;** Alexey Chernobrovkin¹; Consuelo Vicente²; Neus Visa²; Roman Zubarev¹; ¹Karolinska Institute, Stockholm, Sweden; ²Stockholm University, Stockholm, Sweden
- MP 541 **A Hybrid Virology-Proteomics Approach Defines the Mechanisms of Cellular Immune Response to Viral DNA;** Benjamin A. Diner; Tuo Li; Krystal K. Lum; Todd M. Greco; Marni S. Crow; Ileana M. Cristea; *Princeton University, Princeton, NJ*
- MP 542 **Global Proteomic Analysis of Ovarian High-Grade Serous Carcinomas using SWATH-MS for Targeted Verification of Proteome Changes Associated with Genomic Alterations;** Stefani Thomas; Paul Aiyetan; Li Chen; Zhen Zhang; Daniel Chan; Hui Zhang; *Johns Hopkins University, Baltimore, MD*
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- MP 543 **Proteomics Identifies Distinct Immunoglobulin Light Chain Variable Region Usage in Clinical Subsets of Amyloidosis;** Surendra Dasari¹; Jason D Theis¹; Julie Vrana¹; Ahmet Dogan²; Paul Kurtin¹; ¹Mayo Clinic, Rochester, MN; ²Memorial Sloan Kettering Cancer Center, New York, NY
- MP 544 **The Structure and Function of the Synaptic Proteome Vary by Sex, Neuropsychiatric Disease Diagnosis, and Brain Region;** Stephanie L. Willard¹; Anamika Banerjee¹; Ailin Cao¹; Karin E. Borgmann-Winter^{1,2}; Chang-Gyu Hahn¹; ¹University of Pennsylvania Dept of Psychiatry, Philadelphia, PA; ²Children's Hospital of Philadelphia, Philadelphia, PA
- MP 545 **Effect of Ion Mobility Measurements on the MS Analyses of Proteins Associated with Autoimmune Diseases;** Jeffrey F. Kuhn¹; Leesa Deterding²; ¹NIEHS/NIH/DHHS, Research Triangle Park, NC; ²NIEHS, RTP, NC
- MP 546 **Quantitative Measurements of a Specific Hydroxylated Collagen Peptide in Urine Improves the Detection of Colorectal Liver Metastases;** Nick Van Huijzen; Zarina Lalmahomed; Mirelle Broker; Robert Coebergh van den Braak; Jan IJzermans; Theo Luider; Lennard Dekker; *Erasmus Medical Center, Rotterdam, the Netherlands*
- MP 547 **Investigating the Contribution of Karyotype Changes to Multidrug Resistance using Quantitative Proteomics;** Lilian Kabeche^{1,2}; Andrew Grasseti^{1,2}; Mark Adamo¹; Scott Gerber^{1,2}; ¹Norris Cotton Cancer Center, Lebanon, New Hampshire; ²Geisel School of Medicine at Dartmouth, Hanover, NH
- MP 548 **The Function of Pathogenic Human Torsin A;** Jong Bok Seo; Soo Jeong Park; *Korea Basic Science Institute, Seoul, South Korea*
- MP 549 **Accurate Clinical Detection of Hemoglobin Variants via Combined Top-Down and Bottom-Up Proteomics;** Raymond Moore; Roman Zenka; Patricia Wendt; Kenneth Swanson; Jennifer Oliveira; James Hoyer; Surendra Dasari; *Mayo Clinic, Rochester, MN*
- MP 550 **Selective Proteomics Analysis Using Congo Red as a Precipitating Reagent;** Hongwu Jing¹; Irina A. Buhimschi^{2,3}; Guomao Zhao²; Michelle Axe⁴; Catalin S. Buhimschi³; Vicki Wysocki¹; ¹Dept. Chem. Biochem., The Ohio State University, Columbus, OH; ²Research Inst. at Nationwide Children's Hospital, Columbus, OH; ³Dept. OB/GYN, The Ohio State University, Columbus, OH; ⁴Dept. Biochem. Mol. Biol., Otterbein University, Westerville, OH
- MP 551 **Determination of EGFR and VEGF Signaling Pathway Activity by immuno-MALDI to Predict the Outcome of Targeted Colorectal Cancer (CRC) Treatment;** Robert Popp¹; Andrew Chambers¹; Adriana Aguilar-Mahecha²; Oliver P  tz³; Mark Basik²; Christoph Borchers^{1,2}; ¹UVic - Genome BC Proteomics Centre, Victoria, Canada; ²Jewish General Hospital, McGill University, Montreal, Canada; ³Natural and Medical Sciences Institute (NMI), Reutlingen, Germany
- MP 552 **Absolute Quantification of Proteins from Different Types of Dried Blood Spot (DBS) Cards using LC-MS/MS;** Jerome Vialaret¹; Christophe Hirtz¹; Karine Hirtz²; Alan Barnes⁴; Audrey Gabelle²; Sylvain Lehmann¹; ¹LBPC-IRB, CHU de Montpellier, Montpellier, France; ²Centre M  moire Ressources Recherche, Montpellier, France; ³Spot to Lab, Cap Om  ga, Montpellier, France; ⁴Shimadzu Research Laboratory, Manchester, UK

- MP 553 **From Venome to Syndrome: Using Mass Spectrometry to Understand the Correspondence of Rattlesnake Venom Composition and Clinical Symptoms of Snakebite**; William K. Hayes¹; Aaron Corbit¹; Sean P. Bush³; Eric C.K. Gren¹; Allen M. Cooper¹; Chip Cochran¹; Gerad A. Fox¹; Carl E. Person¹; Wayne Kelln¹; Kevin Kim²; Zachary Travis²; Ben D. Gardner¹; ¹Loma Linda University, Loma Linda, CA; ²La Sierra University, Riverside, CA; ³East Carolina University, Greenville, NC
- MP 554 **Quantitative Proteomic Discovery of Candidate Serum Biomarkers for Early Detection of Ovarian Cancer**; Matthew Russell^{1,4}; Michael Walker^{1,4}; Andrew Williamson¹; Aleksandra Gentry-Maharaj²; Andy Ryan²; Evangelia-Ourania Fourkala²; Phillip Humphries¹; Usha Menon²; Anthony Whetton¹; Ian Jacobs^{1,3}; Robert Graham¹; ¹University of Manchester, Manchester, UK; ²University College London, London, UK; ³University of New South Wales, Sydney, Australia
- MP 555 **Bottom-up Proteomic Analysis of Single HCT 116 Colon Carcinoma Multicellular Spheroids**; Peter Feist^{1,2}; Xin Liu¹; Liangliang Sun¹; Norman Dovichi¹; Amanda Hummon^{1,2}; ¹University of Notre Dame, Notre Dame, Indiana; ²Integrated Biomedical Sciences Program, Notre Dame, IN
- MP 556 **Zoledronic Acid Potentiates $\gamma\delta$ T-Cell Anti-Leukemic Activity in Patients Receiving $\alpha\beta$ + T and CD19+ Depleted Grafts from Haplo-Identical Donors**; Andrea Petretto¹; Irma Airoidi¹; Chiara Lavarello¹; Elvira Inglesse¹; Alice Bertaina²; Barbarella Lucarelli²; Alessia Zorzoli¹; Pietro Merli²; Giulia Barbarito²; Letizia Brescia²; Valentina Bertaina²; Giuseppe Milano²; Franco Locatelli²; ¹Institute Giannina Gaslini, Genoa, Italy; ²Bambino Gesù Children's Hospital, Rome, Italy
- MP 557 **Barcoding Primary Human B-cells via Analysis of Membrane Proteins on the Cell Surface**; Nicole A. Haverland¹; Matthew Waas²; Tim Toby¹; Ioanna Ntai¹; Rebekah Gundry²; Neil L. Kelleher¹; ¹Northwestern University, Evanston, IL; ²Medical College of Wisconsin, Milwaukee, WI
- MP 558 **Detecting Recombinant Insulin Drugs in Amyloid Plaques of Diabetes Patients using Shotgun Proteomics**; Jason D Theis; Surendra Dasari; Julie Vrana; Roman Zenka; Paul Kurtin; *Mayo Clinic, Rochester, MN*
- MP 559 **Nanomaterial Based Sub-Proteome Selection for Analysis of the Activation State Of Macrophages**; Arnaud Millet; Magali Court; Adrien Mombrun; Vera Aiello; Frederic-Xavier Gaillard; Francois Berger; Ali Bouamrani; *Grenoble, France*
- MP 560 **The Associations between Enterovirus Infections and Type 1 Diabetes**; Niina Lietzen¹; Sami Oikarinen²; Young Ah Goo³; David Goodlett³; Jorma Toppari¹; Jorma Ilonen¹; Riitta Veijola⁴; Mikael Knip^{5,6}; Heikki Hyöty²; Riitta Lahesmaa¹; ¹University of Turku, Turku, Finland; ²University of Tampere, Tampere, Finland; ³University of Maryland, Baltimore, Maryland; ⁴University of Oulu, Oulu, Finland; ⁵Children's Hospital, University of Helsinki, Helsinki, Finland; ⁶Helsinki University Central Hospital, Helsinki, Finland
- MP 561 **Measuring Minimum Residual Disease in Multiple Myeloma by LC-MS/MS: A comparison to Multicolor Flow Cytometry**; H. Robert Bergen, III¹; Angela Dispenzieri¹; John Mills²; David Barnidge²; David Murray²; ¹Mayo Clinic, Rochester, MN; ²Mayo Clinic / DLMP, Rochester, MN
- MP 562 **Diagnostic Accuracy for Proteomic Cancer Markers in the Face of Autoantibodies: Can We Assume Trypsin Does All the Work?** Christopher Shuford; Patricia Holland; Russell Grant; *Laboratory Corporation of America, Burlington, NC*
- MP 563 **Mass Spectrometry-based Phosphoproteomics for the Identification of Phosphorylation Signaling Pathways in Chronic Lymphocytic Leukemia (CLL)**; Stephen Swatkoski; Sarah Herman; Deanna Wong; Adrian Wiestner; Marjan Gucek; *-NIH/NHLBI, Bethesda, MD*
- MP 564 **Tandem MS/MS with Isotope Dilution Identifies a Cluster of Proteins Implicated in Kidney Disease in HDL of Hemodialysis Subjects**; Baohai Shao; Ian de Boer; Philip S. Mayer; Leila Zelnick; Maryam Afkarian; Jay W. Heinecke; Jonathan Himmelfarb; *University of Washington, Seattle, WA*
- MP 565 **Ultrasensitive Tissue Proteomics using an Enhanced Workflow with Para-Magnetic Beads for Clinical Proteomics Research Applications**; Christopher Hughes; Melissa McConechy; David Huntsman; Gregg Morin; *British Columbia Cancer Agency, Vancouver, BC*
- MP 566 **Mass Spectrometry Based Study of Human Body Adaptation during the Space-flight and MARS 105 Days Isolation Experiment**; Irina Larina¹; Alexey Kononikhin^{2,5}; Lyudmila Pastushkova¹; Igor Popov^{4,5}; Alexander Bzhozovskiy¹; Igor Dobrokhotov¹; Evgeny Tiys³; Vladimir Ivanisenko³; Eugene Nikolaev^{2,6}; ¹Institute of Biomedical Problems RAS, Moscow, Russia; ²Institute for Energy Problems of Chemical Physics, Moscow, Russia; ³Institute of Cytology and Genetics SB RAS, Novosibirsk, Russia; ⁴Emanuel Institute of Biochemical Physics, Moscow, Russia; ⁵Moscow Institute of Physics and Technology, Moscow, Russia; ⁶Skolkovo Institute of Science and Technology, Skolkovo, Russia
- MP 567 **Differential Proteomic Analysis of Human Saliva using Tandem Mass Tags for Gastric Cancer Detection**; Hua Xiao¹; David T.W. Wong²; ¹Shanghai Jiao Tong University, Shanghai, China; ²UCLA, CA
- MP 568 **Single Point Calibrator for Protein Quantification in Formalin-Fixed Paraffin Embedded Tissues**; Han-Yin Yang¹; James G. Bollinger¹; Ying Sonia Ting¹; Christine Wu²; Andrew Hoofnagle¹; Michael J. Maccoss¹; ¹University of Washington, Seattle, WA; ²Stratus Biosciences, Seattle, WA
- MP 569 **Developing a Robust Urine UMOD and Albumin Assay By Liquid Chromatography-Targeted Mass Spectrometry**; Qin Fu¹; Eric Grote²; Jie Zhu²; Christine Jelinek³; Josef Coresh⁴; Jennifer Van Eyk¹; ¹Cedars Sinai Medical Center, Los Angeles, CA; ²Johns Hopkins University, Baltimore, MD; ³Johns Hopkins School of Medicine, Baltimore, MD; ⁴Johns Hopkins Bloomberg School of Public Health, Baltimore, MD

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- MP 571 **Automation Enables Highly Reproducible Phosphopeptide Enrichment from Complex Mixtures by IMAC using High-Capacity Fe(III)-NTA Microchromatography Cartridges**; Jason Russell; Steve Murphy; *Agilent Technologies, Inc., Madison, WI*
- MP 572 **Spatial Extraction and Enrichment of Phosphopeptides from Tissues using Hydrogels Containing Metal Ion-functionalized Nanopolymers**; M. Lisa Manier; Jamie Wenke; Jeremy L. Norris; Kevin L. Schey; Richard Caprioli; *Vanderbilt University, Nashville, TN*
- MP 573 **Single Shot Phosphoproteomics**; Alex Hebert; Nicholas Kwiecien; Alicia Richards; Anna Merrill; Michael S. Westphall; Joshua J. Coon; *University of Wisconsin-Madison, Madison, WI*

- MP 574 **Enrichment of Phosphorylated Peptides using Polymeric Reverse Micelles for MALDI-MS Analysis;** Meizhe Wang; Bo Zhao; Mijanur Rahaman; Sankaran Thayumanavan; Richard Vachet; *University of Massachusetts Amherst, Amherst, MA*
- MP 575 **In-Depth Phosphoproteome Analysis in *E. coli* Using High-pH Reversed-Phase and TiO₂ Chromatography;** Gerhard Saalbach¹; Sivaramesh Wigneshwararaj²; Rita Figueira²; ¹*John Innes Centre, Norwich, UK*; ²*Imperial College, London, UK*
- MP 576 **PTM- and Protein-Based Proteome Profiling of Drug Response in Human Gastric Carcinoma Cells using Antibody-Based and Metal Affinity-Based Phosphopeptide Enrichment;** Matthew P. Stokes¹; Charles L. Farnsworth¹; Hongbo Gu¹; Jian Min Ren¹; Vicky Yang¹; Camilla R. Worsfold²; Kimberly A. Lee¹; Jeffrey C. Silva¹; ¹*Cell Signaling Technology, Danvers, MA*; ²*Emory University, Atlanta, GA*
- MP 577 **Investigation of Changes in Protein Phosphorylation During Cell Differentiation: Combined Extraction-Fractionation at High pH to Facilitate Phosphopeptide Isolation;** Alice Harnacke^{1,2}; Wolfgang Fischer¹; ¹*The Salk Institute, La Jolla, CA*; ²*University of Freiburg, Freiburg, Germany*
- MP 578 **StageTip-based IMAC for Rapid and Deep Phosphoproteomic Typing in One-Shot LC-MS/MS Analysis;** Chia-Feng Tsai; Yi-Ting Wang; Miao-Hsia Lin; Pei-Yi Lin; Yu-Ju Chen; *Academia Sinica, Taipei, Taiwan*
- MP 579 **Comparing Multi-Step IMAC and Multi-Step TiO₂ Methods for Phosphopeptide Enrichment;** Xiaoshan Yue; Amanda B. Hummon; *University of Notre Dame, Notre Dame, IN*
- MP 580 **Tyrosine Phosphorylation Profiling and Phosphoproteome Mapping of Three Mouse Tissues;** Ling Zhong; Mark Raftery; *UNSW, Sydney, Australia*
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- MP 581 **Automated Structural Characterization of Intact N- and O-linked Glycopeptide using a Orbitrap Fusion Tribrid Mass Spectrometer;** Chein-Hung Chen; Ya-Ping Lin; Fang-Chi Liu; Chi-Lin Wu; Jung-Lee Lin; Chung-Hsuan Chen; *Academia Sinica, Taipei, Taiwan*
- MP 582 **Glycan Composition and Charge State Influence upon Collision Cross Sections of High Mannose N-Linked Glycopeptides;** Abby S. Gelb; Eric D. Dodds; *University of Nebraska - Lincoln, Lincoln, NE*
- MP 583 **Glycoproteomic and Proteomic Analyses of Hearts from Hypertrophic Cardiomyopathy Mice;** Shuang Yang¹; Sumita Mishra²; Lijun Chen¹; Jian-Ying Zhou¹; Yuri Poluektov¹; Daniel W. Chan¹; Subroto Chatterjee²; Hui Zhang¹; ¹*John Hopkins Dept. of Pathology, Baltimore, MD*; ²*Department of Pediatrics, Johns Hopkins University, Baltimore, MD*
- MP 584 **Effects of Charge Carrier and Composition on the Energy-Resolved Collision-Induced Dissociation of Tryptic N-Glycopeptides;** Forouzan Aboufazel; Venkata Kolli; Abby S. Gelb; Eric D. Dodds; *University of Nebraska - Lincoln, Lincoln, NE*
- MP 585 **Improving the ETD Performance of Glycopeptides through Chemical Charge Enhancement;** William Alley; Yanyan Qu; Rebecca Sosa; *University of Texas at San Antonio, San Antonio, TX*
- MP 586 **High-Throughput Profiling of Protein N-Glycosylation by MALDI-TOF-MS Employing Linkage-Specific Sialic Acid Esterification;** Karli Reiding¹; Dennis Blank¹; Dennis Kuijper²; André Deelder¹; Manfred Wuhrer^{1,2}; ¹*Leiden University Medical Center, Leiden, Netherlands*; ²*VU University, Amsterdam, Netherlands*
- MP 587 **Analysis of Site-specific N/O-Glycosylation of Targeted Proteins;** Shu-Hui Chen; *National Cheng Kung University, Tainan, Taiwan*
- MP 588 **O-linked Glycopeptide Analysis via Negative Electron Transfer Dissociation;** Nicholas M. Riley¹; Nichollas E. Scott²; Mario F. Feldman³; Michael S. Westphall¹; Joshua J. Coon¹; ¹*University of Wisconsin, Madison, Wisconsin*; ²*Center for High-Throughput for Biology, UBC, Vancouver, Canada*; ³*Alberta Glycomics Centre, Dept. of Biology, Edmonton, Canada*
- MP 589 **Characterization of Intact Prostate Specific Antigen (PSA) and Its Glycoforms by CESI-MS under Native and Denaturing Conditions;** Marcia R. Santos¹; Chitra K. Ratnayake¹; David M. Horn²; Barry L. Karger³; Alexander R. Ivanov³; Rosa I. Viner²; ¹*Scienc, Brea, CA*; ²*Thermo Fisher Scientific, San Jose, CA*; ³*Northeastern University, Boston, MA*
- MP 590 **N-glycan Analysis: Combining the Power of a Novel Glycan Label and Customized Scientific Library for Confident Glycan Assignment;** Mark Hilliard¹; Niaobh McLoughlin¹; Pauline Rudd¹; Ying Qing Yu²; ¹*NIBRT, Dublin, Ireland*; ²*Waters Waters Corporation, Milford, MA*
- MP 591 **Highly Specific Enrichment of N-glycoproteome through Nonreductive Amination Reaction using Fe₃O₄@SiO₂-Aniline Nanoparticles;** Ying Zhang; Liqi Xie; Haojie Lu; *Fudan University, Shanghai, China*
- MP 592 **Glycosylation Patterns on HIV-1 Envelope Glycoprotein and Its Structural Implications;** Audra Laube¹; Milan Raska^{1,2}; Qing Wei¹; Barbora Knoppova²; Stacy Hall¹; Katerina Zachova²; Zhi-Qiang Huang¹; Zina Moldoveanu¹; Jan Novak¹; Matthew Renfrow¹; ¹*University of Alabama at Birmingham, Birmingham, AL*; ²*Palacky University in Olomouc, Olomouc, Czech Republic*
- MP 593 **In-planta Deglycosylation and Mass Spectrometry;** Ranjith Munigunt; Lindsay Bennett; Brian Berquist; Vally Komminen; Earl White; Sylvain Marcel; *Caliber Biotherapeutics, Bryan, TX*
- MP 594 **Site-specific N- and O-glycosylation Analysis of Human IgG3 Assisted by Integrated C18-PGC-LC-ESI-MS/MS Analysis;** Kathrin Stavenhagen¹; Rosina Plomp²; Gillian Dekkers³; Yoann Rombouts^{2,4}; Paul J. Hensbergen²; Gestur Vidarsson³; Manfred Wuhrer^{1,2}; ¹*BioAnalytical Chemistry, VU University Amsterdam, Amsterdam, The Netherlands*; ²*CPM, Leiden University Medical Center, Leiden, The Netherlands*; ³*Sanquin Research and Academic Medical Center, Amsterdam, The Netherlands*; ⁴*Dep. Rheumatology, Leiden University Medical Center, Leiden, The Netherlands*
- MP 595 **An Improved Workflow using Rapid PNGase F to Quickly Deglycosylate IgG for Accurate N-glycan Analysis;** Paula Magnelli; Beth McLeod; Colleen McClung; Rengpeng Liu; Alicia Bielik; Ellen Guthrie; *New England Biolabs, Ipswich, MA*
- MP 596 **High-Throughput Electron Capture Dissociation Mass Spectrometry in A Novel Branched Radio-Frequency Ion-Trap as a Platform for Glycoproteomics;** St John Skilton; J.C. Yves Leblanc; Takashi Baba; James Hager; J. Larry Campbell; *SCIEX, Concord, On, Canada*
- MP 597 **Development of a Novel Work Flow for the Enrichment of Glycated Peptides from Complex Matrices;** Sara Eun Lendal; Johannes Graumann; *Weill Cornell Medical College in Qatar, Doha, Qatar*
- MP 598 **Glycosylation of Vascular Endothelial Growth Factor Receptor 2 (VEGFR-2) in Angiogenesis;** Kevin Brown Chandler; Nader Rahimi; Catherine E Costello; *Boston University School of Medicine, Boston, MA*
- MP 599 **Site-specific Quantification of the Surface N-Sialoglycoproteome in Cancer Cells with Distinctive Invasiveness;** Weixuan Chen; Johanna Smeekens; Ronghu Wu; *Georgia Tech, Atlanta, GA*

- MP 600 **Rapid Preparation of Released N-Glycans for HILIC Analysis Using a Novel Fluorescence and MS-Active Labeling Reagent;** [Matthew Lauber](#)¹; Ying-Qing Yu¹; Darryl Brousmiche¹; Jeffrey Thomson²; Seamus O'Connor²; Zhengmao Hua¹; Stephan Koza¹; Paula Magnelli³; Ellen Guthrie³; Chris Taron³; Kenneth Fountain¹; ¹Waters Corporation, Milford, MA; ²Regeneron Pharmaceuticals, Rensselaer, NY; ³New England Biolabs, Ipswich, MA
- MP 601 **Site-Specific N-glycoform Analysis of Human Alpha-1-Acid Glycoprotein: Towards an Integrated Approach for Complete Molecular Characterization;** [Katherine N. Schumacher](#); Eric D. Dodds; *University of Nebraska - Lincoln, Lincoln, NE*
- MP 602 **A Novel Quantitative Mass Spectrometry Platform for Determining Site-Specific Protein O-GlcNAcylation Dynamics;** [Xiaoshi Wang](#)¹; Zuo-Fei Yuan¹; Jing Fan²; John M. Denu²; Benjamin A. Garcia¹; ¹University of Pennsylvania, Philadelphia, PA; ²University of Wisconsin-Madison, Madison, WI
- MP 603 **A Systematic Investigation of CID Q-TOF-MS/MS Collision Energies to Improve N- and O-glycopeptide Identification by LC-MS/MS;** Hannes Hinneburg^{1,2}; Kathrin Stavenhagen³; Ulrike Schweiger-Hufnagel⁴; Dirk Wunderlich⁴; Stuart Pengelley⁴; [Arndt Asperger](#)⁴; Wolfgang Jabs⁴; Peter H. Seeberger^{1,2}; Daniel Varón Silva¹; Manfred Wuhrer³; Daniel Kolarich¹; ¹Max-Planck-Institute of Colloids and Interfaces, Potsdam, Germany; ²Free University Berlin, Berlin, Germany; ³VU University Amsterdam, Amsterdam, Netherlands; ⁴Bruker, Bremen, Germany
- MP 604 **Glycoprofiling by HILIC-FLR-MSⁿ of Procainamide-Labeled Glycans;** [Brian C. Gau](#); Benjamin Cutak; Kevin Ray; *Sigma-Aldrich, St. Louis, MO*
- MP 605 **Parallel Data Acquisition of In-source Fragmented Glycopeptides to Characterize the Peptide Backbones and Glycan Structures;** [Jingfu Zhao](#); Ehwang Song; Yehia Mechref; *Texas Tech University, Lubbock, Texas*
- SYSTEMS BIOLOGY: PROTEOMICS**
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- MP 606 **Comprehensive Characterization of the Differentiation of Human Embryonic Stem Cells into Mesenchymal Stem Cells;** [Anja M Billing](#); Shaima S Dib; Hisham Ben-Hamidane; Aditya M Bhagwat; Shahina Hayat; Pankaj Kumar; Rasha Al-Mismar; Neha Goswami; Karsten Suhre; Arash Rafii; Johannes Graumann; *Weill Cornell Medical College in Qatar, Doha, Qatar*
- MP 607 **Subcellular Trafficking of Cholera Toxin Revealed by Proteome-wide Dose Response Time Course Profiling;** [Christoher Ebmeier](#); Tristan McClure-Begley; Douglas Chapnick; Xuedong Liu; William Old; *University of Colorado, Boulder, CO*
- MP 608 **Regulation of the Primary Human Trophoblast Cell Secretome by Mechanistic Target of Rapamycin (mTOR) Signaling;** [Susan T. Weintraub](#)¹; Frederick Rosario²; Sammy Pardo¹; Thomas Jansson²; ¹Univ. of Texas Health Science Center, San Antonio, TX; ²Univ. of Colorado Denver Anschutz Med. Campus, Aurora, CO
- MP 609 **The Nuclear Proteome of a Vertebrate;** [Martin Wühr](#); Thomas Güttler; Leonid Peshkin; Graeme Mcalister; Matthew Sonnett; Aaron C. Groen; Marc Presler; Brian Erickson; Timothy J. Mitchison; Marc W. Kirschner; Steven Gygi; *Harvard Medical School, Boston, MA*
- MP 610 **Chemical and Computational Approaches to Integrate Redox Signaling in the Study of Systems Biology;** Nelmi O. Devarie-Baez; Zhiwei Ji; Elsa Silva-Lopez; Jade Mims; Xiaofei Chen; Allen W. Tsang; Xiaobo Zhou; [Cristina M. Furdui](#); *Wake Forest School of Medicine, Winston-Salem, NC*
- MP 611 **The Dynamic Phosphoproteome of Peripheral Nerve Injury and Chronic Pain;** [Christopher B. Lietz](#)¹; Dana M. Tilley²; Courtney Kelley²; Ricardo Vallejo²; Ramsin Benyamin²; Joseph Williams³; David L. Cedeño^{2,3}; Lingjun Li¹; ¹University of Wisconsin, Madison, WI; ²Millennium Pain Center, Bloomington, IL; ³Illinois Wesleyan University, Bloomington, IL
- MP 612 **Phosphoproteomic Analysis of Signal Integration in Cancer;** [Robert Lawrence](#); Judit Villén; *University of Washington, Seattle, WA*
- MP 613 **Targeted Proteomics-Driven Computational Modeling of Macrophage S1P Chemosensing;** [Nathan Manes](#)¹; Bastian Angermann¹; Eunkyung An¹; Virginie Sjoelund¹; Jing Sun¹; Masaru Ishii²; Ronald Germain¹; Martin Meier-Schellersheim¹; Aleksandra Nita-Lazar¹; ¹NIH, Bethesda, MD; ²Osaka University, Osaka, Japan
- MP 614 **Proteomic and Phosphoproteomic Characterization of Breast Cancer Progression in MCF10A Model Cell-line;** [Hongjie Pan](#); Harsha P. Gunawardena; Xian Chen; *University of North Carolina at Chapel Hill, Chapel Hill, NC*
- MP 615 **Kinase Profiling, Expression Proteomics, and Phosphoproteomics Reveal Adaptive Signaling in Melanoma after Targeted Therapy;** [Ritin Sharma](#)¹; Inna Fedorenko¹; Bin Fang¹; David Britton²; Sasa Koncarevic²; Gitte Boehm²; Ian Pike²; Keiran Smalley¹; John Koomen¹; ¹H. Lee Moffitt Cancer Center & Research Institute, Tampa, FL; ²Proteome Sciences PLC, Surrey, UK
- MP 616 **Deep Proteomic and Phosphoproteomic Profiling Reveals Different Gliomagenesis Mechanism between Two Pediatric High-grade Glioma Subtypes;** [Hong Wang](#)^{1,2}; Tim Shaw¹; Xusheng Wang¹; Yuxin Li¹; Ji-Hoon cho¹; Barbara Paugh¹; Alex Diaz^{1,2}; Yanling Yang¹; Zhiping Wu¹; Haiyan Tan¹; Bing Bai¹; Anthony High¹; Vishwajeeth Pagala¹; Suzanne Baker^{1,2}; Junmin Peng^{1,2}; ¹St Jude Children's Research Hospital, Memphis, TN; ²University of Tennessee Health Science Center, Memphis, TN
- MP 617 **Global and Targeted Quantification of Seven Human Cell Lines Reveals the Correlation of Cell Type-Specific Responses with Feedback Regulators ;** Tujin Shi¹; Yuqian Gao¹; Matthew Gaffrey¹; William Chrisler¹; Thomas Fillmore¹; Carrie Nicora¹; Meng Markillie¹; karin rodland¹; Jason McDermott¹; Mario Niepel²; Peter Sorger²; Richard Smith¹; Steven Wiley¹; [Wei-Jun Qian](#)¹; ¹Pacific Northwest National Lab, Richland, WA; ²Harvard Medical School, Boston, MA
- MP 618 **Metaproteomics Based on SWATH-MS Approach to Analyse a Complex Synthetic Microbial Community;** [Mélanie Béraud](#); giuseppe giambarresi; David Gillan; [Ruddy Wattiez](#); *Dept of Proteomic and Microbiology, UMONS, Mons, Belgium*
- MP 619 **PhosphoPath; Visualization of Phosphosite Specific Dynamics in Molecular Network Analysis of Large Phosphoproteomic Datasets;** [Linsey Raaijmakers](#)¹; Piero Giansanti¹; Patricia A. Possik²; Judith Mueller²; Daniel S. Peeper²; Albert J.R. Heck¹; A.F. Maarten Altelaar¹; ¹Utrecht University, Utrecht, Netherlands; ²Netherlands Cancer Institute, Amsterdam, Netherlands
- MP 620 **Monitoring Protein-Protein Interactions in Live Cells with a Wide Scope by Rapid Photo-Activated Cross-Linking and LC-MS/MS;** [Anthony Persechini](#)¹; Boris Kornilayev¹; Andrew Keightley¹; Paul M Stemmer²; ¹Univ Missouri-Kansas City, Kansas City, MO; ²Wayne State University, Detroit, MI
- MP 621 **Probing Paradoxical Effects of RAF Inhibition by Dynamic Phosphoproteomics;** [Peter Kubiniok](#); H. Lavoie; M. Therrien; P. Thibault; *Universite de Montreal, Montreal, Canada*

- MP 622 **Quantitative Proteomic and Systems Analysis of Human Immune Cells in Response to Adjuvanted Influenza Vaccine**; [Allison Galassie](#)¹; Parimal Samir²; Andrew Link^{1,2}; ¹Vanderbilt University, Nashville, TN Tennessee; ²Vanderbilt University School of Medicine, Nashville, TN
- MP 623 **Global Analysis of Protein Folding Thermodynamics for the Characterization of Disease States**; Jagat Adhikari¹; Graham West^{2,3}; [Michael C. Fitzgerald](#)¹; ¹Duke University, Durham, NC; ²The Scripps Research Institute, Jupiter, FL; ³Current Address: Pfizer, Inc, Groton, CT
- MP 624 **Pharmacoproteomic Analysis of the Resveratrol and DMSO**; Tanya Porras-Yakushi; Michael J Sweredoski; [Sonja Hess](#); Caltech, Pasadena, CA
- MP 625 **Protease Inhibitors PZP and α2MG as Biochemical Keys to Find Unknown Mechanisms of Alzheimer's Disease**; [Diana Nijholt](#); Peter Koudstaal; Arfan Ikram; Peter Sillevius-Smitt; Theo Luider; Erasmus Medical Centre, Rotterdam, The Netherlands
- MP 626 **A Systems Biology Approach for the Investigation of the Mechanism of Action of the Neurotrophic Drug Cerebrolysin**; [Florian Füssl](#)¹; Stefan Winter²; Christian Huber¹; ¹University of Salzburg, Salzburg, Austria; ²Ever Neuro Pharma GmbH, Unterach, Austria
- MP 627 **Defining the Physical Interactome of the Active Kinome from the Intrinsic Subtypes of Human Breast Cancer**; [Matthew R. Meyer](#)¹; Jing Wang³; Kelly V. Ruggles⁴; Petra Erdmann-Gilmore¹; Jeanne Rumsey¹; Robert Kitchens¹; Jacqueline Snider¹; Jeremy Hoog¹; Shunqiang Li¹; Sherri R. Davies¹; Matthew J. Ellis²; David Fenyö⁴; Bing Zhang³; Gary L. Johnson⁵; R. Reid Townsend¹; ¹Washington University School of Medicine, St. Louis, MO; ²Baylor College of Medicine, Houston, TX; ³Vanderbilt University, Nashville, TN; ⁴New York University, New York, NY; ⁵University of North Carolina, Chapel Hill, NC
- SYSTEMS BIOLOGY: OTHER**
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- MP 628 **Integrated Proteomics and Metabolomics Reveal Molecular Mechanism of Symbiotic Relationship between Fungal *Mortierella elongata* and Bacterial Endosymbiont *C. Glomeribacter* sp.**; [Zhou Li](#)¹; Stephen Dearth²; Qiuming Yao¹; Jessie Uehling³; Hector Castro-Gonzalez²; Shawn Campagna²; Gregory Hurst¹; Jessy Labbé¹; Chongle Pan¹; ¹Oak Ridge National Laboratory, Oak Ridge, TN; ²University of Tennessee, Knoxville, TN; ³Duke University, Durham, NC
- MP 629 **Discovering Metabolic Dynamics and Regulation by Real-Time Mass Spectrometry**; [Tobias Fuhrer](#)¹; Hannes Link²; Andreas Kühne¹; Uwe Sauer¹; Nicola Zamboni¹; ¹Institute of Molecular Systems Biology, ETH Zürich, Zürich, Switzerland; ²Max Planck Institute for Terrestrial Microbiology, Marburg, Germany
- MP 630 **LC-MS/MS Characterization of the Microbiome Stability in Post-Surgery Crohn's Disease Patients**; [J. Alfredo Blakeley-Ruiz](#)^{1,2}; Weili Xiong^{1,2}; Robert Hettich¹; ¹Oak Ridge National Laboratory, Oak Ridge, TN; ²University of Tennessee, Knoxville, TN
- MP 631 **Studies of Heart Regeneration in Zebrafish: A Multi-Omics/System Biology Approach**; [Leanne C. Nye](#)¹; Lee Gethings²; Cheng Shuk Han³; Yun Wah Lam³; Fatemeh Babaei³; Chi Chi Liu³; Alfred W. H. Chan³; Robert Plumb⁴; Ian D. Wilson¹; ¹Imperial College, London, UK; ²Waters Corporation, Wilmslow, UK; ³City University, Hong Kong, Hong Kong; ⁴Waters, Milford, MA
- MP 632 **Systematic Identification of the Lysine Succinylation in the Protozoan Parasite *Toxoplasma gondii***; [Xiaolong Li](#)²; Di Che³; Zhongyi Cheng¹; Xingling Yi¹; Feng Tan³; ¹PTM Biolabs, Inc, Hangzhou, China; ²The First Affiliated Hospital of Wenzhou Medical U, Wenzhou, CN; ³Wenzhou Medical University, Wenzhou, CN
- MP 633 **Systematic Integration Of "Omics" Data To Improve Innovation In Beer**; [Barbara Dunn](#)¹; Dan Kvitck²; Xiaoyue Jiang³; Daniel Lopez Ferrer³; Gina Tan³; Andreas Huhmer³; ¹Dept. of Genetics, Stanford University, Palo Alto, CA; ²Invitae, San Francisco, CA; ³Thermo Fisher Scientific, San Jose, CA
- MP 634 **LOPIT Proteomics Reveals Proteome-Wide Relocalisation upon Nitrogen Starvation in Yeast**; [Daniel J. H. Nightingale](#)¹; Duygu Dikicioglu²; Stephen G. Oliver²; Kathryn S. Lilley¹; ¹Cambridge Centre for Proteomics, Cambridge, UK; ²Cambridge Systems Biology Centre, Cambridge, UK
- MP 635 **Quantitative SWATH Proteomics Analysis of Tree-Fungal Interactions under Nutrient Limiting Conditions**; [Landon Wilson](#)¹; Geetika Trivedi²; Avinash Sreedasyam³; Helen Kim¹; Xiangqin Cui¹; Leland J Cseke²; Stephen Barnes¹; ¹University of Alabama at Birmingham, Birmingham, AL; ²University of Alabama in Huntsville, Huntsville, AL; ³HudsonAlpha Institute for Biotechnology, Huntsville, AL
- MP 636 **Towards High-Throughput Analysis of Salmonella Serotypes: A Fundamental Look at Protein Profiles, Proteomes and Secretomes of Salmonella typhimurium and enteritidis**; [Amornmart Jararungtawe](#)¹; Jaran Jainhuknan¹; Saw Yen Ow²; Onrapak Reamtong³; Tipparat Thiangtrongjit³; Yuphakhun Chaturongkasumrit⁴; Mongkol Vesaratchavest⁴; ¹Brucker Corporation, Bangkok, Thailand; ²Brucker Corporation, Kuala Lumpur, Malaysia; ³Mahidol University, Bangkok, Thailand; ⁴Research and Development Center, Betagro Group, Bangkok, Thailand
- MP 637 **Enhanced Informatics Methods for Integrating Metagenome and Metaproteome Information for the Pre-term Human Gut Microbiome**; [Robert Hettich](#)¹; Weili Xiong^{1,2}; Alison Erickson¹; J.J. Chai¹; Chongle Pan¹; ¹Oak Ridge National Laboratory, Oak Ridge, TN; ²University of Tennessee, Knoxville, TN
- MP 638 **Quantitative Proteomic Analysis Reveals Environmental Interaction and Epistasis in the Responses to Complex Stimuli in *Saccharomyces cerevisiae***; [Parimal Samir](#)¹; Rahul²; Andrew Link¹; ¹Vanderbilt University School of Medicine, Nashville, TN; ²University of Waterloo, Waterloo, Canada
- MP 639 **Proteome-in-motion: Deep Study of Protein Dynamics and Regulation in Yeast Proliferating Cells**; [Miguel Martin Perez](#); Judit Villen; University of Washington, Seattle, WA
- MP 640 **Comprehensive Quantitation of 1,000 Proteomes**; [Alicia L. Richards](#); Alexander S. Hebert; Jonathan A. Stefely; Elyse C. Freiburger; Nicholas W. Kwiecien; Adam Jochem; Xiao Guo; Michael S. Westphall; David J. Pagliarini; Joshua J. Coon; University of Wisconsin, Madison, WI
- MP 641 **Proteomic Visualization of Nanoparticle Cellular Entry Pathways**; [Linna Wang](#); Li Yang; Naveen Kadasala; Li Pan; Alexander Wei; Weiguo Andy Tao; Purdue University, West Lafayette, IN
- ENERGY: HYDROCARBON AND PETROCHEMICAL**
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- MP 642 **Correlation of Boiling Point, Molecular Weight and Composition by Mass Spectrometry: The Development of Class Dependent Equations**; [Yuri E. Corilo](#)^{1,2}; Priscila M. Lalli²; Steven M. Rowland²; Logan C. Krajewski¹; Alan G. Marshall^{1,3}; Ryan P. Rodgers¹; ¹National High Magnetic Field Laboratory, FSU, Tallahassee, FL; ²Future Fuels Institute, FSU, Tallahassee, FL; ³Department of Chemistry and Biochemistry, FSU, Tallahassee, FL
- MP 643 **Structural Identification of Naphthyl Compounds in 2,6-naphthalenedicarboxylic Acid by UPLC-QTOF Tandem Mass Spectrometry**; [Junyan Liu](#); Liyan Jiang; Sinopec Shanghai Research Institute of Petrochemical, Shanghai, China



- MP 644 **Probing Nanoaggregation of Asphaltene Model Compound using Electropray Ionization Mass Spectrometry**; Lan Liu¹; Johan Sjöblom²; Zhenghe Xu¹; ¹University of Alberta, Edmonton, Canada; ²Norwegian University of Science and Technology, Trondheim, Norway
- MP 645 **Comprehensive Characterization of Petroleum – Crude Oil, Asphaltenes and Sulfur Compounds**; Jeffrey Patrick; Joe Binkley; Jonathan Byer; Clécio Klitzke; *LECO Corporation, St. Joseph, MI*
- MP 646 **Characterization of Semi-Synthetic Motor Oil using FT-ICR**; Sung Hwan Yoon; David Goodlett; David Kilgour; *University of Maryland, Baltimore, MD*
- MP 647 **Study of Asphaltene Adsorption on Mineral Surfaces by High-Resolution Mass Spectrometry**; Martha Chacón-Patiño¹; José J. Villarreal¹; Andrea Gomez-Escudero²; Jorge A. Orrego-Ruiz²; Cristian Blanco-Tirado¹; Marianny Y. Combariza¹; ¹UIS, Bucaramanga, Colombia; ²ECOPETROL, Piedecuesta Santander
- MP 648 **Identification of Challenging Components in Complex Hydrocarbon Mixtures using High Resolution GC/Q-TOF with an Innovative EI Source**; Pierre Giusti¹; Sabrina Marceau¹; Benoit Paupy¹; Sofia Nieto²; Mingda Wang²; Harry Prest²; ¹TOTAL Refining and Chemicals, TRTG, Gonfreville l'Orcher, France; ²Agilent Technologies, Inc., Santa Clara, CA
- MP 649 **MS/MS of Aromatic Surfactants, Structure Determination of Mixture by Charge Remote Fragmentation at High Resolving Power**; Michael T. Cheng¹; Matthew Hurt²; ¹Chevron Research, Richmond, CA; ²Chevron, Richmond, CA
- MP 650 **Application of Design of Experiment (DOE) and Optimization by Atmospheric Pressure Photoionization (APPI) Source Parameters for Studies in Petroleomics**; Jandyson Machado Santos¹; Marcos A. Pudenzi¹; Eduardo M. Schmidt¹; Heliara D. L. Nascimento¹; Alberto Wisniewski Jr.²; Marcos N. Eberlin¹; ¹University of Campinas, Campinas, SP; ²Federal University of Sergipe, São Cristóvão, SE
- MP 651 **Supercritical Fluid Chromatography Coupled with Ion Mobility-Mass Spectrometry for Comprehensive Profiling of Petroleum Samples**; Eleanor Riches¹; Yunju Cho²; Sunghwan Kim²; ¹Waters Corporation, Wilmslow, UK; ²Chemistry Department, Kyungpook National University, Daegu, South Korea
- MP 652 **Characterization of Heteroatom-Containing Species in Lignite with Orbitrap Mass Spectrometry and Statistical Analysis**; Lu Chen; Xing Fan; Chun-Yan You; Xian-Yong Wei; Yun-Peng Zhao; Jun-Liu Xia; Miao Wang; *China University of Mining & Technology, Xuzhou, China*
- MP 653 **Analysis of Dibenzothiophenes in Diesel by GC-APCI Ion Mobility High Resolution Mass Spectrometry**; Sheher Bano Mohsin¹; David Wong²; Robert Ley²; ¹Agilent Technologies, Schaumburg, IL; ²Agilent Technologies, Inc., Santa Clara, CA
- MP 654 **Standard Compounds Analysis as a Tool for the Establishment of Ionization/Intrinsic Characteristics Relationship on Crude Oil Polar Compounds**; Marcos Albieri Pudenzi¹; Clécio Fernando Klitzke¹; Vanessa Gonçalves Santos¹; Heliara D. Lopes Nascimento¹; Pedro Henrique Vendramini¹; Eduardo Morgado Schmidt¹; Rosana Cardoso Lopes Pereira²; Wagner Leonel Bastos²; Marcos Nogueira Eberlin¹; ¹Unicamp, Campinas, Brasil; ²CENPES, PETROBRAS, Rio de Janeiro, RJ - Brasil
- MP 655 **Application of Molecular Dynamic Simulation for More Accurate CCS Calculations of Aromatic Compounds with Long Alkyl Chains**; Arif Ahmed¹; Dongwan Lim¹; Jong Wha Lee²; Hugh I. Kim²; Sunghwan Kim^{1,3}; ¹Kyungpook National University, Daegu, Republic of Korea; ²Pohang University of Science and Technology, Pohang, Republic of Korea; ³Green-Nano Materials Research Center, Daegu, Republic of Korea
- MP 656 **Comparison of Interface-Active Materials in Crude Oils with Different Emulsifying Propensities by using Solid Phase Extraction and an LTQ-Orbitrap Mass Spectrometer**; Xueming Dong; Chunfen Jin; Ravikiran Yerabolu; Hilka Kenttamaa; *Purdue University, West Lafayette, IN*
- MP 657 **Nitrogen Speciation in Petroleum Distillates using a Complementary and Powerful Approach by GC×GC-NCD and FT-ICR/MS**; Fabien Chainet; Lyes Assam; Vincent Souchon; Jérémie Ponthus; Florian Albrieux; *IFPEN, Solaize, France*
- MP 658 **A Model Compound Study to Assess Potential Complications of Using APPI for Mass Spectrometric Analysis of Crude Oil**; Matthew Hurt; Michael T. Cheng; *Chevron Research, Richmond, CA*
- MP 659 **Pretreatment of Oil Samples for GCMS Analysis of Polycyclic Aromatic Hydrocarbons and Their Hetero-Analogs**; Nino Todua¹; Natela Khetsuriani²; Elza Topuria²; Levan Megutnishvili¹; Alexey Mayorov¹; Anzor Mikaia¹; ¹National Institute of Standards & Technology, Gaithersburg, MD; ²Melikishvili Institute of Phys. & Org. Chemistry, Tbilisi, Georgia
- MP 660 **Development of an Analytical Method for Complex Downstream Hydrocarbons of Gas Cracker by GC/GC-MS**; Syed Ali; Asraf Ali; Momdoh Al-Enzi; Ibrahim Al-Ghamdi; Nasser M. Al-Harbi; Khalid H. Al-Assaf; *SABIC Research Center, Riyadh, Saudi Arabia*
- MP 661 **Analysis of Complex Aromatic Mixtures Such as Asphaltenes using Online Coupling LC-MS Methods**; Lilla Molnárné Guricza; Schrader Wolfgang; *Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany*
- MP 662 **Characterization of Isomers in Petroleum Interfacial Material by Ion Mobility Mass Spectrometry**; Priscila M. Lalli^{1,2}; Jacqueline M. Jarvis¹; Alan G. Marshall^{1,3}; Ryan P. Rodgers^{1,2}; ¹National High Magnetic Field Laboratory, Tallahassee, FL; ²Florida State University Future Fuels Institute, Tallahassee, FL; ³Department of Chemistry, Florida State University, Tallahassee, FL
- MP 663 **Analysis of Naphthenic acids by Matrix Assisted Laser Desorption Ionization Time of Flight Mass Spectrometry**; Jeferson Valencia; Marianny Yajaira Combariza; Cristian Blanco Tirado; *Universidad Industrial de Santander, Bucaramanga, Colombia*
- MP 664 **Unprecedented Inventory of Coal Tar Compounds by an Integrative Approach Comprising GC×GC-TOF MS and APPI(+)-FT-ICR MS**; Hector Koolen¹; Robert Swarthout¹; Robert Nelson¹; Huan Chen²; Logan Krajewski²; Christoph Aeppli³; Amy McKenna²; Ryan Rodgers²; Christopher Reddy¹; ¹Woods Hole Oceanographic Institution, Woods Hole, MA; ²National High Magnetic Field Laboratory, Tallahassee, FL; ³Bigelow Laboratory for Ocean Sciences, East Boothbay, ME
- MP 665 **Evaluation of Biodegradation of Crude Oils by Gc×gc using New Strategies Chemometrics**; Paloma Santana Prata; Noroska Gabriela Salazar Mogollón; Fabio Augusto; *Unicamp, Campinas, BR*
- MP 666 **Determination of Molecular Changes in Asphaltene Composition during Hydroconversion and Thermal Cracking Processes by High Resolution Mass Spectrometry**; Martha L. Chacón-Patiño¹; Cristian Blanco-Tirado¹; Jorge A. Orrego-Ruiz²; Andrea Gómez-Escudero²; Marianny Y. Combariza¹; ¹Universidad Industrial de Santander, Bucaramanga, Colombia; ²Instituto Colombiano del Petróleo, Piedecuesta, Colombia

CARBOHYDRATES I
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- MP 667 **Evaluation of the INLIGHT™ strategy for LC-MS/MS Disaccharide Analysis;** Adam Hawkrigde; John Mangrum; Umesh Desai; *Virginia Commonwealth University, Richmond, VA*
- MP 668 **Development of Bioinformatics Support for High Throughput Isomeric Separation and the Structural Identification of Glycans by LC-MS;** Ningombam Sanjib Meitei¹; Arun Apte²; Udayanath Aich³; Julian Saba⁴; ¹PREMIER Biosoft, Indore, India; ²PREMIER Biosoft, Palo Alto, CA; ³Thermo Fisher Scientific, Sunnyvale, CA; ⁴Thermo Fisher Scientific, San Jose, CA
- MP 669 **Intelligent Glycomics Data-Independent-Acquisition Method (iGODIA) for Targeted Glycotope Analysis;** Hsin-Hung Huang^{1,2}; Kay-Hooi Khoo^{1,2}; ¹IBC, Academia Sinica, Taipei, Taiwan; ²IBS, National Taiwan University, Taipei, Taiwan
- MP 670 **MultiGlycan: A Software Tool for Automated Glycan Quantification using Labeling-Based and Label Free Approaches;** Chuan-Yih Yu¹; Yunli Hu²; Shiyue Zhou²; Yehia Mechref²; Haixu Tang¹; ¹Indiana University, Bloomington, IN; ²Texas Tech University, Lubbock, TX
- MP 671 **Development of Structural Analysis Techniques for Keratan Sulfate Using Chemical Derivatization and LC-MS/MS;** David Fischler; *Complex Carbohydrate Research Center, UGA, Athens, GA*
- MP 672 **Towards Absolute Quantification in Glycomics Facilitating New Labeling Strategies for *Pichia pastoris* N-glycans;** Evelyn Rampler; Gunda Koellensperger; *University Vienna, Vienna, Austria*
- MP 673 **Using an Isotopically Labelled Glycoprotein Internal Standard to Enable Comparison of Glycan Quantitation across Mass Spectrometer Types;** Emily Betchy¹; Barry Boyes²; Ron Orlando¹; ¹University of Georgia, Athens, GA; ²Advanced Materials Technology, Wilmington, DE
- MP 674 **Towards the Discrimination of Sialyl Linkages in Glycopeptides: A New Derivatization Approach;** Takashi Nishikaze; Shinichi Iwamoto; Koichi Tanaka; *Shimadzu Corporation, Kyoto, Japan*
- MP 675 **Semi-Automatic Site Specific Analysis of High Mannose and Hybrid Type Glycosylation of Human Serum Glycoproteins in Liver Disease;** Miloslav Sanda¹; Nathan J Edwards²; Radoslav Goldman¹; ¹Department of Oncology, Lombardi Comprehensive, Washington, DC; ²Department of Biochemistry and Molecular & Cell, Washington, DC
- MP 676 **Survey of Cationizing Metals for CID and ETD of Metal-Adducted Oligosaccharides;** Ranelle M. Schaller-Duke; Carolyn J. Cassidy; *The University of Alabama, Tuscaloosa, AL*
- MP 677 **Determination of *Caulobacter crescentus* Glycan Strand Length Distribution by LC-UV-MS;** Ludmila Alexandrova¹; Allis Chien¹; Leigh Harris²; Julie Theriot²; ¹Stanford University Mass Spectrometry, Stanford, CA; ²Biophysics Program, Department of Biochemistry, Stanford, CA
- MP 678 **Rapid Characterization of Model Glycosaminoglycans using Negative Electron Transfer Dissociation;** Matthew Rush; Nicholas Riley; Christopher Rose; Alexander Hebert; Michael Westphall; Joshua Coon; *University of Wisconsin, Madison, WI*
- MP 679 **Electrospray Ionization of Saccharides by Amino Acids;** Abdil Ozdemir²; Chung-Hsuan Chen¹; ¹Academia Sinica, Genomics Research Center, Taipei, Taiwan; ²Sakarya University, Adapazari, Turkey
- MP 680 **Mass Spectrometric Analysis to Identify arabino-xylo-oligomers Generated from Hydrothermal Processing Of Switchgrass;** Michael Bowman; Victoria Nguyen; Bruce Dien; *USDA-NCAUR, Peoria, IL*
- MP 681 **The Coolest Sugars in the Universe: Characterizing Complex Carbohydrates in Liquid Helium Nanodroplets;** Christiane Stachl¹; Ana Isabel González Flórez¹; Doo-Sik Ahn¹; Johanna Hofmann¹; Heung Sik Hahm²; Peter Seeberger²; Gert von Helden¹; Kevin Pagel¹; ¹Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany; ²Max Planck Institute of Colloids and Interfaces, Potsdam, Germany
- MP 682 **Reliable Quantitative Glycomics using LC-MS and iGlycoMab Stable Isotope Labeled Glycan Standard;** Nadia Tello¹; Shiyue Zhou¹; Alex Harvey²; Barry Boyes²; Ron Orlando²; Yehia Mechref¹; ¹Texas Tech University, Lubbock, TX; ²GlycoScientific, Athens, GA
- MP 683 **Addition of Basic Sites to the Glycans of *Helicobacter pylori* to Increase MS/MS Peak Abundance;** Haley S. Miller; Danielle Dube; Elizabeth A. Stemmler; *Bowdoin College, Brunswick, ME*
- MP 684 **Improved Sensitivity in Tandem MS Quantification of Heparan Sulphate by Depolymerisation Using Acid Butanolysis Reaction;** Paul J Trim; John Hopwood; Marten Snel; *South Australian Health and Medical Research Insti, Adelaide, Australia*
- MP 685 **Analysis of Fructosylamino Acids in Dried Fruit Utilizing Deuterated *n*-butyl-ketoximes as Standards by Gas-Liquid Chromatography/Mass Spectrometry;** Thomas P. Mawhinney; Deborah Chance; Valeri Mossine; Brock Evans; Carl Cheadle; James Waters; *University of Missouri, Columbia, MO*
- MP 686 **Quantification and Structural Characterization of Glycans and Glycopeptides by TQMS: The Energy-Resolved Oxonium Ion Monitoring (Erexim) Platform;** Atsuhiko Toyama¹; Shuichi Nakaya¹; Shinji Funatsu¹; Koji Ueda²; Yoshihiro Hayakawa¹; Ichiro Hirano¹; ¹Shimadzu Corporation, Kyoto, Japan; ²The University of Tokyo, Tokyo, Japan
- MP 687 **Branched Oligosaccharides by Microwave Assisted Hydrolysis, HILIC Separation, and MSⁿ (n>2);** Jia Ren; *Purdue University, West Lafayette, IN*
- MP 688 **Esterification of Glycopeptides for the Determination of Sialylation Levels in Antibodies;** Andrey Oliveira¹; Rini Roy¹; Paul Lopez¹; Edward Bodnar¹; Celine Raymond²; Yves Durocher²; Helene Perreault¹; ¹University of Manitoba, Winnipeg, Canada; ²National Research Council of Canada, Montreal, Qc
- MP 689 **LC-MS/MS Analysis of Permethylated Free Oligosaccharides and N-glycans Released from Human Milk;** Xue Dong; Shiyue Zhou; Nadia Tello; Yehia Mechref; *Texas Tech University, Lubbock, TX*
- MP 690 **Mass Spectral Patterns Obtained by Field Ionization GC/MS of Methyloxime-TMS-derivatized Primary Metabolites;** Takeshi Furuhashi¹; Takemichi Nakamura²; ¹RIKEN, Yokohama, Japan; ²RIKEN, Wako, Japan
- MP 691 **Advanced LC-MS Based Approaches for Orthogonal Determination of N- and O-linked Glycosylation Structures in Therapeutic Proteins;** Chen Li¹; Peter Li¹; Douglas Richardson²; Huijuan Li²; Yuetian Chen²; Daisy Richardson²; Mohammed Shameem²; David Pollard²; Shiao-Lin Wu¹; ¹BioAnalytix, Cambridge, MA; ²Merck & Co, Kenilworth, NJ
- MP 692 **Heparan Sulfate Libraries Derived From Robo-1 Affinity Pulldowns;** Morgan Stickney¹; David Fischler²; Rongrong Huang²; Joshua S. Sharp²; Jon Amster¹; ¹University of Georgia, Athens, GA; ²Complex Carbohydrate Research Center, UGA, Athens, GA



These special posters will be displayed Monday through Thursday.

Special **iPRG 2015 Study: Differential Abundance Analysis in Label-free Quantitative Proteomics**; Eugene Kapp⁷; Henry Lam¹⁰; Brett Phinney²; John S. Cottrell³; Michael R. Hoopmann⁴; Sangtae Kim⁸; Thomas Neubert⁵; Magnus Palmblad⁶; Olga Vitek⁹; **Susan T. Weintraub¹**; ¹Univ. of Texas HSC, San Antonio, TX; ²Univeristy of CA, Davis, Davis, CA; ³Matrix Science, Ltd., London, UK; ⁴Institute for Systems Biology, Seattle, WA; ⁵Skirball Institute, NYUMC, New York, NY; ⁶Leiden University, Leiden, Netherlands; ⁷Walter and Eliza Hall Institute of Medical Researc, Parkville, Australia; ⁸Pacific Northwest National Laboratory, Richland, WA; ⁹Northeastern University, Boston, MA; ¹⁰Hong Kong University of Science and Technology, Hong Kong, Hong Kong

Special **Mapping Scientific Pedigrees and Collaborative Patterns using Bibliometrics: Six Former Presidents of the ASMS**; **Arzu Tugce Guler¹**; Cathelijn Waaijer²; Magnus Palmblad¹; ¹Leiden University Medical Center, Leiden, Netherlands; ²Leiden University, Leiden, Netherlands

TUESDAY POSTERS

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

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 Ion Spectroscopy.....029-038
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 Instrumentation: General.....061-079
 Instrumentation: New Developments in Ionization and Sampling.....080-099
 High Mass Accuracy/High Performance MS: Applications 100-117
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 Informatics: Workflow and Data Management.....127-140
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 Proteomics: Quantitative - Stable Isotope Labeling Methods...587-605
 Biomarker: Quantitative Analysis (non-protein, lipids/metabolites/compounds).....606-629
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 Imaging MS: Pharmaceutical Applications655-667
 Imaging MS: Disease Markers668-694

AMBIENT IONIZATION: APPLICATION
 001-028

- TP 001 **Optimization and Application of Continuous Solvent Addition and Controlled Elution to Paper Spray Ionization**; **Elizabeth Dhummakupt**; Michael Wei; Richard A. Yost; *University of Florida, Gainesville, FL*
- TP 002 **Characterization of Sterols in Vegetable Oils by Transmission Mode Direct Analysis in Real Time Mass Spectrometry**; **Rosana Alberici¹**; Gabriel Fernandes²; Andréia Porcari¹; Marcos Eberlin¹; Daniel Barrera-Arellano²; Facundo Fernandez³; ¹Thomson Mass Spectrometry Laboratory-UNICAMP, Campinas, Brazil; ²Fats and Oils Laboratory-UNICAMP, Campinas, Brazil; ³Georgia Institute of Technology, Atlanta, GA
- TP 003 **Direct Analysis in Real Time-Mass Spectrometry (DART-MS) for the Study of Gas-Surface Heterogeneous Reactions: Focus on Ozone and PAHs**; Shouming Zhou; **Matthew W. Forbes**; Jonathan P.D. Abbatt; *Department of Chemistry, University of Toronto, Toronto, Canada*
- TP 004 **Continuous-Wavelength Laser Desorption Coupled with ESI/APCI Dual Ion Source for Rapid Characterization of Packaging Materials**; **Yi Lun Chen**; Siou Sian Jhang; Min Zong Huang; Jentaie Shiea; *National Sun Yat- Sen University, Kaohsiung, Taiwan*
- TP 005 **Direct Analysis from TLC Plate using Matrix Assisted Ionization (MAI)**; **Khoa Hoang**; Charles McEwen; *Philadelphia, PA*

- TP 006 **Thermal Gravimetric Analysis Coupled with Ambient Mass Spectrometry (TG-AMS) for Rapid Determination of Chemical Components in Plastic and Rubber Products**; **Siou Sian Jhang**; Min Zong Huang; Jentaie Shiea; *National Sun Yat- Sen University, Kaohsiung, Taiwan*
- TP 007 **Ambient Analysis of Leachable Compounds from Single-Use Bioreactors with Desorption Electrospray Ionization Time-of-Flight Mass Spectrometry**; **Jian Liu¹**; Joseph H Kennedy²; Mike Ronk¹; Liliana Marghitoiu¹; Hans Lee¹; Yasser Nashed-Samuel¹; ¹Amgen, Thousand Oaks, California; ²Prosolia, Inc., Indianapolis, IN
- TP 008 **Gas Chromatography Coupled with ESI/APCI Dual Ion Source for Simultaneous Detection of Polar and Nonpolar Compounds**; **Ban Hsin Wu**; Siou Sian Jhang; Min Zong Huang; Jentaie Shiea; *National Sun Yat-Sen Univ., Kaohsiung, Taiwan*
- TP 009 **Using DART Mass Spectrometry for an Undergraduate Analytical Chemistry Laboratory**; **Nathan Cunningham**; Hong Hanh Nguyen; Joseph A. Loo; *UCLA, Los Angeles, CA*
- TP 010 **Rapid, Direct Technique for the Discrimination of Meat Tissues Originating from Different Animal Species for Food Authenticity**; **Sara Stead**; Simon Hird; Julia Balog; Alex Hooper; Steve Pringle; Mike Wilson; Mike Morris; *Waters corp, Manchester, UK*

- TP 011 **Integration of GC/LC with ESI+APCI/MS for Analysis of Complicated Mixtures over a Wide Polarity Range;** Sy chyi Cheng; Siou Sian Jhang; Min Zong Huang; Jentaie Shiea; *National Sun Yat-Sen Univ., Kaohsiung, Taiwan*
- TP 012 **Direct Quantitative Analysis of Drugs of Abuse in Urine and Saliva;** Chris Hopley; Bryan McCullough; Camilla Liscio; *LGC, Teddington, UK*
- TP 013 **Liquid Microextraction Coupled with Thermal Desorption Electrospray Ionization Mass Spectrometry for Rapid Screening of Veterinary Drug Residues in Foods;** Peng Yu Chen; Jo Han Chou; Min Zong Huang; Jentaie Shiea; *National Sun Yat-Sen University, Kaohsiung, Taiwan*
- TP 014 **Mobile Screening of Glycerin Contaminants using Paper Spray Portable Mass Spectrometry;** Samanthi I Wickramasekara; Hongli Li; Dinesh Patwardhan; Steven Wolfgang; *US Food and Drug Administration, Silver Spring, MD*
- TP 015 **Rapid Differentiation of Ganoderma Species by Direct Ionization Mass Spectrometry;** Ho-Yi Wong; Bin Hu; Pui-Kin So; Chi-On Chan; Daniel Kam-Wah Mok; Zhong-Ping Yao; *Department of Applied Biology & Chemical Technology, The Hong Kong Polytechnic University, Hong Kong*
- TP 016 **Molecular Analyses of Algae using Desorption Electrospray Ionization (DESI) and Laser Desorption/Ionization (LDI) Mass Spectrometry;** Dilrukshika S. W. Palagama; Raymond E. West III; Dragan Isailovic; *The University of Toledo, Toledo, OH*
- TP 017 **Desorption Ionization of Illicit Drugs from Solid Phase Micro-Extraction Fibers at Increasing Temperature;** Joseph Lapointe¹; Brian Musselman¹; Craig Aurand²; ¹*Ionsense Inc., Saugus, MA*; ²*Sigma Aldrich, Bellefonte, PA*
- TP 018 **Defining Limit of Detection of Mini Surface Acoustic Wave Nebulization Chip by Using Different Types of Mass Spectrometer;** Tao Liang¹; Andrew Dennison²; Sung Hwan Yoon¹; Gloria Yen⁵; Yifan Li⁴; Scott Heron¹; Adam Stokes³; Anthony Walton²; Erik Nilsson⁵; David Goodlett¹; ¹*Pharmacy School, University of Maryland Baltimore, Baltimore, MD*; ²*School of Chemistry, The University of Edinburgh, Edinburgh, UK*; ³*School of Engineering, The University of Edinburgh, Edinburgh, UK*; ⁴*Department of Engineering, Northumbria University, Newcastle, UK*; ⁵*Deurion LLC, Seattle, WA*
- TP 019 **Rapid Screening and Identification of Designer Drugs in Powders or Plant Materials using Paper Spray Ionization-Mass Spectrometry;** Joseph H Kennedy¹; Kevin G. Shanks²; Justin Wiseman¹; Brian C. Laughlin¹; ¹*Prosofia, Inc., Indianapolis, IN*; ²*AIT Laboratories, Indianapolis, IN*
- TP 020 **Thermal Desorption Electrospray Ionization Mass Spectrometry Combined with Principal Component Analysis for Rapid Classification of Cooking Oils;** Ting Hao Chang; Siou Sian Jhang; Min Zong Huang; Jentaie Shiea; *National Sun Yat-Sen University, Kaohsiung, Taiwan*
- TP 021 **Using Desorption Electrospray Ionization with Mass Spectrometry (DESI-MS) to Identify Silicone Oil Contamination on Components;** Lance Miller; James Hochrein; *Sandia National Laboratories, Albuquerque, NM*
- TP 022 **DART-MS Determination of Malachite Green and Leucomalachite Green in Fish Extract;** Jia Shi¹; Xiaokun Duan²; Kai Liu²; Charles C. Liu²; Hongwei Zhao³; ¹*Sichuan Aquaculture Bureau, Chengdu, Sichuan*; ²*ASPEC Technologies LTD, Beijing, China*; ³*Xiangpu Technology, Chengdu, Sichuan*
- TP 023 **In situ Detection and Imaging of Ergot Alkaloids in Ipomoea tricolor Seeds by LAESI-MS/MS;** Gregory Boyce¹; Callee Walsh¹; Daniel Panaccione²; ¹*Protea Biosciences, Morgantown, WV*; ²*West Virginia University, Morgantown, WV*
- TP 024 **A Continuous Microplasma-Coupled Sampling Device for Real-Time Monitoring of Environmental Quality during Space Missions;** Matthew C. Bernier¹; Joel D. Keelor¹; Rosana M. Alberici²; Prabha Dwivedi¹; Daniel B. Gazda³; Thomas F. Limerio³; William T. Wallace³; Ariel V. Macatangay⁴; Joshua M. Symonds¹; Thomas M. Orlando¹; Facundo M. Fernandez¹; ¹*Georgia Institute of Technology, Atlanta, GA*; ²*Thomson Mass Spectrometry Laboratory, UNICAMP, Campinas, Brazil*; ³*Wyle Science, Technology, and Engineering Group, Houston, TX*; ⁴*NASA Johnson Space Center, Houston, TX*
- TP 025 **Monolayer-Coated Probe Electrospray Ionization Mass Spectrometry for Analysis of Individual Small Organisms and Single Cells;** Jiewei Deng¹; Yunyun Yang²; Mingzhi Xu¹; Xiaowei Wang¹; Zhong-Ping Yao³; Tiangang Luan¹; ¹*Sun Yat-Sen University, Guangzhou, China*; ²*China National Analytical Center Guangzhou, Guangzhou, China*; ³*The Hong Kong Polytechnic University, Hong Kong SAR, China*
- TP 026 **Analysis of Butylene Glycol Oligomer Samples by Temperature-Rising Direct Analysis in Real Time Mass Spectrometry (TR-DART-MS);** Jun Watanabe¹; Kazumasa Kinoshita²; Takao Nishiguchi²; Chikako Takei²; Motoshi Sakakura³; Teruhisa Shiota³; ¹*Shimadzu Corporation, Kyoto, Japan*; ²*Bio Chromato, Inc., Fujisawa, Japan*; ³*AMR, Inc., Tokyo, Japan*
- TP 027 **Development of a Simultaneous Analysis Method of Volatile Compounds by DART MS;** Takehito Sagawa¹; Keiko Matsumoto²; Jun Watanabe²; Motoshi Sakakura³; Teruhisa Shiota³; ¹*S & B Foods Inc., Tokyo, Japan*; ²*Shimadzu Corporation, Kyoto, Japan*; ³*AMR, Inc., Tokyo, Japan*
- TP 028 **DART in Forensic Toxicology - Fast and Accurate Detection of Toxicants and Illicit Drugs in Human Blood and Urine Samples;** Ying Zhang¹; Wei Zhang¹; Wenfang Zhang¹; Shiyang Qin¹; Daming Zhang¹; Xiaokun Duan²; Xiangtao Chen²; Charles C. Liu²; ¹*Beijing Public Security Bureau, Beijing, China*; ²*ASPEC Technologies LTD, Beijing, China*

ION SPECTROSCOPY 029-038

- TP 029 **Gas-Phase IRMPD Modeling of Deprotonated Peptide Binding Frameworks for Divalent Transition Metal Ions;** Robert C. Dunbar¹; Jonathan Martens²; Giel Berden²; Jos Oomens^{2,3}; ¹*Case Western Reserve Univ, Cleveland, OH*; ²*Radboud University, Nijmegen, Netherlands*; ³*University of Amsterdam, Amsterdam, Netherlands*
- TP 030 **Conformation-Specific IR-JV Double-Resonance Spectroscopy and Structural Analysis of Methyl Esterified Leucine Enkephalin;** Nicole Burke; Andrew DeBlase; James Redwine; John Hopkins; Timothy Zwier; Scott McLuckey; *Purdue University, Lafayette, IN*
- TP 031 **Proton Migration in Tryptophan-Containing Radicals Elucidated by Infrared Laser Spectroscopy;** Ning Zhao; *University of Florida, Gainesville, FL*
- TP 032 **Unimolecular Decomposition of M(Pro2-H)+ (M=Mg, Ca, Sr, Ba, Mn, Fe, Co, Ni, Cu, Zn) by IRMPD, SORI-CID, and Theoretical Studies;** Yasaman Jami Alahmadi; Travis D Fridgen; *Memorial University of NL, St. John's, Canada*
- TP 033 **Charge Solvation or Salt Bridge : Proton Affinity as a Structural Probe for Protonated Amino Acid Homodimers;** Xianglei Kong; *Nankai University, Tianjin, China*
- TP 034 **UltraViolet Action Spectroscopy of Peptidic Diazirines and Their Peptide Ion Complexes;** Robert Pepin¹; Frantisek Turecek²; Steen Bronsted Nielsen³; ¹*U of Washington, Chemistry, Lakewood, WA*; ²*University of Washington, Seattle, WA*; ³*University of Aarhus, Aarhus, Denmark*

- TP 035 **Towards Probing Hydrogen Bonded Networks and Electron Transfer States through the Characterization of Fluorophores;** [Vaishnavi Rajagopal](#); Alessandra Ferzoco; *Rowland Institute at Harvard, Cambridge, MA*
- TP 036 **Unravelling Environmental Effects on Light-Harvesters: Photodissociation Action Spectroscopy of Gas-Phase Chlorophylls and Porphyrins;** [Sydney Wellman](#); Rebecca Jockusch; *Department of Chemistry, University of Toronto, Toronto, Canada*
- TP 037 **“Turn-On” Fluorophores to Probe the Conformation of Gaseous Biomolecules?** Martin Czar; Stephen Sciuto; [Rebecca A. Jockusch](#); *Chemistry Department, University of Toronto, Toronto, Canada*
- TP 038 **Ultraviolet and Vacuum Ultraviolet Light Sources for Advanced Mass Spectrometry Techniques in Support of Nuclear Non-Proliferation;** [David Willingham](#); Benjamin Naes; Mindy Zimmer; *Pacific Northwest National Laboratory, Richland, WA*
- ION/MOLECULE, ION/ION, ION/ELECTRON INTERACTIONS**
039-060
- TP 039 **Strategies for Selective and Non-Selective Oxidative Labeling of Peptides and Proteins in the Gas-Phase via Ion/Ion Reactions;** [Alice Pilo](#); Jiexun Bu; Scott McLuckey; *Purdue University, West Lafayette, IN*
- TP 040 **Roles of Metal-Peptide Interactions in Electron Capture Dissociation of Metal- α B Complexes;** [Tao Jiang](#); Kristina Hakansson; *University of Michigan, Ann Arbor, MI*
- TP 041 **Gas-Phase Nucleophilic Substitution in Atmospheric Pressure Photoionization in the Presence of Halogenated Dopants;** [Tiina J. Kauppila](#)¹; Hendrik Kersten²; Thorsten Benter²; ¹*University of Helsinki, Helsinki, Finland*; ²*University of Wuppertal, Wuppertal, Germany*
- TP 042 **Multiply Charged Non-Covalent Complexes by UV/Vis-Photodissociation with Electron Transfer Dissociation and Collision-Induced Dissociation;** [Andy Dang](#); Christopher Shaffer; Frantisek Turecek; *University of Washington, Seattle, WA*
- TP 043 **Design of Isoxazolium Reagents for the Gas-Phase Amidation of Carboxylic Acids via Ion/Ion Reactions;** [Zhou Peng](#); Scott A. McLuckey; *Purdue University, West Lafayette, IN*
- TP 044 **Generation of Hydroxyalkyl Radicals with Photoinitiator and Their Reactions with CysteinyI Peptides;** [Sarju Adhikari](#); Lei Tan; Yu Xia; *Purdue University, West Lafayette, IN*
- TP 045 **Alkali Metal Adduct Radical Cations of Cysteine Derivatives: A Gas-Phase Reactivity and Structural Elucidation Study;** [Michael Lesslie](#)¹; Sandra Osburn²; Giel Berden³; Jos Oomens³; Michael J. Van Stipdonk⁴; Victor Ryzhov¹; ¹*Northern Illinois University, Dekalb, IL*; ²*Duquesne University, Munhall, PA*; ³*Radboud University Nijmegen, Nijmegen, Netherlands*; ⁴*Duquesne University, Pittsburgh, PA*
- TP 046 **Ion-Ion and Ion-Electron Activation Experiments in a Novel Linear Ion Trap;** [Dimitris Papanastasiou](#)¹; Alexander Lekkas¹; Diamantis Kounadis¹; Ioannis Orfanopoulos¹; Andreas Mpozatzidis¹; Emmanuel Raptakis²; ¹*Fasmatech, Athens, Greece*; ²*Fasmatech SA, Athens, Greece*
- TP 047 **Bending Gold(I) Dicoordinate Complexes to Switch on C-X σ -Bond Activation;** [Athanasios Zavras](#)¹; Abderrahmane Amgoune²; Didier Bourissou²; Richard A. J. O’hair¹; ¹*University of Melbourne, Victoria, Australia*; ²*universite Paul Sabatier, Toulouse, France*
- TP 048 **Considerations for Attaining Improved ETD Performance for Top Down Applications;** [Christopher Mullen](#); Lee Earley; Chad Weisbrod; John E. P. Syka; Jean-Jacques Dunyach; *Thermo Fisher Scientific, San Jose, CA*
- TP 049 **Conformational Differences of Leucine-Enkephalin Complexes Evaluated using Gas-Phase Hydrogen/Deuterium Exchange;** [Yinjuan Chen](#)¹; Lei Yue²; Xunlei Ding³; Yuanjiang Pan²; Chuan-Fan Ding¹; ¹*Fudan University, Shanghai, China*; ²*Zhejiang University, Hangzhou, China*; ³*North China Electric Power University, Beijing, China*
- TP 050 **Gas-Phase Ion/Molecule Reaction of CO₂ with Anilide Anions;** [Chongming Liu](#); Athula B. Attygalle; *Stevens Institute of Technology, Hoboken, NJ*
- TP 051 **Gas-Phase Click Chemistry: 1,3-dipolar Cycloaddition of Alkynes with Azides via Ion/Ion Reactions;** [Jiexun Bu](#); Scott McLuckey; *Purdue University, West Lafayette, IN*
- TP 052 **Impact of a Localized Radical Site on Dissociation of Peptides Modified Using an Alkyl-Nitroxide Spin Label Reagent;** [Julia Aponte](#); Jennifer Brodbelt; *University of Texas Austin, Austin, TX*
- TP 053 **Identification of the Protonated Carboxylic Acid Functionality and Differentiation of Protonated Isomeric Hydroxybenzoic Acids via Regioselective Ion-Molecule Reactions;** [Ravikiran Yerabolu](#)¹; John Kong¹; Joann Max¹; Raghavendhar Kotha¹; Minli Zhang²; Hilka Kenttamaa¹; ¹*Purdue University, West Lafayette, Indiana*; ²*AstraZeneca, Boston, MA*
- TP 054 **Which Ion and Neutral Multipole and Anisotropic Polarizability Terms are Important in Ion—Molecule Collision Rates in Extreme Temperature Environments?** Kent M. Ervin; *University of Nevada, Reno, Reno, NV*
- TP 055 **Apparent Activation of H₂O and Elimination of H₂ from Gas-Phase Mixed Metal Complexes;** [Sandra Osburn](#); Alexandra Plaviak; Michael J. Van Stipdonk; *Duquesne University, Pittsburgh, PA*
- TP 056 **Integrated Ion Dynamics Simulations in OpenFOAM: Flow, Transport, Chemical Reactions and Space-Charge;** [Walter Wissdorf](#); Thorsten Benter; *University of Wuppertal, Wuppertal, Germany*
- TP 057 **A Comparison of the Reactions of N-Methyl-6-dehydroquinolinium Cation with Nucleosides and Dinucleoside Phosphates in the Gas Phase and Aqueous Solution;** [Joann Max](#); Ashley Wittrig; Fanny Widjaja; Hilka Kenttamaa; *Purdue University, West Lafayette, IN*
- TP 058 **Conformational Effects on the Proton Affinity of Lysine Homolog Containing Oligopeptides Studied by Mass Spectrometry and Infrared Multiphoton Dissociation Spectroscopy;** [Patrickhenry Batoon](#); Jianhua Ren; *University of the Pacific, Stockton, CA*
- TP 059 **Probing Chemistry Using Molecular Beams and Vacuum Ultraviolet Synchrotron Radiation;** [Biswajit Bandyopadhyay](#); Yigang Fang; Oleg Kostko; Musahid Ahmed; *Lawrence Berkeley National Laboratory, Berkeley, California*
- TP 060 **Identification of the N-Monosubstituted N-Hydroxylamino Functionality in Protonated Analytes via Ion/Molecule Reactions in Tandem Mass Spectrometry;** [John Kong](#)¹; Huaming Sheng¹; Weijuan Tang¹; Ravikiran Yerabolu¹; Peggy Williams¹; Minli Zhang²; Hilka Kenttamaa¹; ¹*Purdue University, West Lafayette, IN*; ²*AstraZeneca, Boston, MA*
- INSTRUMENTATION: GENERAL**
061-079
- TP 061 **PALMS: A Parallel Computational Engine for SIMION Simulating Multiple Ion Interactions;** [Konstantin Novoselov](#); Vladimir M. Doroshenko; Alexander Misharin; *MassTech, Inc., Columbia, MD*
- TP 062 **Optimization of Ion Trap Isolation Methodology for Simultaneous Precursor Selection at the MS Level;** [Philip M Remes](#)¹; Romain Huguet¹; Jarrett Egerton²; Michael J. Maccoss²; Vlad Zabrouskov¹; ¹*Thermo Fisher Scientific, San Jose, CA*; ²*Univ of Washington, Seattle, WA*

- TP 063 **Tracing Ions and Visualizing Charged Clusters in the Aerolens Under Transitory Gas Flow Conditions;** Emmanuel Raptakis¹; Diamantis Kounadis¹; Alexander Lekkas¹; Athanasios Zacharos³; Ioannis Nikolos³; Dimitris Papanastasiou²; ¹Fasmatech SA, Athens, Greece; ²Fasmatech, Athens, Greece; ³Technical University of Crete, Chania, Greece
- TP 064 **Sub 500ps Magnetic Ion Detector with Extended Operating Life;** Dick Stresau; Yair Benari; Kevin Hunter; Peter Raffin; Wayne Sheils; Sid Sondur; Scott Morgan; *ETP Electron Multipliers, Clyde, Australia*
- TP 065 **Every Ion Counts: Optimization of the Quadrupole Mass Spectrometer for Improved Ion Transmission and Flat-Top Peaks;** Mariya J. Antony Joseph¹; Simon Maher^{1,2}; Fred P. M. Jjunju¹; S. U. A. H. Syed³; John R. Gibson¹; Iain S. Young²; Ron M. A. Heeren³; Stephen Taylor¹; ¹Dept. of Electrical Engineering and Electronics, University of Liverpool, UK; ²Institute of Integrative Biology, University of Liverpool, UK; ³FOM Institute for Atomic and Molecular Physics, Amsterdam, Netherlands
- TP 066 **Improve Single Reaction Monitoring (SRM) Screening Speed by Using Parallel System Design on Mass Spectrometer Control System;** Qingyu Song; Eric Hemenway; Jew-Dong Kuo; Mary Blackburn; *Thermo Fisher Scientific, San Jose, CA*
- TP 067 **A New High-Resolution, Temperature-Variable Ion Mobility Mass Spectrometer;** Jakub Ujma¹; Kevin Giles²; Michael Morris²; Perdita Barran¹; ¹The University of Manchester, Manchester, UK; ²Waters Corporation, Wilmslow, UK
- TP 068 **Next Generation Long Life Discrete-Dynode Detector;** Kevin Hunter; Russell Jurek; Dick Stresau; Scott Morgan; Wayne Sheils; *ETP Electron Multipliers, Clyde, Australia*
- TP 069 **Massively Parallel Simion Model of Quadrupole Analyzer Peak Shape;** Ken Newton; *Agilent Technologies, Santa Clara, CA*
- TP 070 **Enabling Fast Prototyping and Customization of Mass Spectrometer Control Software;** Jeff Brown; Emmy Hoyes; Richard Newton; Christopher Jones; Darren Hewitt; Wright Steven; Rennie Birch; David Langridge; Keith Richardson; Richard Chapman; *Waters Corporation, Wilmslow, UK*
- TP 071 **Simulation Results for Tolerance of Misalignment in Six Degrees of Freedom in Ceramic Plate Linear Ion Traps;** Qinghao Wu; Yuan Tian; Ailin Li; Daniel Austin; *Brigham Young University, Provo, UT*
- TP 072 **Fully Automated On-Line Sample Extraction and Analysis of Residual Pesticides in Agricultural Products by using On-Line SFE-SFC-MS;** Takanari Hattori¹; Takato Uchikata¹; Hidetoshi Terada¹; Chigusa Ichikawa¹; Yasuhiro Funada¹; Yayoi Ichiki²; Miho Sakai³; Takashi Ando³; Yoshihiro Izumi^{4,5}; Eiichiro Fukusaki⁵; Takeshi Bamba^{4,5}; ¹Shimadzu Corporation, Kyoto, Japan; ²Miyazaki Enterprise Promotion Organization, Miyazaki, Japan; ³Miyazaki Agricultural Research Institute, Miyazaki, Japan; ⁴Kyushu University, Fukuoka, Japan; ⁵Osaka University, Suita, Japan
- TP 073 **Surface Induced Dissociation Utilized to Characterize Protein Complexes Trapped in the Trap Cell of a Q-TOF Instrument;** Jing Yan¹; Sophie R. Harvey¹; Jeff Brown²; Emmy Hoyes²; Vicki H. Wysocki¹; ¹The Ohio State University, Columbus, OH; ²Waters Corporation, Wilmslow, UK
- TP 074 **Ion Mobility-Selected Trapping and Enrichment in Structures for Lossless Ion Manipulations (SLIM);** Tsung-Chi Chen; Jeremy A. Sandoval; Spencer A. Prost; William E. Karnesky; Xing Zhang; Ian K. Webb; Ahmed M. Hamid; Randolph V. Norheim; Erin S. Baker; Yehia M. Ibrahim; Richard D. Smith; *Pacific Northwest National Laboratory, Richland, WA*
- TP 075 **Velocity Distribution Measurement of Fullerene Ions with and without Quadrupole Fields;** Avinash Patil; Sin-Ciang Jiang; Kai-Chun Yen; Szu-Wei Chou; Wen-Ping Peng; *National Dong Hwa University, Shoufeng, Hualien, Taiwan*
- TP 076 **Enhancing Ion Sampling Efficiency, Ion Transmission and Detection on a Triple Quadrupole Platform;** Natsuyo Asano; Manabu Ueda; Wataru Fukui; Tairo Ogura; Kazuo Mukaibatake; *Shimadzu Corporation, Kyoto, Japan*
- TP 077 **Quantifying and Improving the Lifetime of Hybrid Detectors;** Stephen Ritzau; Matthew Breuer; Bruce Laprade; Jason Alston; *PHOTONIS USA, Sturbridge, MA*
- TP 078 **High-Throughput Serum Peptide Profiling of a Clinical Cancer Cohort on a Novel MALDI-TOF-MS Platform;** Yuri E.M. Van Der Burg²; Hans Dalebout²; Simone Nicolardi²; Marco R. Bladergroen²; Wilma E. Mesker¹; Rob A.E.M. Tollenaar¹; Magnus Palmblad²; ¹Leiden University Medical Center, Leiden, Netherlands; ²Center for Proteomics and Metabolomics, LUMC, Leiden, Netherlands
- TP 079 **Trajectory Calculations of Space Charge Effects in Ion Traps via an Iterative Solution of the Poisson Equation;** David Langridge; *Waters, Wilmslow, UK*
- INSTRUMENTATION: NEW DEVELOPMENTS IN IONIZATION AND SAMPLING**
080-099
- TP 080 **Characterizing an ESI-MS Interface Based on the Ion Utilization Efficiency;** Jonathan Cox¹; Ioan Marginean²; Richard Smith¹; Keqi Tang¹; ¹Pacific Northwest National Laboratory, Richland, WA; ²GWU, Washington, DC
- TP 081 **The Correlations between Ions and Neutrals in Matrix-Assisted Laser Desorption/Ionization;** I-Chung Lu; Yuan Tseh Lee; Chi-Kung Ni; *Institute of Atomic and Molecular Sciences, Academ, Taipei, Taiwan*
- TP 082 **Aerodynamic Focusing Extractive Electrospray Ionization;** Bijay Banstola; Fabrizio Donnarumma; Kermit K. Murray; *Louisiana State University, Baton Rouge, LA*
- TP 083 **Soft Ionization, NIST identification and Capabilities for Quantitative Analysis in Conditioned Glow Discharge Ion Source;** Alexander Kolosov; Anatoly Verenchikov; *MSC-CG, Bar, Montenegro*
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- TP 117 **Low-Abundance Isotope Enrichment in Individual Muscle Proteins Measured by High-Resolution Mass Spectrometry;** Kelly Hines^{1,2}; G. Charles Ford¹; Katherine Klaus²; Brian Irving²; Beverly Ford¹; Kenneth Johnson³; Ian Lanza^{1,2}; K. Sreekumaran Nair^{1,2}; ¹Mayo Clinic Metabolomics Resource Core, Rochester, MN; ²Mayo Clinic Division of Endocrinology, Rochester, MN; ³Mayo Clinic Medical Genome Facility Proteomic Core, Rochester, MN
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- TP 119 **Investigation of Self-Calibrated, Fine-Isotope-Line Fit Scoring in Combined HPLC-Fourier Transform Orbital Trapping MS for Candidate Formulae Elimination;** Yongdong Wang; Ming Gu; *Cerno Bioscience, Norwalk, CT*
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- TP 122 **Absorption Mode Gets Even Better with its Svelte New Curves;** David Kilgour¹; Konstantin Nagornov²; Steven Van Orden³; Anton Kozhinov²; Konstantin Zhurov²; Yury Tsybin^{2,4}; David Goodlett¹; ¹University of Maryland Baltimore, Baltimore, MD; ²Ecole Polytechnique Fédérale, Lausanne, Switzerland; ³Bruker Daltonics Inc., Billerica, MA; ⁴Spectroswiss Sàrl, Lausanne, Switzerland
- TP 123 **A Novel Method of m/z Drift Correction for oa-TOF Mass Spectrometers based on Construction of Libraries of 'Matrix' Components;** Martin Green; Keith Richardson; Martin Palmer; Nick Tomczyk; *Waters Corporation, Manchester, UK*
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- TP 126 **Frequency Multiplication for High-Throughput Fourier-Transform Ion Cyclotron Resonance Mass Spectrometry;** Tzu-Yung Lin¹; Mikhail V. Gorshkov²; Aleksey V. Tolmachev¹; Jared B. Shaw¹; Rosalie K. Chu¹; Richard Harkewicz¹; R. James Ewing¹; Mowei Zhou¹; David W. Koppenaal¹; Errol W. Robinson¹; Ljiljana Pasa-Tolic¹; ¹Pacific Northwest National Lab, Richland, WA; ²INEPCP RAS, Moscow, Russian Federation
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- TP 133 **Mass Spectrometry Quality Control: Instrument Monitoring and Pattern Mining Insights;** Wout Bittremieux¹; Hanny Willems²; Lennart Martens³; Dirk Valkenborg²; Kris Laukens¹; ¹University of Antwerp, Antwerp, Belgium; ²VITO, Mol, Belgium; ³University of Ghent, Ghent, Belgium

- TP 134 **Performing Quality Control on Targeted Proteomics Assays using Skyline and Panorama;** Josh Eckels¹; Vagisha Sharma²; Yuval Boss³; Huilin Shi³; Tom Dunkley⁴; Kristin Wildsmith⁵; Cory Nathe²; Aaron Robinson²; Richard S. Johnson⁶; Jacob D. Jaffe⁷; Michael J. Maccoss³; Brendan Maclean³; ¹LabKey Software, San Diego, CA; ²LabKey Software, Seattle, WA; ³University of Washington, Seattle, WA; ⁴F. Hoffmann-La Roche Ltd, Basel, Switzerland; ⁵Genentech, Inc, San Francisco, CA; ⁶University of Washington, Mercer Island, WA; ⁷The Broad Institute, Cambridge, MA
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- Research Center, Academia Sinica, Taipei, Taiwan; ³Institute of Biological Chemistry, Academia Sinica, Taipei, Taiwan; ⁴Dept. of Clin. Chem., Univ. Med. Center Goettingen, Goettingen, Germany
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- TP 173 **Integrated Metabolomics and Transcriptomics Reveal Enhanced Specialized Metabolism in *Medicago truncatula* Root Border Cells**; Bonnie Watson¹; Mohamed Bedair²; Ewa Urbanczyk-Wochniak²; David V. Huhman¹; Dong Sik Yang¹; Stacy Allen¹; Wensheng Li²; Yuhong Tang¹; Lloyd Sumner¹; ¹*The Samuel Roberts Noble Foundation, Ardmore, OK*; ²*Monsanto, Chesterfield, MO*
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- TP 176 **Parameter Optimization for Data Dependent Acquisitions in Metabolomics on an Orbitrap Fusion Tribrid Mass Spectrometer**; Ulli Hohenester¹; Pierre Barbier Saint Hilaire¹; Benoit Colsch¹; Francois Fenaille¹; Marie-Françoise Olivier¹; Richard B. Cole²; Jean-Claude Tabet¹; Christophe Junot¹; ¹*CEA de Saclay, Gif sur Yvette Cedex, France*; ²*Univ. P. et M. Curie (Paris 6), Paris Cedex 05, France*
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- TP 180 **Elucidation of Biochemical Basis of Scab Resistance in Pecan Using Metabolomics**; [Zhentian Lei](#); Shelagh Henson; David Huhman; Bonnie Watson; Lloyd Sumner; *The Samuel Roberts Noble Foundation, Ardmore, OK*
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- TP 183 **Differentiating Yeast Strains by Untargeted Metabolomics Using UHPLC-HRMS/MS**; [Biao Ji](#)¹; Joanie Emond¹; Jennifer Chiang²; Guri Giaever²; Corey Nislow²; Lekha Sleno¹; ¹UQAM, Montreal, Canada; ²UBC, Vancouver, Canada
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- Langridge¹; Robert Plumb¹; Albert Fornace Jr²; Giuseppe Astarita^{1,2}; ¹Waters Corporation, Milford, MA; ²Georgetown University, Washington, DC; ³Leiden University, Leiden University, Netherlands; ⁴Janssen Pharmaceutica, Discovery Sciences, Beerse, Belgium
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- TP 206 **Non-Targeted Metabolite Profiling of Dried Blood Spots in a Field Based Epidemiological Study**; Corey Broeckling; Jay Kirkwood; Maggie Clark; Jennifer Peel; Jessica Prenni; *Colorado State University, Fort Collins, CO*
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- TP 210 **Effect of Mealybug Infestation on Grape Metabolomics**; Shabeer TP Ahammed¹; Amala Udayakumar¹; Akanksha Singh²; Manoj Pillai²; ¹National Research Centre for Grapes, Pune, Maharashtra, India; ²SCIEX, 121, Udyog Vihar Phase IV, Gurgaon, Haryana, INDIA
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- TP 245 **Retinoic Acid Analysis with Differential Mobility Mass Spectrometry for Improved Selectivity and Sensitivity**; Leo (Jinyuan) Wang¹; Jace W. Jones²; Maureen A. Kane²; Pauk R.S. Baker¹; ¹*AB SCIEX, Redwood City, CA*; ²*University of Maryland, School of Pharmacy, Baltimore, MD*
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- TP 248 **Bacteria Identification by Laser Desorption Ionization Mass Spectrometry (LDI-MS) – Enhancement of Signal Consistance using Amorphous Silicon (a-Si) Thin Films**; Sohee Yoon¹; Shin Hye Kim¹; Jeong Hee Moon²; Kyung Joong Kim¹; Tae Geol Lee¹; ¹*KRISS, Daejeon, Republic of Korea*; ²*KRIBB, Daejeon, Republic of Korea*

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- TP 250 **Supercritical Fluid Chromatography - Mass Spectrometry and Lipids – A Perfect Marriage**; [G. John Langley](#)¹; Julie Herniman¹; Caroline Sayer¹; Joost Brandsma²; Tom Sutton²; Waraporn Ratsameepakai¹; Tim Jenkins³; ¹Chemistry, University of Southampton, Southampton, UK; ²Medicine, University of Southampton, Southampton, UK; ³Waters Corporation, Wilmslow, UK
- TP 251 **Chromatographic Separation of Phosphatidylcholine Isomers on a UHPLC-MS Timeframe with Quadrupole Orbitrap Mass Spectrometer Detection**; [Josef Ruzicka](#)¹; David A. Peake²; ¹Thermo Fisher Scientific, Somerset, NJ; ²Thermo Fisher Scientific, San Jose, CA
- TP 252 **Comprehensive Lipid Analysis by MALDI Imaging and Spatially Resolved MS/MS Sequencing in Three Dimensional Cell Culture Models of Colorectal Carcinoma**; [Eric Weaver](#)¹; Andrew Palmer^{2,3}; Michael Becker⁴; Jens Fuchser⁴; Theodore Alexandrov^{2,5}; Amanda B. Hummon¹; ¹University of Notre Dame, Notre Dame, IN; ²EMBL Heidelberg, Heidelberg, Germany; ³University of Bremen, Bremen, Germany; ⁴Bruker Daltonik GmbH, Bremen, Germany; ⁵SCILS, Bremen, Germany
- TP 253 **An Interactive Software for LC-MS/MS Lipid Identification and Quantitation**; [Kevin L. Crowell](#)¹; Yong J. Kil¹; Marshall W. Bern¹; Chris H. Becker¹; Jennifer E. Kyle²; Richard D. Smith²; Thomas O. Metz²; ¹Protein Metrics Inc., San Carlos, California; ²Pacific Northwest National Laboratory, Richland, WA
- TP 254 **A Comprehensive Data-Independent Lipidomic Survey in Serum after Chronic Exposure to Strontium-90 *in vivo***; [Maryam Goudarzi](#)¹; Waylon Weber²; Tytus Mak³; Juijung Chung¹; Melanie Doyle-Eisele²; Dunstana Melo²; Steve Strawn¹; David Brenner⁴; Raymond Guilmette²; Albert Fornace Jr.¹; ¹Georgetown University, Washington Dc, DC; ²Lovelace Respiratory Research Institute, Albuquerque, NM; ³National Institute of Standards and Technology, Gaithersburg, MD; ⁴Columbia University, New York, NY
- TP 255 **Application of an Integrated Ion Cyclotron Based High Resolution Lipidomics Platform on RORy Ligand Search**; [Harald Koefeler](#)¹; Bettina Meissburger^{2,5}; Troetzmueller Martin¹; Alexander Triebel¹; Alexander Fauland³; Juergen Hartler⁴; Christian Wolfrum²; ¹Medical University Graz, ZMF, Graz, AUSTRIA; ²Eidgenössische Technische Hochschule, Zürich, Switzerland; ³Karolinska Institutet, Stockholm, Sweden; ⁴Graz University of Technology, Graz, Austria; ⁵DKFZ, Heidelberg, Germany
- TP 256 **Profiling and Quantitation of Globosides (Gb4) in Biological Samples Using Ultra-Fast Mass Spectrometry**; [Ruth Gordillo](#)¹; William L. Holland¹; Benjamin J. Figard²; Erin McAllister²; David Jorissen²; Philipp E. Scherer¹; ¹UTSW Medical Center, Touchstone Diabetes Center, Dallas, Texas; ²Shimadzu Scientific Instruments, Columbia, MD
- TP 257 **HR/AM Mass Spectrometry Methodologies for Rapid Screening and Comprehensive Studies of Lipid Deposition Correlation to Contact Lens Properties**; [Andrew J. Hotelling](#)¹; William Nichols²; ¹Bausch + Lomb, Rochester, NY; ²Mass2Charge Consulting LLC, Romulus, NY
- TP 258 **Lipidomic Profiling of Gut commensal *Bacteroidales* and Elucidating Immunomodulatory Sphingolipid Biosynthesis**; [Sungwhan Oh](#); Naama Geva-Zatorsky; Wen Zheng; Dennis Kasper; Harvard Medical School, Boston, MA
- TP 259 **Comprehensive Two-Dimensional HPLC Analysis Coupled with Mass Spectrometric Detection and Informative Data Processing for Lipids Analysis**; [Tetsuo Iida](#)¹; Yoshiyuki Watabe¹; Daisuke Nakayama¹; Kanya Tsujii¹; Saki Ueda¹; Kenichiro Tanaka²; Tadayuki Yamaguchi¹; Junichi Masuda¹; Yoshihiro Hayakawa¹; ¹Shimadzu Corporation, Kyoto, Japan; ²Shimadzu Scientific Instruments, Inc., Columbia
- TP 260 **Phospholipid Oxidation Products as Biomarkers for Oxidative Stress in Inflammatory Liver Disease**; Beate Fuchs; University of Leipzig, Leipzig, Germany
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- TP 262 **Lipidomics Approach Reveals Potential Xanthohumol Anti-Obesity Mechanism through Triglycerides Identification and Fatty Acids Composition**; [Jaewoo Choi](#)¹; Cristobal L. Miranda^{1,2}; Hyi-Seung Lee^{1,3}; Hye-Kyeong Kim^{1,4}; Jan F. Stevens^{1,2}; ¹Linus Pauling Institute, Oregon State University, Corvallis, Oregon; ²College of Pharmacy, Oregon State University, Corvallis, Oregon; ³Korea Institute of Ocean Science and Technology, Ansan, South Korea; ⁴The Catholic University of Korea, Bucheon, South Korea
- TP 263 **Lipid Profiling Analysis of Liver Tissues between Obesity-Prone and Obesity-Resistant Mice under High Fat Diet**; [Sunhee Jung](#)^{1,2}; Miso Nam^{1,2}; Youngae Jung¹; Do Hyun Ryu²; Geum-Sook Hwang^{1,3}; ¹Korea Basic Science Institute, Seoul, Republic of Korea; ²Sungkyunkwan University, Suwon, Republic of Korea; ³Graduate School of Analytical Science and Technol, Daejeon, Republic of Korea
- TP 264 **Fetal Sex-dependent Effects of Maternal Obesity on Dysregulation of Lipid Metabolic Pathways in the Placenta**; [Xiaoli Gao](#); Sribalashubashini Muralimanoharan; Susan T Weintraub; Leslie Myatt; Alina Maloyan; UT Health Science Center at San Antonio, San Antonio, TX
- TP 265 **Lipidomics of Marine Microorganisms under Stress. Solving the Needle / Haystack Problem with a Large Database and Open-Source Software**; [Helen Fredricks](#); James Collins; Bethanie Edwards; Benjamin Van Mooy; Woods Hole Oceanographic Institution, Woods Hole, MA
- TP 266 **Lipidomic Discrimination of omega-3 Polyunsaturated Fatty Acid Status in Whole Blood and Dried Blood Spots**; Juan Aristizabal Henao; [Richard W Smith](#); Ken D Stark; University of Waterloo, Waterloo, Canada
- TP 267 **High Resolution LC-MS Demonstrates Serum Triglyceride Composition is Affected Qualitatively and Quantitatively by Interactions of Dietary Fat and Carbohydrate**; [Bruce Kristal](#)^{1,2}; Irina Stavrovskaya¹; Susan Bird^{1,3}; Vasant Marur¹; Caryn Porter^{1,4}; ¹Brigham + Women's Hospital, Boston, MA; ²Harvard Medical School, Boston, MA; ³ThermoFisher (Current), Boston, MA; ⁴Mass General Hospital (Current), Boston, MA
- TP 268 **Can "Classic" Lipid Profiling Data on a QQQ Justify Diving into a Full Profile of the Sphingolipid Pool?** [Todd Williams](#); Lei Jiang; Elias Michaelis; Marylou Michaelis; University of Kansas, Lawrence, KS
- TP 269 **Lipidomic Profiling of Plasma from Patients with Atrial Fibrillation by UPLC/Q-TOF MS**; [Youngae Jung](#)¹; Doo-Hae Lee^{1,2}; Geum-Sook Hwang^{1,2}; ¹KBSI Western Seoul Center, Seoul, Republic of Korea; ²GRAST in Chungnam University, Daejeon, Republic of Korea



- TP 270 **Development of a Comprehensive Monitoring Method of Lipid Mediator Species for Human Plasma Profiling;** Masaki Yamada^{1,2}; Yoshihiro Kita¹; Takahiro Kohira^{1,3}; Suzumi M. Tokuoka¹; Takao Shimizu^{1,4}; ¹The University of Tokyo, Tokyo, Japan; ²Shimadzu Corporation, Kyoto, Japan; ³Japanese Red Cross Society, Tokyo, Japan; ⁴National Center for Global Health and Medicine, Tokyo, Japan
- TP 271 **Comprehensive and Quantitative Analysis of Fatty Acids in Biological Samples by Gas Chromatography-Mass Spectrometry;** Jaeman Byun; Anna Mathew; Subramaniam Pennathur; *University of Michigan, Ann Arbor, MI*
- TP 272 **Lipidomic Profiling of Plasma from Radiation Animal Models;** Jace W. Jones¹; Claire L. Carter¹; Gregory Tudor²; Alexander Bennett¹; Ann Farese¹; Catherine Booth²; Thomas J. MacVittie¹; Maureen A. Kane¹; ¹University of Maryland, Baltimore, MD; ²Epistem Ltd., Manchester, UK
- TP 273 **LC-MS/MS Profiling of Gangliosides in Mouse Retina;** Ashta Lakshmi Prasad Gobburu¹; Dr. Denise M. Inman²; Dr. Renliang Zhang³; Dr. Belinda Willard³; Dr. David J Anderson¹; ¹Cleveland State University, Department of Chemistr, Cleveland, OHIO; ²Northeast Ohio Medical University, Rootstown, Ohio; ³Cleveland Clinic, Cleveland, Ohio
- TP 274 **Comparison of LC-Orbitrap-MS with Infusion-based Shotgun MS for Lipidomic Profiling;** Russell Pickford¹; Magda Montgomery¹; Simon Brown²; Todd W Mitchell²; Nigel Turner¹; ¹University of New South Wales, Sydney, Australia; ²University of Wollongong, Wollongong, Australia
- TP 275 **Lipid Data Analyzer 2: Flexible and Automatic Identification of Lipid Structures in High-Throughput LC-MSⁿ Data from Various Instruments;** Juergen Hartler^{1,2}; Alexander Triebel³; Martin Troetzmueller³; Andreas Ziegler¹; Gerald N. Rechberger⁴; Friedrich Spener⁴; Harald C. Koefeler³; Gerhard G. Thallinger^{1,2}; ¹Bioinformatics, IKD, Graz University of Technology, Graz, Austria; ²Omics Center Graz, Graz, Austria; ³ZMF, Medical University of Graz, Graz, Austria; ⁴Institute of Molecular Biosciences, University of Graz, Austria
- TP 276 **Determining the Potential Underlying Mechanism of Anesthetic-Induced Neurotoxicity in the Developing Monkey Brain Using Shotgun Lipidomics;** Jessica Frisch-Daiello¹; Fang Liu²; Cheng Wang²; Xianlin Han¹; ¹Sanford-Burnham Medical Research Institute, Orlando, FL; ²National Center for Toxicological Research - FDA, Jefferson, AR
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- TP 278 **SIFT-MS - a 24/7 Analytical Technique;** Daniel Milligan¹; John Gray¹; Vaughan Langford¹; Murray McEwan²; ¹Syft Technologies Ltd, Christchurch, New Zealand; ²University of Canterbury, Christchurch, New Zealand
- TP 279 **Automation of Calibration Curve Redaction for Absolute Quantitation by LC/MS;** Lyle Burton; Michael J. Y. Jarvis; *SCIEX, Concord, Ontario*
- TP 280 **Highly Sensitive Quantitative Analysis of Amoxicillin and Clavulanic Acid from Plasma Using LC/MS/MS;** Deepti Bhandarkar; Rashi Kochhar; Shailendra Rane; Shruti Raju; Shailesh Damale; Ajit Datar; Pratap Rasam; Jitendra Kelkar; *Shimadzu Analytical (India) Pvt. Ltd., Mumbai, INDIA*
- TP 281 **Quantification of Total and Free Metal-Based Oncology Drugs Using ICP-MS Methods for Clinical and Pre-Clinical Studies;** Nicole Greer; Xuefei Guo; Elise Snider; Yong-Xi Li; *Medpace Bioanalytical Laboratories, Cincinnati, OH*
- TP 282 **The Control of the Formation and Degradation of Omega-3 Ethyl Esters in Human Plasma;** Luc Bouchard; Genevieve Emond; François Viel; Philippe Bélanger; Nadine Boudreau; Ann Lévesque; *inVentiv Health Clinical, Québec, Canada*
- TP 283 **Low level quantitation of Fluticasone and Salmeterol from plasma using LC/MS/MS;** Shruti Raju; Rashi Kochhar; Shailendra Rane; Deepti Bhandarkar; Shailesh Damale; Ajit Datar; Jitendra Kelkar; Pratap Rasam; *Shimadzu Analytical (India) Pvt. Ltd., Mumbai, INDIA*
- TP 284 **Efficient Method for the Analysis of Ticagrelor and its Metabolite AR-C124910XX in Human EDTA K2 Plasma by LCMSMS;** Pierre-Yves Caron; François Viel; Nadine Boudreau; Ann Lévesque; *inVentiv Health Clinical, Québec, Canada*
- TP 285 **Hydrolysis Conditions Investigation for Analysis of Total Dabigatran in Human Plasma;** Pierre-Yves Caron; Nancy Lampron; François Viel; Nadine Boudreau; Ann Lévesque; *inVentiv Health Clinical, Québec, Canada*
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- TP 287 **Determination of Selenomethionine in Animal Feed by High Performance Liquid Chromatography – Inductively Coupled Plasma – Mass Spectrometry;** Paula Fisher; *Novus International, St. Charles, MO*
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- TP 289 **An Ultra-Sensitive Method for Femtogram Level Detection of Dexamethasone in Human Plasma using LC/MS/MS;** Jason Bilodeau; François Viel; Nadine Boudreau; Ann Lévesque; *inVentiv Health Clinical, Québec, Canada*
- TP 290 **Development and Validation of an LC-MS/MS Method for the Quantification of Hydroxypropyl β -Cyclodextrin in Human Plasma;** Chun-Yi Wu¹; Ihid C. Leao²; James E. K. Hildreth²; Ai-Ming Yu¹; ¹UC Davis PK/PD Bioanalytical Core Facility, Sacramento, CA; ²Dept of Molecular and Cellular Biology, UC Davis, Davis, CA
- TP 291 **Complex Quantification of modified β -Cyclodextrin in Human EDTA K2 Plasma using Monolithic Column by LCMSMS;** Guy Havaard; François Viel; Nadine Boudreau; Ann Lévesque; *inVentiv Health Clinical, Québec, Canada*
- TP 292 **HeadSpace Gas Chromatography-Mass Spectrometry Analysis of Volatile Compounds in Biological Samples;** Wanqing Lu; Aiping Zhu; Nelson Santiago; Yong-xi Li; *Medpace Bioanalytical Laboratories, Cincinnati, OH*
- TP 293 **A Simple LC-MS/MS Method for Determination of Fluticasone Propionate and Salmeterol Xinafoate in Human Plasma at pg/mL Level;** Huafang Jiang; Peipei Zhang; Hongxia Chai; Xiaohang Shen; Xin Zhang; Wenzhong Liang; *WuXi AppTec (Shanghai) Co. Ltd., Shanghai, China*
- TP 294 **Determination of Digoxin in Human Urine Using High Performance Liquid Chromatography-mass Spectrometry;** Wuyi Zha; Runlan Huo; Mohamed Osman; Jinn Wu; Xinpeng Fang; *XenoBiotic Laboratories, Inc., WuXi AppTec, Inc, Plainsboro Township, NJ*

- TP 295 **A Sensitive LC-MS/MS Method for Quantitation of Buprenorphine and Norbuprenorphine in Human Plasma;** Xinping Fang; Dawei Zhou; Shu Zhang; Jinn Wu; *XenoBiotic Laboratories, Inc., WuXi AppTec, Inc., Plainsboro, NJ*
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- TP 297 **Impurity Characterisation of the Fungicide Flutriafol using Liquid Chromatography and Time of Flight MS Detection to Aid Pesticide Product Registration;** Marian Twohig¹; Oliver Burt²; Gordon Fujimoto³; Peter Lee¹; John McCauley⁴; ¹Waters Corporation, Milford, MA; ²Waters Corporation, Wilmslow, UK; ³Waters Corporation, Beverly, MA; ⁴Waters Corporation, New Castle, DE
- TP 298 **LC/MS/MS Analysis of Urinary Biomarkers of the Fungicide Pyrimethanil following Experimental Exposure in Humans;** Moosa Faniband; Eva Ekman; Margareta Littorin; Margareta Maxe; Bo A. Jönsson; Christian Lindh; *Lund University, Lund, Sweden*
- TP 299 **Highly Sensitive Determination of Acidic Pesticides Residues in Agricultural Commodities by Paired Ion Electro Spray Ionization (PIESI) Mass Spectrometry;** Hongyue Guo^{1,2}; Leah Riter¹; Chad Wujcik¹; Daniel Armstrong²; ¹Monsanto, St Louis, MO; ²University of Texas at Arlington, Arlington, TX
- TP 300 **Novel Approach to Sample Preparation for Contaminant Analysis in Food using the Thomson eXtreme Filter Vials® by LC-MS/MS and GC-MS;** Samuel Ellis; Lisa Wanders; *Thomson Instrument Company, Oceanside, CA*
- TP 301 **Direct Determination of Trace Hormones in Drinking Water by Large Volume Injection at Sub ng/L Levels Using LC-MS/MS;** David R. Baker; Neil J Loftus; *Shimadzu, Manchester, UK*
- TP 302 **Supercritical Fluid Chromatography Triple-Quadrupole Mass Spectrometry: An Alternative to LC/MS/MS for High-Sensitivity and -Throughput Analysis of Multiresidue Pesticides;** Yoshihiro Izumi^{1,2}; Eiichiro Fukusaki²; Takeshi Bamba^{1,2}; ¹Medical Institute of Bioregulation, Kyushu Univ., Fukuoka, Japan; ²Dept. Biotech., Grad. Sch. Eng., Osaka Univ., Osaka, Japan
- TP 303 **Structural Elucidation and Estimation of the Acute Toxicity of the Major UV-Visible Photoproduct of Fludioxonil – Detection in Grape Samples;** Yannick Lassalle; Édith Nicol; Christophe Genty; Sophie Bourcier; Stéphane Bouchonnet; *LCM UMR-9168, École Polytechnique, Palaiseau, France*
- TP 304 **Rapid Screening of the Potential Chemical Contaminants in Underground Water Using UHPLC-QTOF Mass Spectrometry;** Jing Guo¹; Bing Du¹; Meiling Lu²; Jerry Zweigenbaum³; Thomas Glauner⁴; Yeru Huang¹; ¹Natl Res Center for Environ Anal Measurement, Beijing, China; ²Agilent Technologies (China) Limited, Beijing, China; ³Agilent Technologies US, Wilmington, DE; ⁴Agilent Technologies GmbH, Waldbronn, Germany
- TP 305 **Direct Analysis of Pharmaceuticals and Personal Care Products (PPCPs) in Environmental Waters using a Newly Developed Triple Quadrupole Mass Spectrometer;** Jian-Zhong Li²; Michael Thurman⁴; Imma Ferrer⁴; Craig Marvin³; Anabel Fandino¹; Na Pi Para¹; ¹Agilent Technologies, Inc., Santa Clara, CA; ²Agilent Technologies, Inc., Beijing, China; ³Agilent Technologies, Wilmington, DE; ⁴University of Colorado, Boulder, Colorado
- TP 306 **Applications of a Novel, High Performance LC-MS/MS Ion Source;** Heather Gamble¹; Sha Joshua Ye¹; Ellie Majdi¹; Donald Gamble²; ¹IONICS Mass Spectrometry Group, Bolton, ON; ²St. Mary's University, Halifax, Canada
- TP 307 **Cross Validation between LDTD-MS/MS and LC-MS/MS for 5 Neonicotinoids Insecticides in Water;** Gregory Blachon; Alex Birsan; Serge Auger; Jean Lacoursière; Pierre Picard; *Phytronix Technologies, Inc., Quebec, QC*
- TP 308 **Development of Electrochemical Methods Capable of Mimicking Oxidative Degradation Pathway of Model Pharmaceuticals;** Marc-André Lecours; Gessie Brisard; Pedro A. Segura; *University of Sherbrooke, Sherbrooke, Canada*
- TP 309 **Measuring a Slice of the Exposome: Targeted GC-MS/MS Analysis of Persistent Organic Pollutants (POPs) in Small Volumes of Human Plasma;** Anthony Macherone^{1,2}; Sarah Daniels³; Alex L. Maggitti⁴; Melissa Churley¹; Matthew McMullin⁴; Martyn T. Smith³; ¹Agilent Technologies, Wilmington, DE; ²Johns Hopkins School of Medicine, Baltimore, MD; ³University of California, Berkeley, CA; ⁴NMS Labs, Willow Grove, PA
- TP 310 **Fate of Anti-Inflammatory Drug Diclofenac in Municipal Wastewater Treatment Plant: Quantification using LDTD Coupled with Tandem Mass Spectrometry;** Linson Lonappan¹; Rama Pulicharla¹; Serge Auger²; Satinder K. Brar¹; Mausam Verma³; Roa Y. Surampalli⁴; ¹INRS-ETE, Université du Québec, Québec, Canada; ²Phytronix Technologies, Quebec, Canada; ³CO2 Solutions Inc., Quebec, Canada; ⁴University of Nebraska-Lincoln, Lincoln, NE
- TP 311 **Determination of leachables in Orally Inhaled and Nasal Drug Products (OINDP) by GCMS/MS;** Prashant Hase; Ankush Bhone; Durvesh Sawant; Dheeraj Handique; Sanket Chiplunkar; Ajit Datar; Jitendra Kelkar; Pratap Rasam; *Shimadzu Analytical India Pvt. Ltd., Mumbai, India*
- TP 312 **Comparative Quantitation of Calibration Methods in Surface Water Analysis Using Online Preconcentration with Orbitrap Mass Spectrometry;** Jaewon Choi¹; Wonseok Choi¹; Yun S. Kim¹; Charles Yang²; Dipankar Ghosh²; ¹K-water, 200 Shintanjinro Daeduck, KOREA; ²Thermo Fisher Scientific, San Jose, CA
- TP 313 **Atmospheric Pressure Ionization Coupled to Tandem Quadrupole Mass Spectrometry for the Analysis of Pyrethroids in Waste Water;** Adam Ladak¹; Lauren Mullin³; Hernando Olivos¹; Douglas Stevens²; ¹Waters, Beverly, MA; ²Waters, Milford, MA; ³MTM Research Centre, Örebro University, Örebro, Sweden
- TP 314 **Application of LC-MS/MS for the Improved Detection of Pesticides in Cannabis Samples;** Jared Russell¹; Jeff Dah²; Liling Fang¹; Willard Bankert¹; ¹Shimadzu Scientific Instruments, Pleasanton, CA; ²Shimadzu, Columbia, MD
- TP 315 **Fast and sensitive analysis of drug residues in water using on line SPE-UHPLC-MS/MS with ultra-fast polarity switching;** Mikael LEVI¹; Caroline DUFOUR²; Isabelle VECCHIOLI²; Stephane MOREAU³; ¹Shimadzu France, Noisiel, France; ²CARSO-LSEHL, Lyon, France; ³Shimadzu Europe GmbH, Duisburg, Germany
- TP 316 **Research and Identification of Veterinary Antibiotic Residues in Environmental and Biological Matrices using LC-HESI-HRMS;** Morgan Sollie; Audrey Roy-Lachapelle; Sébastien Sauvé; *Université de Montréal, Montréal, Canada*
- TP 317 **Transformation of Antidepressant Pharmaceuticals During Chlorination Disinfection Processes in Wastewater Treatment;** Melissa M. Schultz; Derrick Marshall; Kent Nakamoto; *The College of Wooster, Wooster, OH*
- TP 318 **Screening and Quantitation of Micro Pollutants from Sewage Water in the Process of Bank Filtration Using UHPLC-HRMS;** Patricia van Baar¹; Florian Wode¹; Uwe Duennbier¹; Maciej Bromirski²; Olaf Scheibner²; ¹Berliner Wasserbetriebe, Berlin, Germany; ²Thermo Fisher Scientific, Bremen, Germany

- TP 319 **Highly Sensitive Detection of Pharmaceuticals and Personal Care Products (PPCPs) in Water Using Direct Injection**; Dan-Hui Dorothy Yang; Yanan Yang; *Agilent Technologies, Inc, Santa Clara, CA*
- TP 320 **Comparison of matrix effects in multi-residue pesticide analysis when using online SPE or direct injection in Liquid Chromatography-tandem Mass Spectrometry**; Sigrid Baumgarten¹; Vincent Gohier²; Mikael Levi¹; ¹*Shimadzu France, Noisiel, France*; ²*Laboratoire Départemental d'Analyse de Corrèze, Tulle, France*
- TP 321 **Quantitative Analysis of Source Water PPCP by Offline SPE with Orbitrap MS and LC-Tandem MS**; Jaewon Choi¹; Wonseok Choi¹; Yun S. Kim¹; Charles T. Yang²; Dipankar Ghosh²; ¹*Kwater, Daejeon, South Korea*; ²*Thermo Fisher Scientific, San Jose, California*
- TP 322 **Screening and Quantitation of 240 Pesticides in Difficult Food Matrices Using the Agilent 6545 QTOF Mass Spectrometer**; Dorothy Yang; Christian Klein; Crystal Cody; Huy Bui; *Agilent Technologies, Inc, Santa Clara, CA*
- TP 323 **Environmental Site Assessment using LC/MS/MS and GC/MS for Phenoxy Family of Pesticides: Data Comparison**; Vyacheslav N. Fishman; Ying Yang; *The Dow Chemical Company, Midland, MI*
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- TP 324 **Simultaneous Determination of Allergens in Food Products Discovered to Validated Using Microfluidic Chip-Based Nano-Liquid Chromatography/Quadrupole Time Of Flight(Chip/Q-TOF) and Ultra High Performance Liquid Chromatography Ifunnel/Tandem Mass Spectrometry(iFunnel/QQQ)**; Wen-Yen Lee; Shan-An Chan; *Agilent, Taipei, Taiwan*
- TP 325 **High Sensitive Detection and Quantification of Synthetic PDE-5 Inhibitors Drugs and Analogues Adulterated in Health Supplements Using LC/MS/MS**; Zhe Sun; Jie Xing; Zhaoqi Zhan; *Customer Support Centre, Singapore (Asia Pacific) Pte Ltd, 79 Science Park Drive, #02-01/08, Singapore 118264*
- TP 326 **Food Contact Material (FCM) Migration Study using HR-LCMS and Novel Software Database Suite**; Allan Brown¹; Kate Comstock²; Ekong Bassy²; David Kage²; Daniel Quinn²; ¹*Scholle Packaging, Northlake, IL*; ²*Thermo Fisher Scientific, San Jose, CA*
- TP 327 **Direct Detection of Chlorpyrifos in Honey by Neutral Desorption-Extractive Electrospray Ionization Mass Spectrometry**; Xingxing Liu¹; Li-Ping Luo¹; Xiaowei Fang²; Eric Handberg²; Huanwen Chen²; ¹*School of Life Sciences, Nanchang University, Nanchang, China*; ²*East China Institute of Tech., Nanchang, China*
- TP 328 **Differentiating Rice Varieties by SPME-GC-MS and NMR Chemical Profiling**; Xinyi Wang; Peter B. Harrington; *Department of Chemistry and Biochemistry, Ohio U, Athens, OH*
- TP 329 **Atmospheric Pressure Ionization GC Coupled to Time of Flight Mass Spectrometry for the Analysis of Agriculture Residues in Food Safety**; Gordon Fujimoto¹; Andrew Baker²; Adam Ladak¹; Kerri Smith¹; ¹*Waters Corporation, Beverly, MA*; ²*Waters, Inc., Pleasanton, CA*
- TP 330 **LC-MS/MS Analysis of Perfluoroalkyl Acids in Environmental Samples, Food Packaging Material and Food – A Migration and Accumulation Study**; Andre Schreiber¹; Liesl Krone²; KC Hyland³; Tom Biesenthal¹; Tanya Gamble¹; Chris Higgins⁴; ¹*SCIEX, Concord, Canada*; ²*Granbury High School, Granbury, TX*; ³*SCIEX, Redwood City, CA*; ⁴*Colorado School of Mines, Golden, CO*
- TP 331 **Investigating the Impact of Frozen Storage on the Anthocyanin Content of American Elderberry Fruit Juice Using Mass Spectrometry**; Mitch Johnson¹; Andrew Thomas^{2,3}; C. Michael Greenleaf^{1,2}; ¹*University of Missouri, Columbia, MO*; ²*Center for Botanical Interaction Studies, MU, Columbia, MO*; ³*Southwest Research Center, University of Missouri, Mt. Vernon, MO*
- TP 332 **Quantitative Determination of Seven Fluorescent Whitening Agents Migration of paper cups by High Performance Liquid Chromatography Tandem Mass Spectrometry**; ZhiFeng Du¹; XinDong Guo²; JinFeng Huang²; LiJun Li³; WenHai Jin⁴; HuaFen Liu⁵; HuaiEn Zhu⁴; ¹*Sciex, GuangZhou, China*; ²*National Centre for Quality Supervision, GuangZhou, China*; ³*Sciex, BeiJing, BeiJing*; ⁴*Sciex, ShangHai, China*; ⁵*Sciex, America, America*
- TP 333 **HR-LCMS and GC-MS/MS Analyses of Non-Intentionally Added Substances and other Migrants from Plastic Food Contact Materials**; Ian Cooper¹; Andrew Feilden²; Kate Comstock³; Cristian Cojocariu⁴; Paul Silcock⁴; ¹*Smithers Pira, Leatherhead, UK*; ²*Smithers Rapra, Shrewsbury, UK*; ³*Thermo Fisher Scientific, San Jose, CA*; ⁴*Thermo Fisher Scientific, RunCorm, UK*
- TP 334 **Quantitative Analysis of Illegal Dyes in Eggs Using LC/MS/MS**; Rashi Kochhar; Shailendra Rane; Shruti Raju; Deepti Bhandarkar; Shailesh Damale; Ajit Datar; Jitendra Kelkar; Pratap Rasam; *Shimadzu Analytical (India) Pvt. Ltd., Mumbai, INDIA*
- TP 335 **Simultaneous Determination of 20 Polyfluoroalkane Substances in Dietary Milk by QuEChERS Combining with On-Line Interference Trapping LC-MS/MS**; Yucheng Yu¹; Dunming Xu¹; Meiling Lu²; Shan Zhou²; Yu Zhou¹; ¹*Xiamen Entry-Exit Inspection and Quarantine Bureau, Xiamen, CN*; ²*Agilent Technologies (China) Limited, Beijing, China*
- TP 336 **Puff by puff investigation of New Smoking Products such as e-cigarettes and 'Heat-Not-Burn' Devices Using Online Photoionization Mass Spectrometry**; Sven Ehlert¹; Andreas Walte²; Ralf Zimmermann¹; ¹*University of Rostock, Rostock, Germany*; ²*Photonion GmbH, Schwerin, Germany*
- TP 337 **Illegal Color Dyes in Food Matrix for Multi-Compounds Analysis with Agilent 6460QQQ and 6545Q-TOF**; Shao-Zhen Wang¹; Yong Zhou²; Ping-Ya Wang²; Ai Chen²; Li Huang²; Jin-Lan Sun¹; Heng-Tao Dong¹; Chun-Ye Sun¹; ¹*Agilent Technology, Inc., Shanghai, China*; ²*Institute for Food and Drug Control, Zhoushan, China*
- TP 338 **Determination of Chemical Contaminants in Marine Fish by GCMS/MS using QuEChERS as an Extraction Method**; Ankush Bhone; Durvesh Sawant; Dheeraj Handique; Prashant Hase; Sanket Chiplunkar; Ajit Datar; Jitendra Kelkar; Pratap Rasam; *Shimadzu Analytical (India) Pvt. Ltd., Mumbai, INDIA*
- TP 339 **The Analysis of Chlorinated Dioxins, Difurans and Polychlorinated Biphenyls in Edible Oils**; Justin Blau; Greg Jeter; *Fluid Management Systems, Watertown, MA*
- TP 340 **The Analysis of Chlorinated Dioxins and Difurans in Pet Food**; Greg Jeter; Ryan Balgos; *Fluid Management Systems, Watertown, MA*
- TP 341 **Determination of Brominated Fatty Acids in Brominated Vegetable Oils and Commercial Beverages by UPLC-MS-MS**; Priyanka Chitranshi; Goncalo Gamboa Da Costa; *FDA/NCTR, Jefferson, AR*
- TP 342 **Analysis of Mercury in Grouper by ICP MS: An Evaluation of Mercury Levels in the Commercial Catch**; Marc E. Engel; *FDACS, Tallahassee, FL*
- TP 343 **Analysis of Mycotoxins Using LC-MS/MS and a QuEChERS Sample Preparation Approach**; Brian Kinsella; *UCT, Bristol, PA*
- TP 344 **Development of an Interface for the Analysis of Volatiles Using a Portable Mass Spectrometer**; Pilar Perez Hurtado¹; Elliott Palmer¹; Clive Aldcroft²; Hanna More²; Baker Andrew²; Mark Allen²; Jamey Jones²; Matthew Turner¹; Jim Reynolds¹; ¹*Loughborough University, Loughborough, UK*; ²*Advion UK Ltd, Essex, UK*

- TP 345 **Analysis of 7 Plasticizers Released from Microwave-Treated Food Wraps Using GC-MS;** Matt S. Chang; Sheng Hsiung Yang; Jermiah Y. Shen; Gaston J. Wu*; *Department of Chemistry, NTNU, Taipei City, Taiwan (R.O.C.)*
- TP 346 **Low Level Quantitation of Steroids in Milk Using LC/MS/MS;** Durvish Sawant; Rashi Kochhar; Shaileendra Rane; Shruti Raju; Deepti Bhandarkar; Shailesh Damale; Ajit Datar; Jitendra Kelkar; Pratap Rasam; *Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India*
- TP 347 **Rapid Authentication of Mixed Edible Oils by Matrix-assisted Laser Desorption/Ionization Mass Spectrometry;** Tsz-Tsun Ng; Pui-Kin So; Bo Zheng; Zhong-Ping Yao; *The Hong Kong Polytechnic University, Hong Kong, China*
- TP 348 **ICP-MS Method for the Determination of Boric Acid in Caviar;** Jung Bok Kim¹; Jang So-Young¹; Kim Joo Taek¹; Kim Myung Chul¹; Lee Ok Hwan²; Shin Jae Wook¹; ¹*Korea Advanced Food Research institute, Seocho-Gu, KOREA*; ²*Kang-Won National University, Chuncheon, Korea*
- TP 349 **High Sensitivity Analysis of Diarrhetic Shellfish Poisoning (DSP) Toxins Using Liquid Chromatography Tandem Mass Spectrometry;** Manami Kobayashi¹; Miho Kawashima²; Satoshi Yamaki¹; Yoshihiro Hayakawa³; ¹*Shimadzu Corporation, Kanagawa, Japan*; ²*Shimadzu Corporation, Tokyo, Japan*; ³*Shimadzu Corporation, Kyoto, Japan*
- TP 350 **Determination of a Single Methodology for the Analysis and Quantitation of Multi-class Veterinary Drugs in Different Animal Matrices;** Ed George; Charles T. Yang; Dipankar Ghosh; Mary Blackburn; *Thermo Fisher Scientific, San Jose, CA*
- TP 351 **Accurate Multi-Mycotoxin Quantification in Feed Materials Using LC-MS/MS Methods and Isotopic or Structural Analog Dilution Strategies Revolutionize Mycotoxin Occurrence Understanding;** Alexandros Yiannikouris; Joshua Martinez; Steve Mobley; *Alltech Inc., Nicholasville, KY*
- TP 352 **Rapid Screening and Confirmation of PDE5 Inhibitors in Dietary Ingredients by DART-MS Ambient Ionization;** Robert Goguen; Julie Carbonello; Elizabeth Crawford; Brian D. Musselman; *IonSense, Inc., Saugus, MA*
- TP 353 **ELISA-based Screening for Alternative Nitrogenous Economic Adulterants in Milk Proteins;** Nicholas Cellar¹; Michael Farrow¹; Nicholas Baldauf²; Todime M. Reddy¹; ¹*Abbott, Columbus, OH*; ²*Advance Testing Laboratories, Cincinnati, OH*
- TP 354 **Study on Carbosulfan Metabolites in Vegetable by Ultra-High Performance Liquid Chromatography Tandem Quadrupole-Time Of Flight Mass Spectrometry;** Jianzhong Li; Tao Bo; *Agilent Technologies(China), Beijing, China*
- TP 355 **Quantitation of Chloramphenicol and Nitrofurantol Metabolites in Aquaculture Products Using Microwave-Assisted Derivatization, Automated Solid-Phase Extraction and LC-MS/MS;** Brian Veach; *Food and Drug Administration, Jefferson, AR*
- TP 356 **Simultaneous Identification of Multiple β -Lactamases in *Acinetobacter baumannii* using Liquid Chromatography-Tandem Mass Spectrometry;** Hein Trip¹; Katrin Mende²; Joanna Majchrzykiewicz-Koehorst¹; Norbert Sedee¹; Albert Hulst¹; Hugo-Jan Jansen³; Clinton Murray²; Armand Paauw¹; ¹*CBRN Protection, TNO, Rijswijk, The Netherlands*; ²*Department of Medicine, San Antonio Military Medical Center, Fort Sam Houston, TX*; ³*Expert Centre Force Health Protection, MoD, Doorn, The Netherlands*
- TP 357 **Rapid detection of Fluoroquinolone-Resistant *Escherichia coli* using Mass Spectrometry;** Tiphaine Cecchini^{1,2}; Silpak Biswas³; Tanguy Fortin^{1,4}; Marc Galimand³; Gilles Zambardi⁵; Xavier Lacoux¹; Arnaud Salvador²; Gaspard Gervasi¹; Jerome Lemoine²; Patrice Courvalin³; Jean-Philippe Charrier¹; ¹*bioMerieux, Marcy L'Etoile, France*; ²*ISA, Unit 5280 CNRS/UCBL-1, Villeurbanne, France*; ³*Unité des Agents Antibactériens, Institut Pasteur, Paris, France*; ⁴*Anaquant, Villeurbanne, France*; ⁵*bioMerieux, La Balme-Les-Grottes, France*
- TP 358 **Label-Free Quantitation Reveals the Importance of Host Cell Arginine Uptake in *Francisella phagosome* Escape and Ribosomal Protein Amounts;** Cerina Chhuon^{1,3}; Elodie Ramond^{2,3}; Gael Gesbert^{2,3}; Ida Chiara Guerrero^{1,3}; Marion Dupuis^{2,3}; Mélanie Rigard⁴; Thomas Henry⁴; Monique Barel^{2,3}; Alain Charbit^{2,3}; ¹*Proteomics Platform Necker, Paris, France*; ²*INSERM U1151, Institut Necker-Enfants Malades, Paris, France*; ³*Université Paris Descartes, Sorbonne Paris Cité, Paris, France*; ⁴*Centre International de Recherche en Infectiologie, Lyon, France*
- TP 359 **Application of Mass Spectrometry as a Confirmatory Tool for *Campylobacter* Species Identification;** Philippe Raymond¹; Rebecca A Guy²; Maxime Gosselin-Théberge²; Sylvianne Paul¹; ¹*Canadian Food Inspection Agency, St-Hyacinthe, Canada*; ²*Public Health Agency of Canada, St-Hyacinthe, Canada*
- TP 360 **Enhanced Detection and Identification of Shiga toxin 1 and 2 from Pathogenic Bacteria by MALDI-TOF-TOF-MS/MS-PSD and Top-Down Proteomic Analysis;** Clifton K. Fagerquist; William J. Zaragoza; *USDA/ARS, Albany, CA*
- TP 361 **Top-Down Analysis of Penicillin Binding Protein 2a from Methicillin Resistant *Staphylococcus aureus*;** Jason Neil¹; Helene Cardasis¹; Ping Yip¹; Vikrant Gohil¹; Alexander Cherkassky¹; James Stephenson²; ¹*Thermo Fisher Scientific, Cambridge, MA*; ²*Thermo Fisher Scientific, Raleigh, NC*
- TP 362 **MALDI-TOF-MS for the Differentiation of Strains of Cyanobacteria by Their Secondary Metabolites Profile;** João Luiz Bronzel Junior; Milena Luizete; Ana C. Codo; Humberto Milagre; *UNESP - Univ Estadual Paulista - Institute of Chem, Araraquara, Brazil*
- TP 363 **MALDI-TOF-MS Identification and Characterization of Fungal Pathogens Associated with Cereal Grains;** Kumaran Sivagnanam¹; Helene Perreault²; Tom Gräfenhan¹; ¹*Canadian Grain Commission, Winnipeg, Canada*; ²*University of Manitoba, Winnipeg, Canada*
- TP 364 **Monitoring Chemical Communication and Chemotypical Differentiation in *Pseudomonas aeruginosa* Microbial Communities Using Confocal Raman Microscopy and Secondary Ion Mass Spectrometry;** Sage Dunham¹; Nameera Baig²; Nydia Morales-Soto²; Eric Lanni¹; Joshua Shrouf²; Paul Bohn²; Jonathan Sweedler¹; ¹*University of Illinois at Urbana Champaign, Urbana, IL*; ²*University of Notre Dame, Notre Dame, IN*
- TP 365 **MALDI Biotyper Analysis of Microorganisms Present in Saliva of Chronic Kidney Disease Individuals and their Association with Periodontal Disease;** Levy Alves¹; Taciana Couto¹; Ana Ciamponi¹; Marcelo Fava²; Meriellen Dias³; Maria Anita Mendes³; ¹*Faculdade de Odontologia - São Paulo University, Sao Paulo, Brazil*; ²*Faculdade de Medicina - São Paulo University, São Paulo, Brazil*; ³*Engenharia Química - Poli - São Paulo University, São Paulo, Brazil*
- TP 366 **Metaproteomic Analysis of Human Cervical-Vaginal Fluid in Residual Pap Tests: Insights into the Cervical Microbiome;** Somaieh Afiani-Zadeh¹; Pratik Jagtap²; Timothy Griffin¹; Marnie Peterson¹; Amy Skubitz²; ¹*University of Minnesota, Minneapolis, MN*; ²*Center for Mass Spectrometry and Proteomics, UMN, St.Paul, MN*



- TP 367 **Glycoproteins with Fucosylated O-glycans are Associated with the Nuclear Membrane of Toxoplasma gondii**; [Edwin M Motari](#)¹; Giulia Bandini¹; Catherine E. Costello²; Samuelson John¹; ¹Boston University School of Dental Medicine, Boston, MA; ²Boston University School of Medicine, Boston, MA
- TP 368 **Identification of Food Borne Microorganism by MALDI-TOF MS**; Miyoung Ha²; Eun Kyoung Choi¹; Jun Young Yang¹; Jooyeon Oh¹; [Sung Hun Kim](#)¹; Yongsun Kim¹; Kyu H Park¹; ¹ASTA, Suwon-Si, South Korea; ²Nonghyup Food Safety Research Institute, Seoul, South Korea
- TP 369 **Analysis of Intact Cowpea Mosaic Virus by MALDI TOF Mass Spectrometry Incorporating Superconducting Tunnel Junction Cryodetection**; Logan Plath¹; Jonathan Feldman¹; Anna Czapar²; Nicole Steinmetz²; [Mark E. Bier](#)¹; ¹Carnegie Mellon University, Pittsburgh, PA; ²Case Western Reserve University, Cleveland, OH
- TP 370 **Dental Plaque meta-omics for Diagnosis of Oral and Systemic Disease**; [Timothy W. Rhoads](#)¹; Nicholas W. Kwiecien¹; Anna E. Merrill¹; Michael S. Westphal¹; Sanjay Shukla²; Amit Acharya²; Joshua J. Coon¹; ¹University of Wisconsin, Madison, WI; ²Marshfield Clinic Research Foundation, Marshfield, WI
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- TP 371 **Structural Dynamics of the 180 kDa HIV-1 Initiation Complex Investigated Using Hydrogen-Deuterium Exchange Mass Spectrometry**; [Devrishi Goswami](#)¹; Steve Tuske²; Bruce D. Pascal³; Joseph D. Bauman²; Disha Patel²; Eddy Arnold²; Patrick R. Griffin¹; ¹The Scripps Research Institute, Jupiter, FL; ²Center for Advanced Biotechnology and Medicine, De, Piscataway, NJ; ³Informatics core, The Scripps Research Institute, Jupiter, FL
- TP 372 **Revealing the Architecture of Protein Complexes by an Orthogonal Approach Combining HDXMS, CXMS and Disulphide Trapping**; [Kunhong Xiao](#)¹; Sheng Li²; ¹Duke University Medical Cent, Durham, NC; ²University of California at San Diego, La Jolla, CA
- TP 373 **Electrostatics-Driven Conformational Dynamics of Cellobiose Dehydrogenase Probed by Structural Mass Spectrometry**; [Alan Kadek](#)^{1,2}; Roland Ludwig³; Petr Halada¹; Petr Man^{1,2}; ¹Institute of Microbiology CAS, Prague, Czech Republic; ²Faculty of Science, Charles University in Prague, Prague, Czech Republic; ³U. of Natural Resources and Applied Life Sciences, Vienna, Austria
- TP 374 **Identifying Dynamical Profiles Associated with Toxicity of Rexinoid X Receptor Agonist by use of Hydrogen Deuterium Exchange Mass Spectrometry**; [Emily Cowart](#); Amanda Proper; Matthew Renfrow; Donald Muccio; University of Alabama at Birmingham, Birmingham, AL
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- TP 376 **Combining HDX-MS, Raman and SAXS Provides Low Resolution Models of a Large Intrinsically Disordered Protein, which Folds upon Ligand Binding**; [Darragh Patrick O'Brien](#)¹; Véronique Hourdel¹; Belen Hernandez²; Patrice Vachette³; Ana-Cristina Sotomayor-Pérez¹; Mahmoud Ghomi²; Julia Chamot-Rooke¹; Daniel Ladant¹; Dominique Durand³; Sébastien Brier¹; Alexandre Chenal¹; ¹Institut Pasteur, Paris, France; ²Université Paris 13, Paris, France; ³Université Paris-Sud, Paris, France
- TP 377 **Mapping Calmodulin-Induced Conformational Changes during Activation of Neuronal Nitric Oxide Synthase by H/D Exchange Mass Spectrometry**; [Eric Underbakke](#)¹; Brian Smith²; ¹Iowa State University, Ames, IA; ²Medical College of Wisconsin, Milwaukee, WI
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- TP 379 **Structural Changes during Dimerization of the Type IV Pilin from Pseudomonas aeruginosa strain K122-4 Measured by Time-Resolved Hydrogen-Deuterium Exchange**; [Cristina Lento](#); Gerald Audette; Derek Wilson; York University, Toronto, Canada
- TP 380 **Probing Conformational Changes Occurring at the Calmodulin Interface upon Adenylate Cyclase Binding Using HDX-MS and Statistical Analysis**; Darragh Patrick O'Brien; Stevann Volant; Véronique Hourdel; Maryline Davi; Marie-Agnes Dillies; Daniel Ladant; Julia Chamot-Rooke; Alexandre Chenal; [Sébastien Brier](#); Institut Pasteur, Paris, France
- TP 381 **Changes in Structural Conformation of the C-terminal Domain of Human La Protein upon RNA binding by Hydrogen/Deuterium Exchange Mass Spectrometry**; [Kerene Brown](#); Mark Bayfield; Derek Wilson; York University, Toronto, ON
- TP 382 **Curli Amyloid Protein Aggregation Studies by HDX Mass Spectrometry**; [Hanliu Wang](#); Qin Shu; Don L. Rempel; Carl Frieden; Michael L. Gross; Washington University, St Louis, MO
- TP 383 **Dynamic Changes during Acid-Induced Activation of Influenza Hemagglutinin**; [Natalie Garcia](#); Miklos Guttman; Jamie Ebner; Alexander Mileant; Lee Kelly; University of Washington, Seattle, WA
- TP 384 **Correlating Dynamic Conformational Sampling to Enzyme Catalysis: A Millisecond Timescale Hydrogen/Deuterium Exchange Mass Spectrometry Approach**; [Peter Liuni](#); Derek Wilson; Department of Chemistry, York University, Toronto, ON
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- TP 385 **Top-Down Quantitative Proteomics Reveals Novel Mechanistic Insights in Acute Myocardial Infarction**; [Zachery Gregorich](#); Ying Peng; Ying-Hua Chang; Lichen Xiu; Santosh Valeja; Ying Ge; UW Madison, Madison, WI
- TP 386 **Automated Glyco-Proteoform Network Analysis (PNA) on Top-Down MS (TDMS) Datasets**; [Steven M. Patrie](#)^{1,2}; John Corbett^{1,2}; Daniel Plymire¹; ¹University of Texas Southwestern Medical Center, Dallas, TX; ²University of Texas at Dallas, Richardson, TX
- TP 387 **Rapid Generation of Accurate Information on Proteoforms Distribution and Relative Abundance by UHR-QTOF MS**; Schmit Pierre-Olivier¹; Wolfgang Jabs²; Stuart Pengelley²; Christian Albers²; Klaus Meyer²; [Matt Willets](#)³; ¹Bruker Daltonique S.A., Wissembourg, France; ²Bruker Daltonik GmbH, Bremen, Germany; ³Bruker Daltonics, Billerica, MA
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- TP 389 **pTop 1.0: a Highly Efficient Search Engine for Intact Protein Identification**; [Lan Luo](#); Rui-Xiang Sun; Long Wu; Hao Chi; Chao Liu; Si-Min He; Institute of Computing Technology, CAS, Beijing, China
- TP 390 **Improving Top-Down Proteomics Sequence Coverage through Complementary Fragmentation Approaches**; [Si Wu](#)¹; Da Meng³; Li Cao⁴; Ljiljana Pasa-Tolic³; Xiaowen Liu²; ¹University of Oklahoma, Norman, OK; ²IUPUI, Indianapolis, IN; ³Pacific NW Nat'l Lab, Richland, WA; ⁴vaccine production program laboratory, Gaithersburg, MD
- TP 391 **A Searchable Public Repository for Archiving Known Proteoforms**; [Ryan Fellers](#); Richard Leduc; Bryan Early; Joseph Greer; Paul Thomas; Neil L. Kelleher; Northwestern University, Evanston, IL

- TP 392 **Top-down MS Analysis of Membrane-bound Light Harvesting Complex 2 from Purple Bacteria;** Yue Lu; Hao Zhang; Michael L. Gross; Robert E. Blankenship; *Washington University, St Louis, MO*
- TP 393 **Optimizing Top Down Analysis of Proteins on an Orbitrap Fusion Tribrid Mass Spectrometer;** Seema Sharma¹; Parag Mallick²; Tanya Stoyanova³; Christopher Mullen¹; Chad Weisbrod¹; Jesse Canterbury¹; David Horn¹; Vlad Zabrouskov¹; ¹*Thermo Fisher Scientific, San Jose, CA*; ²*Stanford University, Stanford, CA*; ³*University of California Los Angeles, Los Angeles, CA*
- TP 394 **Characterization of Tropomyosin Proteoforms in Skeletal Muscle by Top-Down Mass Spectrometry;** Yutong Jin; Ying Peng; Yi-Chen Chen; Timothy Hacker; Ying Ge; *University of Wisconsin-Madison, Madison, WI*
- TP 395 **Optimization of LC/MS Intact /Top-Down Protein Analysis on an Orbitrap Fusion Mass Spectrometer;** Rosa Viner; Seema Sharma; Jesse D. Canterbury; David Horn; Vlad Zabrouskov; *Thermo Fisher Scientific, San Jose, CA*
- TP 396 **In-Line Separation by Capillary Electrophoresis prior to Analysis by Top-Down Mass Spectrometry Enables Sensitive Characterization of Protein Complexes;** Xuemei Han¹; Aaron Aslanian¹; Bryan Fonslow^{1,2}; Daniel McClatchy¹; Beth Graczyk³; Trisha N. Davis³; John Yates¹; ¹*The Scripps Research Institute, La Jolla, CA*; ²*AB SCIEX, San Diego, CA*; ³*University of Washington, Seattle, WA*
- TP 397 **Exploring Depth and Breadth of a Protein Complex Mixture with Top-Down Data-Independent Acquisition Using an Orbitrap Fusion Tribrid Mass Spectrometer;** Aaron Bailey; David Horn; Seema Sharma; Romain Huguet; Vlad Zabrouskov; *Thermo Fisher Scientific, San Jose, CA*
- TP 398 **Performance Evaluation of the Q Exactive™ HF Hybrid Quadrupole-Orbitrap Mass Spectrometer for High-Throughput Top-Down Proteomics;** Eugen Damoc¹; Ping Yip²; Leena Valmu³; Alexander Cherkassky²; Bernard Delanghe¹; Eduard Denisov¹; Oksana Gvozdyak²; Helene Cardasis²; Jason Neil²; Alexander Makarov¹; Jim Stephenson²; ¹*Thermo Fisher Scientific, Bremen, Germany*; ²*Thermo Fisher Scientific, Cambridge, MA*; ³*Thermo Fisher Scientific, Vantaa, Finland*
- TP 399 **Automated Multi-Dimensional Top-Down Clinical Proteomics Platform for High Sensitivity and Quantitative Proteoform Analysis on Individual Patient Cerebrospinal Fluid;** John Corbett^{1,2}; Daniel Plymire¹; Steven Patrie^{1,2}; ¹*University of Texas Southwestern Medical Center, Dallas, TX*; ²*University of Texas at Dallas, Richardson, TX*
- TP 400 **Fractionation by Size Exclusion Chromatography of Proteins for Top-Down Analysis;** Lucia Geis-Asteggiate¹; Suzanne Ostrand-Rosenberg²; Catherine Fenselau¹; ¹*University of Maryland, College Park, MD - Maryland*; ²*University of Maryland Baltimore County, Baltimore, MD*
- TP 401 **A Novel Three Dimensional Liquid Chromatography Platform for Top-down Proteomics;** Lichen Xiu; Santosh Valeja; Zachery Gregorich; Huseyin Guner; Song Jin; Ying Ge; *University of Wisconsin-Madison, Madison, WI*
- TP 402 **Top-Down, High-Throughput Proteomics of Thermo-Stable Allergens Using Complementary MS/MS Fragmentation Strategies;** Monica Carrera¹; Daniel Lopez Ferrer²; Chad Weisbrod²; Romain Huguet²; Jose Manuel Gallardo¹; Jae C. Schwartz²; Andreas Huhmer²; ¹*CSIC, Vigo, SPAIN*; ²*ThermoFisher Scientific, San Jose, CA*
- TP 403 **Identification of Proteoforms from Yeast Lysate Using Measurements of Intact Mass and Lysine Count;** Brian L. Erey; Michael R. Shortreed; Mark Scaif; Rachel A. Knoener; Anthony J. Cesnik; Lloyd M. Smith; *University of Wisconsin, Madison, WI*
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- TP 405 **Improving Protein LC/MS Analysis;** Barry Boyes^{1,2}; Stephanie Schuster¹; Joseph Kirkland¹; Benjamin Libert¹; Brian Wagner¹; Joseph Destefano¹; ¹*Advanced Materials Technology Inc., Wilmington, DE*; ²*University of Georgia, Athens, GA*
- TP 406 **Integration of Electrochemistry with Ultra-Performance Liquid Chromatography/Mass Spectrometry (UPLC/MS);** Yi Cai¹; Qiuling Zheng¹; Yong Liu²; Roy Helmy²; Joseph A. Loo³; Hao Chen¹; ¹*Ohio University, Athens, OH*; ²*Merck Research Laboratories, Merck & Co., Inc., Rahway, NJ*; ³*University of California-Los Angeles, Los Angeles, CA*
- TP 407 **Mass Spectrometry of Collagen Preserved in Archaeological Specimens Including Human Bones;** Shunsuke Fukakusa¹; Kazuki Kawahara²; Mehdi Moini³; Takashi Nakazawa¹; ¹*Nara Women's University, Nara, Japan*; ²*Osaka University, Suita, Osaka*; ³*George Washington University, Washington DC*
- TP 408 **General Protein Analysis Using in-source CID and SEC Chromatography;** Dale Schoener; John Cremin; Michael Buonarati; *Intertek Pharmaceutical Services, El Dorado Hills, CA*
- TP 409 **A Knowledge-Based Approach to Developing a Mass Spectrometry Method for Detection of Gluten in "Free-From" Foods;** Sophie Bromilow¹; Lee A Gethings²; Prof. Peter Shewry³; Michael Buckley¹; Michael Bromley⁴; Phil Johnson¹; Prof. Clare Mills¹; ¹*University of Manchester, Manchester, UK*; ²*Waters, Manchester, N/A*; ³*Rothamsted Research, Harpenden, UK*; ⁴*Synergy Health, Swindon, UK*
- TP 410 **Small Molecule Inhibition of Beta-2 Microglobulin Amyloid Formation Studied by Mass Spectrometry;** Tyler Marcinko; Patrick Kiefer; William Warren; Kate Daborowski; Richard Vachet; *University of Massachusetts, Amherst, MA*
- TP 411 **Use of MALDI-MS in the Detection of Non-Covalent Amyloid β Oligomers;** Jasmine S.-H. Wang^{1,2}; Kristina Jurcic¹; Shawn N. Whitehead²; Ken K.-C. Yeung¹; ¹*Department of Chemistry and Biochemistry, London, ON*; ²*Department of Anatomy and Cell Biology, London, ON*
- TP 412 **Development of a Combined Workflow to Study the Relationship Between Cysteine Accessibility in the Active Site and Protein Aggregation;** Natalya Atlasevich; Pilsoo Kang; Jianmei Kochling; *Genzyme, Framingham, MA*
- TP 413 **Protein Characterization Involved in Mussel Byssal Threads Biogenesis by 2D-LC-MS/MS;** Maxime Sansoucy¹; Cynthia Caron¹; Réjean Tremblay²; Isabelle Marcotte¹; Lekha Sleno¹; ¹*UQAM, Montreal, Canada*; ²*UQAR-ISMER, Rimouski, Canada*
- TP 414 **Characterizing High Molecular Weight Glutentin Subunits in Canadian Wheat Varieties Using ESI-MS on Intact Protein;** Ray Bacala; Dave Hatcher; *Canadian Grain Commission, Winnipeg, Canada*
- TP 415 **Mass spectrometric characterization of Coenzyme Q biosynthesis;** Arne Ulbrich; Catherine E. Minogue; Jon A. Stefely; Danielle C. Lohman; Andrew G. Reidenbach; Michael S. Westphal; David J. Pagliarini; Joshua J. Coon; *University of Wisconsin, Madison, WI*
- TP 416 **Correlation between Protein Concentrations and Recovery in SDS PAGE;** David Fabacher; Ute Bahr; Michael Karas; *Goethe University, Frankfurt am Main, Germany*
- TP 417 **Venomomics of *Nephilengis cruentata* Spider by Data Dependent and Data Independent Acquisition Methods in Mass Spectrometry;** Rafael Lomazi¹; Thiago Abreu¹;

- Josias Pagotto¹; Eduardo Kitano²; Solange Serrano²; Pedro Silva Jr.²; Alexandre Keiji Tashima¹; ¹*EPM/Universidade Federal de São Paulo, São Paulo, Brazil*; ²*LETA/ Instituto Butantan, Sao Paulo, Sao Paulo*
- TP 418 **On-target Tryptic Digest and MALDI-MS Analysis of Reproduction Proteins from *Pieridae* Butterflies**; Måns Ekelöf; Maria Khihon Rokhas; Johan Jacksén; Åsa Emmer; *KTH Royal Institute of Technology, Stockholm, SWEDEN*
- TP 419 **Trypsin modified membrane reactors for controlled and limited proteolysis followed by mass spectrometry**; Wenjing Ning; Jinlan Dong; Merlin Bruening; *Michigan State University, East Lansing, MI*
- TP 420 **Investigating the Cellular Interactions of BIRB796 Analogs Using a Novel Chloroalkane Capture Tag**; Marjeta Urh¹; Rachel Friedman Ohana¹; Robin Hurst¹; Thomas Kirkland²; Sergiy Levin²; Michael Ford³; Richard Jones³; Keith Wood¹; ¹*Promega, Madison, WI*; ²*Promega Biosciences LLC, San Luis Obispo, CA*; ³*MS Bioworks LLC, Ann Arbor, MI*
- TP 421 **Characterization of a Novel NUDIX Hydrolase Using Limited Proteolysis, Bottom-Up, and Middle-Down Mass Spectrometry**; Lauren R Devine; Robert O'Meally; Andres H de la Peña; Sandra B Gabelli; Robert N Cole; *Johns Hopkins, Baltimore, MD*
- TP 422 **Protein Fractionation by Subcellular Location to Enhance Proteomic Coverage of Cultured Cells**; Haiyan Wu; Ryan Bomgardner; Kay Opperman; John C. Rogers; Barb Kaboord; *Thermo Fisher Scientific, Rockford, IL*
- TP 423 **Integrating Mass Spectrometry and Structural Biology Techniques to Investigate a Novel Bacterial Ferritin-Like Protein**; Sally Vanden-Hehir¹; Didi He¹; Sophie Harvey²; C. Logan Mackay¹; Jon Marles-Wright¹; David J Clarke¹; ¹*University of Edinburgh, Edinburgh, UK*; ²*Ohio State University, Columbus, OH*
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- TP 425 **The Use of MRM Methods for Glycan Discovery and Extensive Characterization of Site-Specific Glycosylation**; Muchena J. Kailemia; Carlito Lebrilla; *University of California, Davis, CA*
- TP 426 **Investigation of Detergent and Detergent Free Sample Preparations for Membrane Proteomics/ Glycoproteomics of Breast Cancer Cells with different Clinicopathological Features**; Yu Zhang; Rui Zhu; Shiyue Zhou; Yehia Mechref; *Texas Tech University, Lubbock, TX*
- TP 427 **Tissue-Specific Protein Glycosylation and the Detection of Sialic Acid Variants at the Glycopeptide Level**; Katalin F. Medzihradsky; Krista Kaasik; Robert J. Chalkley; *UCSF, San Francisco, CA*
- TP 428 **Developing Methods for Analyzing N-Glycans Released from Low-Abundant Human Plasma Proteins**; Cheylene Tanimoto; Sarah Totten; Sharon Pitteri; *Stanford University School of Medicine, Palo Alto, CA*
- TP 429 **SugarCone: a Software of Automatic Glycopeptide Sequencing by Y1 and peptide ion of N- and O-linked Glycopeptide**; Chein-Hung Chen; Hsin-Yu Hsieh; Jung-Lee Lin; Chung-Hsuan Chen; *Academia Sinica, Taipei, Taiwan*
- TP 430 **Unraveling the Cell Surface Glycoproteome**; Rebecca Sosa; Yanyan Qu; William Alley; *University of Texas at San Antonio, San Antonio, TX*
- TP 431 **Comprehensive Monitoring of Glycopeptides Alternation in Cancer Patients by Multiple Reaction Monitoring and Precursor Ion Scan**; Petra Darebna²; Petr Novak^{1,2}; Radek Kucera³; Ondrej Topolcan³; Miloslav Sanda⁴; Radoslav Goldman⁴; Petr Pompach^{1,2}; ¹*Institute of Microbiology, Prague, Czech Republic*; ²*Charles University, Prague, Czech Republic*; ³*Faculty Hospital in Pilsen, Pilsen, Czech Republic*; ⁴*Georgetown University, Washington, DC, DC*
- TP 432 **Glycomic Profiling of Biofluids and Exosomes by MALDI-FTICR**; Huarong Xu; Thomas Powers; Roper Stephen; Richard R Drake; *Medical University of South Carolina, Charleston, SC*
- TP 433 **Defining a Glycosylation Site of Human PSA Prompted by Missense Mutation by LC-MS/MS**; Ehwang Song¹; Yunli Hu¹; Chuan-Yih Yu²; Haixu Tang²; Yehia Mechref¹; ¹*Texas Tech University, Lubbock, TX*; ²*Indiana University, Bloomington, IN*
- TP 434 **Mass Spectrometry Analysis of Glycoproteins of the Sulfate Reducer *Archaeoglobus fulgidus***; Deborah R. Leon¹; Cheng Lin¹; Nancy Leymarie²; Rachel R. Ogorzalek Loo³; Joseph A. Loo³; Robert P Gunsalus³; Catherine E. Costello²; ¹*Boston University School of Medicine, Boston, MA*; ²*Boston University School of Medicine, Boston, MA*; ³*UCLA, Los Angeles, CA*
- TP 435 **The Characterization of Glycosylated Neuropeptides from the Lobster, *Homarus americanus***; Henry E. Pratt¹; Patsy S. Dickinson¹; Andrew E. Christie²; Elizabeth A. Stemmler¹; ¹*Bowdoin College, Brunswick, ME*; ²*University of Hawaii at Manoa, Honolulu, HI*
- TP 436 **A Method for Simultaneous Analysis of N-Linked Glycans, Glycosites, and Site-Specific Glycan Heterogeneity for Comprehensive Characterization of Glycoproteins**; Shisheng Sun²; Punit Shah¹; Shadi Toghi Eshghi¹; Weiming Yang¹; Namita Trikannad¹; Shuang Yang¹; Lijun Chen¹; Paul Aiyetan¹; Naser Uddin Hoti¹; Daniel W. Chan¹; Hui Zhang¹; ¹*John Hopkins Dept. of Pathology, Baltimore, MD*; ²*Johns Hopkins University, Baltimore, Maryland*
- TP 437 **Site-specific modulation of surface glycoprotein sialylation upon short time stimulation of HeLa cells**; María Ibáñez-Vea; Lylia Drici; Veit Schwämmle; Pernille Lassen; Giuseppe Palmisano; Lene Jakobsen; Martin R. Larsen; *University of Southern Denmark, Odense, Denmark*
- TP 438 **HILIC and ERLIC Enrichment of Glycopeptides Derived From Breast and Brain Cancer Cells**; Lauren Zacharias; Ehwang Song; Alyssa Hartmann; Rui Zhu; Parvin Mirzaei; Yehia Mechref; *Texas Tech University, Lubbock, TX*
- TP 439 **An Optimized Method for the Deglycosylation, Enrichment, and Derivatization of N-linked Glycans from Proximal Biofluids**; Crystal Daniels^{1,2}; Jana Rocker^{1,2}; Lewis Pannell^{1,2}; ¹*University of South Alabama, Mobile, AL*; ²*Mitchell Cancer institute, Mobile, AL*
- TP 440 **Comprehensive and High Throughput Quantitative Site-Specific N-Linked Glycosylation Analysis of Recombinant Glycoproteins**; Xiaoying Jin¹; Dongyu Liu²; Lin Liu¹; Joanne Cotton¹; Clarence Wang²; Xiaokui Kate Zhang¹; ¹*Sanofi Biotherapeutics, Framingham, MA*; ²*Genzyme, Framingham, MA*
- TP 441 **A Pipeline Employing Native MS to Analyze Glycoproteins and Glycoprotein Complexes from Endogenous Samples**; Rafael D. Melani^{1,2}; Luis H. F. do Vale³; Owen Skinner¹; Luca Fornelli¹; Marcelo V. Sousa³; Gilberto Domont²; Philip Compton¹; Neil L. Kelleher¹; ¹*Northwestern University, Evanston, IL*; ²*Univ Federal Do Rio De Janeiro, Rio De Janeiro, Brazil*; ³*Universidade de Brasília, Brasília, Brazil*

- TP 442 **Integrated N-Glycoproteomics-Based Assessment of Equivalence between Induced Pluripotent Stem Cells and Embryonic Stem Cells;** Putty-Reddy Sudhir¹; Madireddy Pavana Kumari¹; Wei-Ting Hsu²; Hung-Chih Kuo²; Chung-Hsuan Chen¹; ¹GRC, Academia Sinica, Taipei, Taiwan; ²ICOB, Academia Sinica, Taipei, Taiwan
- TP 443 **Identification of N-Glycans Using an Accurate Mass and Retention Time Database Yield Oligosaccharides Variations in Individual Serum;** Ting Song¹; Stephen Madden²; Carlito Lebrilla¹; ¹University of California Davis, Davis, CA; ²Agilent Technologies, Inc., Santa Clara, CA
- TP 444 **Quantification of Glycopeptides from Human Prostate Specific Antigen using Multiple Reaction Monitoring;** Masaki Kurogouchi¹; Toshio Nakamura¹; Yusuke Inohana²; Ichiro Hirano²; Junko Amano¹; ¹the noguchi institute, Tokyo, Japan; ²Shimadzu Corporation, Kyoto, Japan
- TP 445 **Analysis of N-Linked Glycopeptides Derived from Human Liver Tissues by LC-MS/MS;** Minkun Wang^{1,2}; Cristina Di Poto¹; Ehwang Song³; Rui Zhu³; Yehia Mechref³; Habtom Resson¹; ¹Georgetown University, Lombardi Cancer Center, Washington, DC; ²Virginia Tech, Arlington, VA; ³Texas Tech University, Lubbock, TX
- TP 446 **In-Depth Analysis of Site-Specific N-Glycosylated alpha 1 Acid Glycoprotein and Vitronectin from Human Plasma;** Juyeon Lee¹; Heeyoun Hwang¹; Gun Wook Park^{1,2}; Hyun Kyoung Lee^{1,2}; Jin Youn Kim¹; Jong Shin Yoo^{1,2}; ¹Korea Basic Science Institute, Chungbuk, South Korea; ²Graduate School of Analytical Science and Technol, Daejeon, South Korea
- TP 447 **Studying the Kinetics of N-glycan Release by PNGase F with MRM Quantitation of the Glycopeptides from Human Serum Glycoproteins;** Yining Huang; Adam Kramer; Ron Orlando; *University of Georgia, Athens, GA*
- TP 448 **Integrative Omics Analysis to Reveal the Molecular Biological Mechanism of Breast Cancer Brain Metastasis;** Wenjing Peng; Rui Zhu; Shiyue Zhou; Ehwang Song; Parvin Mirzaei; Lauren Zacharias; Yunli Hu; Kameswara Rao Kottapalli; Yehia Mechref; *Texas Tech University, Lubbock, TX*
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- TP 449 **A Global Survey of Protein Phosphorylation Reveals its Extensive Regulatory Network in Rat Fetal Neural Stem Cells;** Shuxin Wang¹; Xuyang Zhao²; Qingsong Wang¹; Jianguo Ji¹; ¹Peking University, Beijing, China; ²Peking University Health Science Center, Beijing, China
- TP 450 **Phosphoproteomics of Human Immunodeficiency Virus-1;** Pratikumar Rathod^{1,2}; Hsin-Pin Ho^{1,2}; Xu Yu³; Dr. Mathias Lichterfeld^{3,4}; Dr. Emmanuel Chang^{1,2}; ¹York College- City University of New York, Jamaica, NY; ²Graduate Center- City University of New York, New York, NY; ³Ragon Institute of MGH, MIT and Harvard, Cambridge, MA; ⁴Infectious Disease Division- MGH, Boston, MA
- TP 451 **Using Phosphoproteomics to Reveal the ATM Dependent Mediators in the Late Phase of Replication Stress;** Stephanie Munk; Luis I. Toledo; Louise von Stechow; Jiri Lukas; Jesper V. Olsen; *NNF CPR, University of Copenhagen, Copenhagen, DENMARK*
- TP 452 **Label-free Quantitative Determination of LPS- and TNF α -induced Phosphorylation dynamics on IRAK4 involved in the Host Immune Response;** Li Wang; Harsha P. Gunawardena; Xian Chen; *University of North Carolina at Chapel Hill, Chapel Hill, NC*
- TP 453 **Phospho-Signaling Pathways and Cross-Talk in SKBR3 Breast Cancer Cells;** Fumio Ikenishi; Iuliana Lazar; *Virginia Tech, Blacksburg, VA*
- TP 454 **Microfluidic Reactor for Fast Proteolytic Digestion and Enrichment in Phosphopeptides;** Jingren Deng; Iulia M. Lazar; *Department of Biological Sciences, Virginia Tech, Blacksburg, VA*
- TP 455 **A Scoring Model for Phosphopeptide Site Localization and its Impact on the Question of Whether to Use MSA;** Juliana Fischer²; Marlon dos Santos²; Fabricio Marchini¹; Valmir Barbosa³; Paulo Carvalho²; Nilson Zanchin²; ¹Carlos Chagas Institute, Fiocruz, Pr, Curitiba, Brazil; ²Laboratory for Proteomics and Protein Engineering, Curitiba, Brazil; ³Federal University of Rio de Janeiro, Rio de Janeiro, Brazil
- TP 456 **Functionalized Multivalent Nanoparticles for Top-down Phosphoproteomics;** Leekyoung Hwang; Bifan Chen; Serife Ayaz-Guner; Tania Guardado; Ying Peng; Zachery Gregorich; Song Jin; Ying Ge; *University of Wisconsin-Madison, Madison, WI*
- TP 457 **Automated Phosphopeptide Spectral Library Searching for Fast and Confident Site Localisation;** Veronika Suni¹; Susumu Imanishi¹; Garry Corthals^{1,2}; ¹Turku Centre for Biotechnology, Turku, Finland; ²University of Amsterdam, Amsterdam, The Netherlands
- TP 458 **Identification of Phosphorylation Sites in Marine Microbes;** Noelle Held; Mak Saito; *Woods Hole Oceanographic Institution, Woods Hole, Massachusetts*
- TP 459 **A Sensitive Assay to Measure Total Protein Phosphorylation Level in Complex Protein Samples;** Li Pan; Linna Wang; Chuan-Chih Hsu; Jiazhen Zhang; Anton Iliuk; Weiguang Andy Tao; *Purdue University, West Lafayette, IN*
- TP 460 **Identification of Post-Translational Modifications on HEXIM1 that Regulate the Activation of P-TEFb and HIV Proviral Reactivation;** Benlian Wang¹; Uri Mbonye²; Giridharan Gokulrangan³; Jonathan Karn²; Mark R. Chance¹; ¹Center for Proteomics and Bioinformatics, CWRU, Cleveland, OH; ²Dept. of Molecular Biology and Microbiology, CWRU, Cleveland, OH; ³PDM Department, Pfizer WRD, Andover, MA
- TP 461 **Probing Phosphoproteome Changes Downstream of MAP4K4;** Adam Schwaid¹; Chunyan Su²; Paula Loos⁶; Jiang Wu⁵; Chuong Nguyen⁴; Kathryn L. Stone³; Jean Kanyo³; Kieran Geoghegan⁴; Philip Carpino¹; Leonard Buckbinder²; Samit Bhattacharya¹; Robert Dow¹; ¹Worldwide Medicinal Chemistry, Pfizer, Cambridge, MA; ²CVMED Research Unit, Pfizer, Cambridge, MA; ³Yale School of Medicine, New Haven, CT; ⁴Pfizer Worldwide Research and Development, Groton, CT; ⁵Shire Pharmaceuticals, Lexington, MA; ⁶Neuroscience Research Unit, Pfizer, Cambridge, MA
- TP 462 **Expanding the Role of TAK1 in Immune and Inflammatory Response Through Chemical Genetics and Proteomics;** Rebecca Levin¹; Nicholas Hertz¹; Alma Burlingame¹; Kevan Shokat^{1,2}; ¹University of California, San Francisco, San Francisco, CA; ²Howard Hughes Medical Institute, Chevy Chase, MD
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- TP 463 **Identification of Anti-Tumor Sclerotium rolfsii Lectin Binding Membrane Proteins from HT-29 Cells Using Micro-Fluidic Based LC System Coupled with QTOF-MS;** Ravindra Gudihal¹; Srikanth Barkeer²; Sachin M Eligar²; Prajna Hegde²; Lu-Gang Yu³; Bale M Swamy²; Shashikala R Inamdar²; ¹Agilent Technologies India Pvt. Ltd, Bangalore, INDIA; ²Department of Studies in Biochemistry, KUD, Dharwad, India; ³Department of Gastroenterology, Uni of Liverpool, Liverpool, L69 3BX
- TP 464 **High-pH Reverse Phase StageTip for Sensitive and Rapid Small-Scale Membrane Proteomic Profiling;** Baby Rorielyn T. Dimayacyac-Esleta^{1,3}; Reta Birhanu Kitata^{1,2}; Wai-Kok Choong¹; Chia-Feng Tsai¹; Pei-Yi Lin¹; Shao-Hsing Weng¹; Susan D. Arco³; Ting-Yi Sung¹; Yu-Ju Chen¹; ¹Academia Sinica, Taipei, Taiwan; ²MST, Taiwan International Graduate Program, Taipei, Taiwan; ³University of the Philippines, Diliman Quezon City, Philippines

- TP 465 **Comparative LC-MS Profiling of the Cell Surface of NSCLC Cell Lines Bearing Oncogenic K-RAS Mutations**; Xiaoying Ye; Robert Stephens; Gordon Whiteley; Josip Blonder; *Leidos Biomedical Research, Inc., Frederick Nationa, Frederick, MD*
- TP 466 **Proteomic Analysis of Membrane Protein Glycosylation and its Relationship to Transmembrane (TM) Domains**; Bingyun Sun; *Simon Fraser University, Burnaby, Canada*
- TP 467 **An Effective Method for Plasma Membrane Protein Enrichment for Proteomic Analysis of Small Tissue Samples**; Geert Baggerman^{1,3}; Katrien Smolders²; Nathalie Lombaert²; Dirk Valkenburg^{1,3}; Lutgarde Arckens²; ¹*Vito, Mol, Belgium*; ²*KULeuven, RU Neuroplasticity and Neuroproteomics, Leuven, Belgium*; ³*University Antwerp, Center for proteomics, Antwerp, Belgium*
- TP 468 **Applying Native nESI-IMS-MS and FPOP with LC-MS to the Study of Membrane Proteins**; Tom G Watkinson; Antonio N Calabrese; Sheena E Radford; Alison E Ashcroft; *University of Leeds, Leeds, UK*
- TP 469 **Interaction Landscape Analysis Reveals Porin-Localized Toxin Inactivation in *Acinetobacter baumannii* Cells**; James Bruce; Xia Wu; Devin Schweppe; Chunxiang Zheng; Arti Navare; Juan Chavez; Jimmy Eng; Pradeep Singh; Colin Manoil; *University of Washington, Seattle, WA*
- TP 470 **Effect of Surfactant, Solvents and Digestion Conditions on Digestion Efficiency of Drug Transporter Proteins by Trypsin**; Buyun Chen; Liling Liu; Alan Deng; Brian Dean; Emile Plise; Laurent Salphati; Yuan Chen; Xiaorong Liang; *Genentech, South San Francisco, CA*
- TP 471 **In Vivo, Stable-Isotope Labeling and MS Probe the Interaction of Warfarin with Vitamin K Epoxide Reductase**; Guomin Shen¹; Hao Zhang²; Weidong Cui²; Weikai Li¹; Michael L. Gross²; ¹*Washington University School of Medicine, St. Louis, MO*; ²*Washington University, St. Louis, MO*
- TP 472 **Activation and Oligomerization of Bax Studied by Ion Mobility Mass Spectrometry**; Jeroen Van Dyck¹; Albert Konijnenberg¹; Frank Sobott^{1,2}; ¹*University of Antwerp BAMS group, Antwerp, Belgium*; ²*Center for Proteomics, Antwerp, Belgium*
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- TP 473 **Effects of Charge State on the Structures of Protein Ions: Results from Cation to Anion Proton Transfer Reactions**; Ken Laszlo¹; Eleanor Munger²; Matthew Bush¹; ¹*University of Washington, Seattle, WA*; ²*Carleton College, Northfield, MN*
- TP 474 **Mass Spectrometric Analysis of Surface Exposed Regions in the Hexadecameric Phosphorylase Kinase Complex**; Mary Ashley Rimmer; Antonio Artigues; Owen W Nadeau; Maria T Villar; Victor Vasquez-Montes; Gerald M Carlson; *University of Kansas Medical Center, Kansas City, KS*
- TP 475 **Analysis of Affinity-Isolated Endogenous Protein Complexes by Native Mass Spectrometry Using an Exactive Plus EMR Instrument**; Paul Dominic B. Olinares; Julio C. Padovan; Brian T. Chait; *The Rockefeller University, New York, NY*
- TP 476 **Surface-Induced Dissociation/Ion Mobility of Pyruvate Kinase: Interface Area and Subunit Packing**; Aniruddha Sahasrabuddhe; Vicki Wysocki; *The Ohio State University, Columbus, Ohio*
- TP 477 **Discovery of Lipid Acquisition Mechanism of *Plasmodium vivax* in Liver Stage by Interactome Technique**; Supachai Topanurak¹; Peerut Chienwichai¹; Wang Nguitragool^{1,2}; Jetsumon Prachumsri²; ¹*Faculty of Tropical Medicine, Mahidol University, Bangkok, Thailand*; ²*Mahidol Vivax Research Unit, Mahidol University, Bangkok, Thailand*
- TP 478 **CSNAP – the 9th Subunit of the COP9 Signalosome Complex**; Gili Ben-Nissan; Maria Gabriela Fuzesi-Levi; Rozen Shelly; Michal Sharon; *Weizmann Institute of Science, Rehovot, Israel*
- TP 479 **Analysis of the Apoptosis Signal-Regulating Kinase Signalosome Dynamics by Targeted Mass Spectrometry**; Joel Federspiel; Simona Codreanu; Daniel Liebler; *Vanderbilt University School of Medicine, Nashville, TN*
- TP 480 **Structural Proteomics Analysis of the tau-Protein – Microtubule**; Karl Makepeace¹; Evgeniy Petrotchenko¹; Nicole Sessler¹; Christoph Borchers^{1,2}; ¹*University of Victoria-Genome BC Proteomics Centre, Victoria, BC, Canada*; ²*Dept. of Biochem. & Microbiol., Univ. of Victoria, Victoria, BC, Canada*
- TP 481 **Crosslinking Analysis of Fibrin Polymerization**; Karl Makepeace¹; Evgeniy Petrotchenko¹; Christoph Borchers^{1,2}; ¹*University of Victoria-Genome BC Proteomics Centre, Victoria, BC, Canada*; ²*Dept. of Biochem. & Microbiol., Univ. of Victoria, Victoria, BC, Canada*
- TP 482 **Changes in Ribosome Associated Proteins During Growth of *E.coli***; Santosh Misal; Aditi Dabir; James Reilly; *Indiana University, Bloomington, IN*
- TP 483 **Deciphering the Topology of a Mitochondrial RNA Processing Complex in Trypanosomes with a Combination of Cross-linking and Mass Spectrometry**; Yu Qian^{1,2}; Catherine E Costello¹; Ruslan Afasizhev²; ¹*Boston University School of Medicine, Boston, MA*; ²*Boston University School of Dental Medicine, Boston, MA*
- TP 484 **A Study of the MEK1 Interactome Dynamics by Affinity Purification-Mass Spectrometry Reveals Novel Interactors**; Laura Herring¹; Kyle Grant²; Kevin Blackburn¹; Jason Haugh¹; Michael Goshe¹; ¹*North Carolina State University, Raleigh, NC*; ²*UNC-Chapel Hill, Chapel Hill, NC*
- TP 485 **Proteomic Analysis of the Essential Mitotic Activator Bora and its Regulation in the Human Cell Cycle**; Andrew Grasseti; Mark Adamo; Scott Rusin; Arminja Kettenbach; Scott Gerber; *Dartmouth Medical School, Hanover, NH*
- TP 486 **Structural Elucidation of Metalloprotein Complexes by Top-down Mass Spectrometry**; Piriya Wongkongkathep; Huilin Li; Joseph A. Loo; *UCLA, Los Angeles, CA*
- TP 487 **Affinity Proteomics Establishes NIMA-Related Kinases as Regulators of Cytokinesis through Control of Microtubule Motor Localization**; Sierra Cullati; Scott Gerber; *Geisel School of Medicine at Dartmouth, Lebanon, NH*
- TP 488 **Discovering a New Subunit for an Old Complex**; Shelly Rozen; Maria Fuzesi-Levi; Gili Ben-Nissan Ben-Nissan; Michal Sharon; *Weizmann Institute of Science, Rehovot, Israel*
- TP 489 **Filtering and Scoring of Results from AP-MS Experiments by Spectral Counts, Label-Free Quantitation and Enrichment Factor**; Roman Mylonas^{1,2}; Patrice Waridel²; Manfredo Quadroni²; ¹*Vital-IT Group - Swiss Institute of Bioinformatics, Lausanne, Switzerland*; ²*CIG - University of Lausanne, Lausanne, Switzerland*
- TP 490 **New Developments for the CRAPome Resource for Scoring AP-MS Protein Interaction Data**; Dattatreya Mellacheruvu¹; Zachary Wright¹; Anne-Claude Gingras²; Alexey Nesvizhskii¹; ¹*University of Michigan, Ann Arbor, MI*; ²*Samuel Lunenfeld Research Institute, Mount Sinai H, Toronto, ON*
- TP 491 **Identification of Yeast Mediator Complex Interacting Proteins by 15N Metabolic Labeling**; Henriette Uthe; Jens T. Vanselow; Andreas Schlosser; *Wuerzburg, Germany*

- TP 492 **Improving Detection Efficiency of Large, Complex Ions Generated Under Native Conditions Using an Electrically Biased Pixelated Detector**; Tiffany Porta^{1,2}; Andrey Dyachenko³; Shane R. Ellis^{1,2}; Gert B. Eijkel¹; Bob Hommersom¹; Jerre van der Horst⁴; Dmitry Byelov⁵; Dirk-Jan Spaanderman²; Ronald Buijs²; Frans Giskes¹; Albert J.R. Heck³; Ron M.A. Heeren¹; ¹M4I Institute - Maastricht University, Maastricht, The Netherlands; ²FOM Institute AMOLF, Amsterdam, The Netherlands; ³Utrecht University, Utrecht, The Netherlands; ⁴MS Vision, Almere, The Netherlands; ⁵Omics2Image, Amsterdam, The Netherlands
- TP 493 **Quantitative Measurement of the Protein Complex Landscape of Murine Tissues Using PCP-SILAC**; Nichollas E. Scott; Duncan Ferguson; Marjan Farahbod; Joerg Gsponer; Paul Pavlidis; Leonard J Foster; *University of British Columbia, Vancouver, Canada*
- TP 494 **Stoichiometry Determination of Large Multiprotein Complexes using QConcat: Lessons Learned through Analysis of the 50 MDa Yeast Nuclear Pore Complex**; Wenzhu Zhang; Javier Fernandez-Martinez; Michael P. Rout; Brian T. Chait; *The Rockefeller University, New York, NY*
- PROTEIN THERAPEUTICS: STRUCTURAL CHARACTERIZATION 495-513**
- TP 495 **Substrate-Mimetic Chaperone Binding Sites in human-galactosidase A Identified by Proteolytic Affinity - Mass Spectrometry**; Stefan Maeser¹; Adrian Moise¹; Frederike Eggers¹; Stephan Rawer²; Michael Przybylski¹; ¹Steinbeis Centre Biopolymer Analysis and Biomedica, Ruesselsheim, Germany; ²Thermofisher Scientific, Darmstadt, Germany
- TP 496 **Conformational Differences in Monoclonal Antibody Dimers Revealed by Hydrogen/Deuterium Exchange Mass Spectrometry**; Jun Zhang; Christopher Woods; Mei Han; Feng He; Michael Treuheit; *Amgen, Inc, Seattle, WA*
- TP 497 **Multiple Reaction Monitoring (MRM)-Based Quantitation of Oxidation During Hydroxyl Radical Protein Footprinting for Pharmaceutical Protein Conformation Analysis**; Franklin E. Leach III¹; Peter J. Todd¹; Ron Orlando²; Joshua S. Sharp²; ¹Photochem Technologies, Athens, GA; ²University of Georgia, Athens, GA
- TP 498 **Characterization of IgG and IgM Monoclonal Antibodies by Superconducting Tunnel Junction Cryodetection MALDI TOF Mass Spectrometry**; Logan Plath; Jonathan Feldman; David Sipe; Mark E. Bier; *Carnegie Mellon University, Pittsburgh, PA*
- TP 499 **Analytical Characterization of Therapeutic Monoclonal Antibodies in Cynomolgus Monkey Serum by Immunopurification and Mass Spectrometry**; Rosalynn Molden; Haibo Qiu; Ning Li; Thomas Daly; *Regeneron Pharmaceuticals, Tarrytown, NY*
- TP 500 **Automatic De Novo Identification and Profiling of Disulfide Bonds in Biopharmaceuticals**; Anja Resemann¹; Rainer Paape¹; Jan Wiesner¹; Jason Wood²; Lars Vorwerk¹; Detlev Suckau¹; Wolfgang Jabs¹; ¹Bruker Daltonics, Bremen, Germany; ²Bruker Daltonics, Billerica, MA
- TP 501 **Evaluating Workflows for Sequence Variant Detection**; Hangtian Song; Thomas Slaney; Wei Wu; Richard Ludwig; Li Tao; Tapan Das; *Bristol-Myers Squibb Company, Bloomsbury, NJ*
- TP 502 **LC-MS and LC-MS/MS Characterization of Asparagine Deamidation with Specific Sequence Motifs in Antibodies of Therapeutic Interest**; Jason X. Tang; Yuping Zhou; *Eli Lilly & Company, Indianapolis, IN*
- TP 503 **High Throughput Peptide Mapping with the Vanquish UHPLC and Q Exactive HF**; Martin Samonig¹; Remco Swart¹; Kai Scheffler²; Jonathan L. Josephs³; ¹Thermo Fisher Scientific, Germering, Germany; ²Thermo Fisher Scientific, Dreieich, Germany; ³Thermo Scientific, West Windsor, NJ
- TP 504 **Comprehensive Characterization of Site-specific Engineered Antibody Drug Conjugate by Orbitrap Mass Spectrometer**; Hongxia (Jessica) Wang¹; Terry Zhang¹; Brian J. Agnew²; Rosa Viner¹; Jonathan Josephs¹; ¹Thermo Fisher Scientific, San Jose, CA; ²Thermo Fisher Scientific, Eugene, OR
- TP 505 **Intact Mass Analysis for Glycan Profiling of a Recombinant Therapeutic Protein Directly from Harvest Cell Culture**; Yunqiu (Rachel) Chen; Li Zang; *Biogen Idec, Cambridge, MA*
- TP 506 **Combination of Bottom-Up and Top-Down Characterization of Biologics Using a High Throughput Capable Workflow in Proteome Discoverer software**; Torsten Uecker¹; Kai Scheffler²; Carmen Paschke¹; Bernard Delanghe¹; ¹Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; ²Thermo Fisher Scientific, Dreieich, Germany
- TP 507 **Expression and Characterization of a Trastuzumab-Interferon Fusion Protein in *Nicotiana benthamiana* Plant to include *in vitro* Assay Results**; Earl L. White¹; Lindsay Bennett¹; Brian Berquist¹; Iqbal Grewal³; Sanjay Khare³; Vally Kommineni¹; Sylvain Marcel¹; Ryan Murry²; Ranjith Munigunt¹; Raj Sachdev³; Don Wilkerson¹; Isaac Wong¹; Barry Holtz¹; ¹Caliber Biotherapeutics, LLC, Bryan, TX; ²G-CON Manufacturing, Inc., College Station, TX; ³ImmunGene, Inc., Camarillo, CA
- TP 508 **Characterization of an IgG-Cleaving Protease from *Streptococcus equi* with Improved Activity Against Mouse IgGs**; Chris Hosfield¹; Philip Compton²; Luca Fornelli²; Paul Thomas²; Neil L. Kelleher²; Michael Rosenblatt¹; Marjeta Urh¹; ¹Promega Corp, Madison, WI; ²Northwestern University, Evanston, IL
- TP 509 **IdeS Digest and Peptide Mapping of a Therapeutic Antibody Drug Conjugate for In-Depth Drug Conjugation Sites Analysis Using LC/MS**; Alex Zhu¹; Ning Tang²; ¹Agilent Technologies, Wilmington, DE; ²Agilent Technologies, Santa Clara, CA
- TP 510 **A Novel Data-Directed Approach for Comprehensive Disulfide Bond Mapping in Biotherapeutic Proteins**; Stephane Houel; Scott Geromanos; Steve Ciavarini; Weibin Chen; *Waters Corp, Milford, MA*
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- TP 512 **Mass Spectrometry Based Characterization of Multiple Critical Quality Attribute of Recombinant Human Collagen VII (rC7)**; Sheng Gu; Matthew Traylor; Craig Kaftan; Donald Gillies; Nicole Resendes; Bruce Tangarone; *Shire, Lexington, MA*
- TP 513 **A General Method for Identifying Chromophores in Protein Therapeutics by Liquid Chromatography and Mass Spectrometry**; Hangtian Song¹; Jianlin Xu²; Mi Jin²; Chao Huang²; Jacob Bongers³; Kelvin Bai³; Wei Wu¹; Richard Ludwig³; Li Tao³; Zhengjian Li²; Tapan Das³; ¹Bristol-Myers Squibb, Bloomsbury, NJ; ²Bristol-Myers Squibb, East Syracuse, NY; ³Bristol-Myers Squibb, Hopewell, NJ
- PROTEOMICS: INFECTIOUS DISEASE 514-529**
- TP 514 **Targeted Proteomics of Human Metapneumovirus in Clinical Samples and Viral Cultures**; Matthew Foster¹; Geoff Gerhardt²; Lynda Robitaille³; Guy Boivin³; Jacques Corbeil³; Arthur Moseley¹; ¹Duke University Medical Center, Durham, NC; ²Waters Corp., Milford, MA; ³Université Laval, Québec, Canada
- TP 515 **An Ion-Current-Based, 44-plex Investigation of Influenza A Virus-Infected Mouse Lungs Revealed Altered Integrity of Lung Microvascular Barriers**; Shichen Shen¹; Jun Li¹; Xiaomeng Shen¹; Andrew Ng¹; Chengjian Tu¹; Sina Ghaemmaghami²; Hulin Wu²; Martin Zand²; Jun Qu¹; ¹SUNY at Buffalo, Buffalo, NY; ²University of Rochester, Rochester, NY

- TP 516 **Application of High Sensitivity LC-MS/MS for Autoimmune Antigen Discovery in Antibiotic-refractory Lyme Arthritis or Rheumatoid Arthritis;** Qi Wang¹; Elise E. Drouin²; Chunxiang Yao¹; Jiyang Zhang³; Yu Huang¹; Allen C. Steere²; Catherine E. Costello¹; ¹*Boston University School of Medicine, Boston, MA*; ²*Harvard Medical School, Boston, MA*; ³*National University of Defense Technology, Changsha, Hunan Province, China*
- TP 517 **The Proteome of *Aedes aegypti* Legs from Female versus Male Mosquitoes;** Francine Perler; Colleen McClung; Ashley Luck; Cristian I. Ruse; *New England BioLabs, Ipswich, MA*
- TP 518 **Differential Protein Expression by Pathogenic *Leptospira* in Response to Mammalian Host Signals;** Jarlath Nally¹; Stephen Hyland²; Andre Grassmann³; Melissa Caimano⁴; Kjell Sergeant⁵; Jenny Renaut⁶; ¹*NADC/USDA, Ames, IA*; ²*University College Dublin, Dublin, Ireland*; ³*Universidade Federal de Pelotas, Pelotas, Brazil*; ⁴*University of Connecticut, Farmington, CT*; ⁵*Luxembourg Institute of Science and Technology, Belvaux, Luxembourg*
- TP 519 **Protein Profiling of Three Distinct *Chlamydia trachomatis* Growth Forms;** Ole Østergaard; Anja Olsen; Peter Lawætz Andersen; Frank Follmann; Niels Henrik Helweg Heegaard; Ida Rosenkrands; *Statens Serum Institut, Copenhagen, Denmark*
- TP 520 **Investigation of Redox Control in *Chlamydia* Infection by Novel Chemical Tools and Mass Spectrometry;** Hanzhi Wu; Rosine Dushime; Xiaofei Chen; Nelmi O. Devarie-Baez; Cristina M. Furdul; Allen W. Tsang; *Wake Forest School of Medicine, Winston-Salem, NC*
- TP 521 **Quantitative and Structural Interaction Network of Nosocomial Pathogenesis;** Devin Schweppe; Arti Navare; Xia Wu; Larry Gallagher; Colin Manoil; James Bruce; *University of Washington, Seattle, WA*
- TP 522 **Novel inhibitor-Based Photoaffinity Labeling and MALDI Mass Spectrometry for Identification of Anti-Malarial Drug Targets.;** David Wood; Michael Prinsen; Megh Singh; Christopher Eickhoff; Francis Sverdrup; Marvin Meyers; *Saint Louis University, St. Louis, MO*
- TP 523 **Thioridazine Alters the Cell Envelope Permeability of *Mycobacterium tuberculosis*;** Jeroen De Keijzer¹; Petra de Haas²; Arnoud de Ru¹; Evy Heerkens²; Leonard Amaral³; Dick van Soolingen²; Peter van Veelen¹; ¹*Leiden University Medical Centre, Leiden, the Netherlands*; ²*National Institute for Public Health (RIVM), Bilthoven, the Netherlands*; ³*Universidade Nova de Lisboa, Lisbon, Portugal*
- TP 524 **Membrane Proteome Characterization of Phenotypically Diverse *Pseudomonas aeruginosa* Cystic Fibrosis Isolates Reveals Adaptation to Host Lungs;** Karthik Shantharam Kamath¹; Dana Pascovici²; Apurv Goel²; Anahit Penesyan¹; Vignesh Venkatakrishnan¹; Ian T Paulsen¹; Nicolle H Packer¹; Mark P Molloy^{1,2}; ¹*Macquarie University, Sydney, Australia*; ²*Australian Proteome Analysis Facility, Sydney, Australia*
- TP 525 ***Mycoplasma synoviae* Infection Induced Proteomic Changes In Chicken Serum;** Balamurugan Packialakshmi¹; Rohana Liyanage¹; Vijay Durairaj²; Jackson O Lay, Jr. ¹; Naola Ferguson-Noel²; Narayan Rath³; ¹*University of Arkansas, Fayetteville, AR*; ²*The University of Georgia, Athens, GA*; ³*PPPSRU, USDA-ARS, Fayetteville, AR*
- TP 526 **Molecular Anatomy of *Streptococcus Pyogenes* in Human Blood Plasma Using Absolute Quantification and Targeted Mass Spectrometry.;** Kristoffer Sjöholm; Lotta Happonen; Johan Malmström; *Lund University, Lund, Sweden*
- TP 527 **Succinylome Analysis Reveals the Involvement of Lysine Succinylation in Metabolism in Pathogenic *Mycobacterium tuberculosis* H37Rv;** Mingkun Yang²; Zhongyi Cheng¹; Jing Gu²; Lijun Bi²; Feng Ge²; ¹*PTM Biolabs, Inc, Hangzhou, China*; ²*Chinese Academy of Sciences, Wuhan, CN*
- TP 528 **Dynamic Regulation of Histone Deacetylase 5 (HDAC5) during HIV-1 Infection;** Amanda Guise¹; Yang Luo²; Mark Muesing²; Ileana M. Cristea¹; ¹*Princeton University, Princeton, NJ*; ²*Aaron Diamond AIDS Research Center, New York, NY*
- TP 529 **The Epstein-Barr Virus Protein Kinase BGLF4 Integrates DNA Damage Response and Mitotic Phosphorylation Signaling to Promote Virus Replication;** Renfeng Li¹; Raja Sekhar Nirujogi^{2,3}; Sneha Pinto^{2,3}; Gangling Liao²; Harsha Gowda³; Tai-Chung Huang²; Patrick Shaw²; Xinyan Wu²; Akhilesh Pandey^{2,3}; S. Diane Hayward²; ¹*Virginia Commonwealth University, Richmond, VA*; ²*Johns Hopkins University, Baltimore, MD*; ³*Institute of Bioinformatics, Bangalore, India*

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- TP 530 **Single Cell Proteome Profiling Using Highly Sensitive LC-MS System and In-Capillary Sample Preparation Method;** Masaki Wakabayashi¹; Jordan Aerts²; Elena Romanova²; Stanislav Rubakhin²; Yasushi Ishihama¹; Jonathan Sweedler²; ¹*Kyoto University, Kyoto, Japan*; ²*University of Illinois, Urbana, IL*
- TP 531 **Quantitatively Profiling Dynamic Proinsulin Processing by LC-MS;** Dongwan Cheng; Junjie Hou; Fuquan Yang; Tao Xu; *Institute of Biophysics, CAS, Beijing, China*
- TP 532 **Advancing Untargeted Proteomics to Single Cells for the 16-cell *Xenopus* Embryo using μ CE-ESI-MS/MS;** Camille Lombard; Sally, A. Moody; Peter Nemes; *George Washington University, Washington, DC*
- TP 533 **MassAnalyzer as an Informatics Tool for Proteomics;** Zhongqi Zhang; Da Ren; Gang Xiao; Pavel Bondarenko; *Amgen, Inc., Thousand Oaks, CA*
- TP 534 **Fluorescence Complementation Mass Spectrometry (FCMS) for Identifying Direct Upstream Kinases;** Lingfei Zeng¹; Wen-Hong Wang¹; Robert Geahlen¹; Chang-Deng Hu¹; Andy Tao²; ¹*Department of MCMP, Purdue University, West Lafayette, IN*; ²*Department of Biochemistry, Purdue University, West Lafayette, Indiana*
- TP 535 **Population Proteome Investigation of Pathogenicity and Persistence of *Pseudomonas aeruginosa* in Cystic Fibrosis Patient Airways;** Xia Wu; Benjamin Staudinger; Jayanthi Garudathri; Katherine Hisert; Colin Manoil; Pradeep Singh; James Bruce; *University of Washington, Seattle, WA*
- TP 536 **Absolute Quantitation of Non-Standard Amino Acids in Proteins Guiding the Evolution of Orthogonal Translation Systems;** Hans Rudolf Aerni^{1,2}; Miriam Amiram^{2,3}; Svetlana Rogulina^{1,2}; Farren J. Isaacs^{2,3}; Jesse Rinehart^{1,2}; ¹*Cellular & Molecular Physiology, New Haven, CT*; ²*Systems Biology Institute, West Haven, CT*; ³*Molecular, Cellular and Developmental Biology, New Haven, CT*
- TP 537 **Discovering the Peptide Variants by Targeted Proteomics-Bioinformatics Pipeline;** Jerry C.D. Chen; *Chang Gung University, Taoyuan City, Taiwan (R.O.C)*
- TP 538 **In-Depth Melanoma Immunopeptidome for Anti-Tumor Immunotherapies;** Michal Bassani-Sternberg¹; Eva Bräunlein²; Richard Klar²; Pavel Sinitcyn¹; Julia Slotta-Huspenina³; Angelika Werner⁴; Rüdiger Heine Rüdiger⁵; Christian Peschel²; Dirk H. Busch⁶; Juergen Cox¹; Angela M. Krackhardt²; Matthias Mann¹; ¹*Max Planck Institute of Biochemistry, Martinsried, DE*; ²*Medizinische Klinik III, Klinikum rechts der Isar, Munich, DE*; ³*Institut für Allgemeine Pathologie und Pathologisc, Munich, DE*; ⁴*Institute of Surgery, Klinikum rechts der Isar, Te, Munich, DE*; ⁵*Department of Dermatology and Allergology, Technic, Munich, DE*; ⁶*Institut für Medizinische Mikrobiologie, Immunolog, Munich, DE*

- TP 539 **A Universal Method for Peptide Identification;** Shannon Eliuk; Nina Soltero; Philip M Remes; Michael W. Senko; Vlad Zabrouskov; *Thermo Fisher Scientific, San Jose, CA*
- TP 540 **Enhancing Electrospray Response in Proteomics through Chemical Additives – Better Alternatives to DMSO;** Peng Yu; Hannes Hahne; Bernhard Kuster; *Technische Universität München, Freising, Germany*
- TP 541 **A New Probabilistic Score for the Chemical Cross-Linking Tandem Mass Spectrometry Data Analysis;** Mihir Jaiswal^{1,2}; Boris Zybalyov²; ¹University of Arkansas at Little Rock, University, Little Rock, AR; ²University of Arkansas for Medical Sciences, Little Rock, AR
- TP 542 **Proteomic Analysis of Ancient Dental Calculus Reveals Differences in Host Immune Proteins and Microbiota;** Rosa R. Jersie-Christensen¹; Anna Fotakis^{1,2}; Jan Refsgaard¹; Christian Kelstrup¹; Enrico Cappellini²; Jesper V. Olsen¹; ¹NNF, Center for Protein Research, University of Copenhagen, DK; ²Natural History Museum of Denmark, University of Copenhagen, DK
- TP 543 **Mass Spectrometric Identification of Amino Acids Modified by 4-hydroxy-2-nonenal (HNE) as a Model for Proteome-Scale Analysis of Oxidative Stress;** Roshanak Aslebagh¹; Steven J. Fliesler^{2,3}; Bruce A. Pfeiffer^{2,3}; Costel C. Darie¹; ¹Clarkson University, Potsdam, NY; ²SUNY- University at Buffalo, Buffalo, NY; ³VA Western NY Healthcare System, Buffalo, NY
- TP 544 **Using Advanced Proteome Modeling to Initiate Real-Time Intelligent Time Based Acquisitions;** Scott Geromanos; Steve Ciavarini; *Waters Corporation, Milford, MA*
- TP 545 **Hypoxia-Induced Alternative Splicing Proteomics in Cancer Cell lines;** Liu Chia-Hsiun; Hsu Pang-Hung; , *Keelung, R.O.C.*
- TP 546 **Development of a Generic Proteomics Method Utilizing Self-Optimizing Acquisition Speed on a UHR-QTOF MS;** Stephanie Kaspar¹; Marko Lubeck¹; Annette Michalski¹; Pierre-Olivier Schmit²; ¹Bruker Daltonik GmbH, Bremen, Germany; ²Bruker Daltonique S.A., Wissembourg, France
- TP 547 **Multiplexed Chemoproteomic Profiling as a Tool to Decipher the Intracellular Interactions between Proteins and Small Molecules Identified in Phenotypic Screens;** Michael Ford¹; Richard Jones¹; Ravi Amunugama¹; Christopher Lietz^{2,3}; Danette Daniels³; Rachel Ohana³; Sergiy Levin⁴; Thomas Kirkland⁴; Marjeta Urh³; Keith Wood³; ¹MS Bioworks, Ann Arbor, MI; ²University of Wisconsin, Madison, WI; ³Promega Corporation, Madison, WI; ⁴Promega Biosciences LLC, San Luis Obispo, CA
- TP 548 **Proteomic Methods Comparison for Protein Identification and Quantitation of Muscle Proteins;** Jeremy Keirse¹; Liwen Zhang¹; Hui Meng²; Federica Montanaro³; Michael Lawlor²; Arpad Somogyi¹; ¹Ohio State University, Columbus, Ohio; ²Medical College of Wisconsin, Milwaukee, WI; ³Research Institute-Nationwide Children's Hospital, Columbus, OH
- TP 549 **Spatiotemporal S-Nitrosoproteome Analysis in Cdk5/p25 Mouse Model of Neurodegeneration by SNOTRAP and Mass Spectrometry;** Uthpala Seneviratne¹; Ravindra Kodihalli¹; Vadiraja Bhat²; Alexi Nott¹; John Wishnok¹; Li-Huei Tsai¹; Steven Tannenbaum¹; ¹Massachusetts Institute of Technology, Cambridge, MA; ²Agilent Technologies, Inc, Wilmington, DE
- TP 550 **Deciphering Phenotypic Drug Screening Targets Using a Novel Chloroalkane Capture Tag;** Rachel Friedman Ohana¹; Thomas A. Kirkland³; Carolyn C. Woodroffe³; Sergiy Levin³; Robin Hurst¹; Paul Otto¹; H. Tetsuo Uyeda³; Michael Ford²; Richard C. Jones²; Danette Daniels¹; Marjeta Urh¹; Keith Wood¹; ¹Promega Corporation, Madison, WI; ²MS Bioworks, LLC, Ann Arbor, MI; ³Promega Biosciences LLC, San Luis Obispo, CA
- TP 551 **In-Depth Proteome Coverage by Iterative Data Dependent Acquisition on a Benchtop Orbitrap Mass Spectrometer;** Mathias Mueller; Andreas Kuehn; Yue Xuan; Tabiwang N. Arrey; Thomas Rietpietsch; Florian Grosse-Coosmann; Catharina Crone; Torsten Ueckert; Markus Kellmann; *Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*
- TP 552 **PERSID: A Proteomic Approach for Identification of S-Sulfhydration Sites in Protein Extracts;** Changyuan Lu; Steven S Gross; *Weill Medical College of Cornell, New York, NY*
- TP 553 **Accumulated Ion Monitoring (AIM) Enables Yoctomolar Absolute Sensitivity and Seven Orders of Magnitude Accurate Quantitation in Complex Proteomes;** Paolo Cifani; Avantika Dhabaria; Alex Kentsis; *Memorial Sloan-Kettering Cancer Center, New York, NY*
- TP 554 **Peptides from RNAs Classified as Non-Coding;** Ruchi Chauhan; *Boston Children's Hospital, Neurology, Harvard, Boston, MA*
- TP 555 **Rapid Proteomics Assessment of Toxin Exposed Human Cells to Elucidate Mechanism of Action;** Jamie Allen¹; Jeffrey Spraggins¹; Ashley Jordan¹; William Burns¹; Jeremy L. Norris²; Eric P. Skaar²; D. B. Lacy²; Richard M. Caprioli²; ¹Vanderbilt University, Nashville, TN; ²Vanderbilt University School of Medicine, Nashville, TN
- PROTEOMICS:
NEW APPROACHES – SAMPLE PREPARATION METHODS
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- TP 556 **Achieving Optimal Digestion Faster with Flash Digest: Potential Alternative to Multi-Step Detergent Assisted In-Solution Trypsin Digestion in Quantitative and Qualitative Proteomics Experiments;** Vinit Shah; Michael Lassman; Haihong Zhou; Omar Laterza; *Merck Research Laboratories, Rahway, NJ*
- TP 557 **Rapid, Efficient and Reproducible Sample Preparation for Bottom-Up Proteomics by a Surfactant-Aided Precipitation/On-Pellet Digestion Strategy;** Shichen Shen; Jun Li; Xiaomeng Shen; Chengjian Tu; Jun Qu; *SUNY at Buffalo, Buffalo, NY*
- TP 558 **A Routine QC Method to Monitor High-Level LC and MS Performances on Complex Protein Digests;** Stephanie Kaspar¹; Ole Hoerning¹; Nicolai Bache¹; Alexander Harder¹; Pierre-Olivier Schmit²; ¹Bruker Daltonik GmbH, Bremen, Germany; ²Bruker Daltonique S.A., Wissembourg, France
- TP 559 **On the Advantages of Admixed Lys-C/Lys-N Digests, for Proteome Depth and DeNovo Peptide Sequencing;** Chris Adams; Anna Okumu; Allis S. Chien; Ryan Leib; *Stanford University Mass Spectrometry, Stanford, CA*
- TP 560 **SPARSE – Streamlined Proteomics And Robust Statistics Experiments: An Optimised Proteomics Pipeline to Increase Analytical Robustness, Accuracy, and Precision;** Ronan O’Cualain; Julian Selley; David Knight; , *M13 9Pt Manchester, UK*
- TP 561 **On-chip Mesoporous Functionalized Magnetic Microspheres for Extended Bottom-Up Proteomics;** Natalia Gasilova; Kristina Srzentic; Liang Qiao; Yury Tsybin; Hubert H. Girault; *EPFL, Lausanne, Switzerland*
- TP 562 **A Simplified Affinity Proteomics Workflow for Rapid, Sensitive, Quantitative Analysis of Proteins in Plasma;** John O’Grady¹; Kevin Meyer¹; Michael Stump²; Don Gray²; ¹Perfinity Biosciences, Inc, West Lafayette, IN; ²Bioanalytical Systems, Inc, West Lafayette, IN
- TP 563 **Immuno-Proteomics Using Polyclonal Antibodies and Stable Isotope Labeled Affinity-Purified Recombinant Protein Fragments;** Fredrik Edfors^{1,2}; Tove Boström¹; Masato Habuka²; Björn Forsström^{1,2}; Mathias Uhlén^{1,2}; ¹Proteomics and Nanobiotechnology, KTH, Stockholm, SE; ²Science for Life Laboratory, KTH, Solna, SE

- TP 564 **Closer Towards the Native State of Proteomes via Quantum Mechanical Protein Extraction;** Hartmut Schlüter¹; Marcel Kwiatkowski¹; Refat Nimer¹; Marcus Wurlitzer¹; Sebastian Kruber²; Nils-Owe Hansen²; R.J. Dwayne Miller²; ¹UKE - Mass Spec Proteomics, Hamburg, Germany; ²MPSD, Hamburg, Germany
- TP 565 **Automated Sample Preparation Solutions for MS-Based Proteomics;** Previn Naicker; Isak Gerber; Justin Jordaan; Stoyan Stoychev; CSIR, Pretoria, South Africa
- TP 566 **FACS-Proteomics: Combining Intracellular Staining, Cell Sorting, and Mass Spectrometry for Proteome Analysis of Targeted Cell Subpopulations;** Tony Ly; Arlene Whigham; Rosemary Clarke; Angus Lamond; Centre for Gene Regulation and Expression, Dundee, UK
- TP 567 **Integrated Strong Cation-Exchange Hybrid Monolith with Capillary Zone Electrophoresis and Mass Spectrometry for Proteomic Analysis;** Zhenbin Zhang; Norman J Dovichi; University of Notre Dame, Notre Dame, IN
- TP 568 **Optimizing Virtual 2D gel/MS through the Analysis of *E. coli* and *M. mazei* Cell Lysate;** Neil R. Quebbemann; Kate Liu; Rachel O. Loo; Joseph A. Loo; University of California, Los Angeles, CA
- TP 569 **Title: Secretome Proteomic Analysis of Stimulated Macrophages Using Metabolic Labeling, Click Chemistry Enrichment, and LC-MS/MS;** Jeffrey Martin; Cheryl Lu; Benbo Gao; Ru Wei; Peter Juhasz; Biogen Idec, Cambridge, MA
- TP 570 **Efficient Desalting and Clean-Up Methods of Protein Digests in Proteomics;** Shota Miyazaki¹; Naoyuki Sugiyama²; Chiaki Aoyama¹; Kosuke Osaka¹; Akira Jyukurogi¹; ¹GL Sciences Inc., Saitama, Japan; ²Kyoto University, Kyoto, Japan
- TP 571 **Laser Ablation Sample Transfer for Tissue LC-MS/MS Proteomic Investigation;** Fabrizio Donnarumma; Kermit K. Murray; Louisiana State University, Baton Rouge, LA
- TP 572 **On-Bead Digestion - Tackling the challenges of serum proteomics;** Haiyan Zheng¹; Caifeng Zhao¹; Meiqian Qian¹; Swapan Roy²; Absari Arpa²; Matt Kuruc²; ¹Rutgers Center for Proteomics, Piscataway, NJ; ²Biotech Support Group LLC, Monmouth Junction, NJ
- TP 573 **Optimization of Pulsed Proteolysis Conditions in Plasma Fractions Increases Sequence Coverage and Depth;** Jon Reed^{1,2}; Gogce Crynen^{1,2}; Prashanthi Vallabhaneni¹; Rosa Joy¹; James Evans¹; Laila Abdullah¹; Thinh Nguyen¹; Fiona Crawford¹; ¹Roskamp Institute, Sarasota, FL; ²SRQ Bio, Sarasota, FL
- TP 574 **Novel Method for Target Protein Identification Utilizing Immobilized Streptavidin Tips;** Kim Alving; Aharon Cohen; Bing Wang; Genzyme, a Sanofi company, Waltham, MA
- TP 575 **Preparation of Sequence-Controlled Triblock Copolymer-Grafted Silica Microparticles by Sequential-ATRP for Highly Efficient Glycopeptides Enrichment;** Yiting Pan; Weijie Qin; Xiaohong Qian; Beijing Proteome Research Center, Beijing, China
- TP 576 **Identification of Cow Milk-Derived Caseins with Two Dimensional Thin Layer Chromatography Matrix-Assisted Laser Desorption/Ionization Imaging Mass Spectrometry (2D-TLC-MALDI-IMS);** Egidijus Machtejevas¹; Michael Schulz¹; Knut Behrend²; Sascha Rohn²; Katerina Matheis¹; ¹Merck KGaA, Darmstadt, Germany; ²University of Hamburg, Hamburg, Germany
- TP 577 **Development of a Sample Enrichment Protocol Using Click Chemistry for Identification of Protein Targets of Reactive Metabolites in Liver Microsomes;** André LeBlanc; Tze Chieh Shiao; René Roy; Lekha Sleno; UQAM, Montréal, Canada
- TP 578 **Cysteine-Selective Dimethylation (cysDML) and Oxidized cysDML (OxycysDML) Methods to Study Redox Signaling in Disease;** Liqing Gu; Renā A. S. Robinson; University Of Pittsburgh, Pittsburgh, PA
- TP 579 **A Hydrophobic Label-Based Depletion Methodology for Enrichment of Protein N-Terminal Peptides from Microgram-Level Samples;** Brian Dill; Joseph Fernandez; Milica Tesic Mark; Henrik Molina; The Rockefeller University, New York, NY
- TP 580 **Chemoselective digestion for middle-down proteomics and structural analysis of monoclonal antibodies;** Kristina Srzentić¹; Konstantin Zhurov¹; Gennady Nikitin¹; Mario Cindrić²; Martin Kussmann^{1,3}; Yury Tsybin¹; ¹Ecole Polytechnique Federale, Lausanne, Switzerland; ²Ruder Boskovic Institute, Zagreb, Croatia; ³Nestlé Institute of Health Sciences, Lausanne, Switzerland
- TP 581 **Flexible Automated Sample Preparation Workflows: Modified Automated Systems for Specific Immuno-MS and MS Workflows;** David Colquhoun¹; Mohamed Nazim Boutaghou¹; Nishi Rochelle¹; Brett Noel²; Laurie Parker²; Kevin W. Meyer³; Scott Kuzdzal¹; Brian Feild¹; ¹Shimadzu Scientific Instruments, Columbia, MD; ²University of Minnesota, Minneapolis, MN; ³Perfinity Biosciences, West Lafayette, IN
- TP 582 **Automated Sample Preparation Workflows for Quantitative Proteomics Applications;** Oliver Popp¹; Lucas Luethy²; Tamara Kanashova¹; HaAn Nguyen¹; Julia Kikuchi¹; Guenter Boehm²; Thomas Blenkins³; Andreas Bruchmann³; Gunnar Dittmar¹; ¹MDC, Berlin, Germany; ²CTC Analytics, Zwingen, Switzerland; ³Axel Semrau GmbH, Sprockhovel, Germany
- TP 583 **High pH Reversed-Phase Peptide Fractionation in a Convenient Spin-Column Format;** Sergei Snovidia¹; Xiaoyue Jiang²; Ramesh Ganapathy¹; Sijian Hou¹; Ryan Bomgarden¹; Paul Haney¹; Rosa Viner²; John C. Rogers¹; ¹Thermo Fisher Scientific, Rockford, IL; ²Thermo Fisher Scientific, San Jose, CA
- TP 584 **MStern Blot - High Throughput PVDF Membrane-Based Proteomic Samples Preparation for 96-Well Plates;** Sebastian Berger¹; Saima Ahmed¹; Jan Muntel¹; Nerea Cuevas Polo¹; Richard Bachur²; Alex Kentsis³; Hanno Steen¹; ¹Harvard Medical School/Children's Hospital Boston, Boston, MA; ²Boston Children's Hospital, Boston, MA; ³Cornell University, New York, NY
- TP 585 **Online Membrane-Assisted Buffer Exchanger Coupled with Multijunction Capillary Isoelectric Focusing Device Enables Fractionation of Intact Human Plasma Proteins by pI;** Mohammad Pirmoradian Najafabadi^{1,2}; Juan Astorga-Wells^{1,2}; Roman A. Zubarev¹; ¹Karolinska Institutet, Solna, Sweden; ²Biomotif AB, Stockholm, Sweden
- TP 586 **Automated In-Gel Digestion on a Commercial Autosampler Directly Coupled to Nano LC-MS/MS;** Guenter Boehm²; Achermann François¹; Reto Bolliger²; Natasha Buchs¹; Nicholas Doiron¹; Sophie Lagache Braga¹; Manfred Heller¹; ¹University of Bern, Dpt of Clinical Research, Bern, Switzerland; ²CTC Analytics AG, Zwingen, Switzerland

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QUANTITATIVE – STABLE ISOTOPE LABELING METHODS
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- TP 587 **ITMSQ : A Software Tool for Multiple b, y Ion Pairs based Isobaric Tandem Mass Spectrometry Quantification;** Liqi Xie; Lei Zhang; Aiyng Nie; Ying Zhang; Haojie Lu; Fudan university, shanghai, P.R.China
- TP 588 **9-Plex Proteomic Labeling with Neutron-Encoded Amino Acids;** Elyse Freiburger¹; Anna Merrill¹; Alex Hebert¹; William Wood²; Marwan ElMasri²; Michael S. Westphall¹; Joel Bradley²; Joshua J. Coon¹; ¹University of Wisconsin, Madison, WI; ²Cambridge Isotope Laboratories, Inc., Tewksbury, MA
- TP 589 **Performance Evaluation of NeuCode Mouse labeling;** Christopher Rose¹; Emily Wilkerson¹; Alan Attie¹; Joshua Baughman²; Joel Bradley³; Marwan ElMasri³; Alex Hebert¹;

- TP 590 Mark Keller¹; Donald S Kirkpatrick²; Anna Merrill¹; Timothy Rhoads¹; Donald Stapleton¹; Michael S. Westphall¹; Clay Williams¹; William Wood³; Joshua J. Coon¹; ¹University of Wisconsin, Madison, WI; ²Genentech, Inc., South San Francisco, CA; ³Cambridge Isotope Labs., Andover, MA
Developmental Phosphoproteomics Identifies Casein Kinase 2 as a Therapeutic Target in Medulloblastoma; Teresa Purzner¹; John Sanders¹; Tom Hartl¹; James Purzner¹; Yoon-Jae Cho¹; Josh Elias¹; Matthew Scott²; ¹Stanford University, Stanford, CA; ²Carnegie Institution for Science, Washington, DC
- TP 591 **Mapping Proteolytic Peptide Production Rates in Plasma Using Stable Isotope Labeled Proteins from the SILAC-Labeled HepG2 Secretome;** John B. Mangrum; Erika J. Martin; Donald F. Brophy; Adam M. Hawkrige; Virginia Commonwealth University, Richmond, VA
- TP 592 **Quantitation of Methylation Levels in Specifically-Modified Histone H3 Standards by Stable-isotope Labeling and Mass Spectrometry;** Steven Toth; Wendell P. Griffith; , Toledo, OH
- TP 593 **Identification of p53-Induced Changes to the Non-Small Cell Lung Cancer Proteome;** Emmanuel Cudjoe; Khushboo Sharma; John Mangrum; David Gewirtz; Adam Hawkrige; Virginia Commonwealth University, Richmond, Virginia
- TP 594 **PCSK9 and Its Variants: A Global Proteomic Study to Identify Interactors and Effects on Protein Trafficking;** Ge Chu; Zhibin Ning; Janice Mayne; Daniel Figeys; University of Ottawa, Ottawa, ON
- TP 595 **In-Depth Comparative Mapping of the Global Proteome between Primary and Metastatic Skin Melanoma Cells Derived from the Same Individual;** Lei Guo; Weili Miao; Yongsheng Xiao; Yinsheng Wang; University of California, Riverside, Riverside, CA
- TP 596 **Quantitative Proteomics Deciphers Druggable ALK Signaling in Neuroblastoma;** Kristina B. Emdal; Anna-Kathrine Pedersen; Dorte B. Bekker-Jensen; Chiara Francavilla; Jesper V. Olsen; The NNF Center for Protein Research, Copenhagen, Denmark
- TP 597 **Quantification of the Membrane Differential Proteomes by Stable Isotope Labeling and Spectral Counting Strategies;** Ying Wai Lam^{1,2}; Bin Deng^{1,2}; Julia Fields^{1,2}; Kenneth Smith¹; Richard Voogt¹; Keith Mintz¹; ¹University of Vermont, Burlington, VT; ²UVM/VGN Proteomics Facility, Burlington, VT
- TP 598 **Quantitative Proteomic Profiling of the Newly Synthesized Proteins Associated with T Cell Growth;** Qing Kong; Zengli Guo; Xin Wei; Cui Liu; Xian Chen; Yisong Wan; University of North Carolina at Chapel Hill, Chapel Hill, NC
- TP 599 **Systematic Investigation of Cellular Response and Pleiotropic Effects in Atorvastatin-treated Liver Cells by MS-based Proteomics;** Haopeng Xiao; Weixuan Chen; George Tang; Johanna Smeeckens; Ronghu Wu; Georgia Institute of Technology, Atlanta, GA
- TP 600 **Characterization of Progression-Related Signaling Networks in a Colon Cancer Metastasis Model Using Phosphoproteomics;** Alissa Schunter; Xiaoshan Yue; Amanda B. Hummon; University of Notre Dame, Notre Dame, IN
- TP 601 **Mass Defect-Based Pseudo-Isobaric a1 Ion Pairs Enabled Accurate Proteome Quantification with Wide Dynamic Range and Deep Coverage;** Yuan Zhou; Jianhui Liu; Lihua Zhang; Yukui Zhang; Dalian Institute of Chemical Physics, Dalian, China
- TP 602 **In vitro Metabolic Labeling of Human Gut Microbiota for Quantitative Metaproteomics;** Xu Zhang; Zhibin Ning; Janice Mayne; Alain Stintzi; Daniel Figeys; Ottawa Institute of Systems Biology, Ottawa, Canada
- TP 603 **Application of Stable Isotope-Labeled Protein Fragments to Investigate the Correlation of Protein and mRNA Levels in Human Cell Lines;** Tove Boström¹; Frida Danielsson²; Emma Lundberg²; Henrik J Johansson³; Hanna Tegel⁴; Janne Lehtiö³; Mathias Uhlén²; Sophia Hober¹; Jenny Ottosson Takanen⁴; ¹Department of Protein Technology, KTH, Stockholm, Sweden; ²Science for Life Laboratory, KTH, Stockholm, Sweden; ³Science for Life Laboratory, KI, Stockholm, Sweden; ⁴Department of Proteomics, KTH, Stockholm, Sweden
- TP 604 **Targeted Absolute Quantification of Protein by GeLC-MS/MS: Western Blot Takes the Back Seat;** Mukesh Kumar¹; Shai Joseph¹; Martina Augsburg²; David Drechsel¹; Nadine Vastenhouw¹; Frank Buchholz²; Marc Gentzel¹; Andrej Shevchenko¹; ¹MPI-CBG, Dresden, Dresden, Germany; ²Medical Systems Biology Medical Faculty, TU Dresden, Dresden, Germany
- TP 605 **Characterization of Clinically-Relevant Stable Isotope Labeled Recombinant Proteins For Use As Internal Standards in Quantitative MS Workflows;** Kevin Ray; Pegah Jalili; David Rhee; Yongsheng Xiao; James J. Walters; Sigma-Aldrich, St. Louis, MO
- BIOMARKER: QUANTITATIVE ANALYSIS (NON-PROTEIN, LIPIDS/METABOLITES/COMPOUNDS)
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- TP 606 **Renal Cell Carcinoma Biomarker Screening by High-Performance Liquid Chromatography - Tandem Mass Spectrometry;** Sisi Chen¹; Casey Burton¹; Anthony Kaczmarek²; Honglan Shi¹; Yinfa Ma¹; ¹Missouri University of Science and Technology, Rolla, MO; ²Central Missouri Urology Clinic, Rolla, MO
- TP 607 **A Fit-for-Purpose LC-MS/MS Method for the Quantitative Measurement of Creatinine in Human Plasma;** Yue Zhao; Guowen Liu; Aida Angeles; Lisa Christopher; Xuewen Ma; Jim Shen; Mark Arnold; Bristol-Myers Squibb Co., Princeton, NJ
- TP 608 **The analysis of Sweat Biomarkers in Mechanically-Loaded Tissues Using SFC-MS;** Julie Herniman¹; G. John Langley¹; Rachel Greenhill¹; Peter Worsley²; Dan Bader²; Tim Jenkins³; ¹Chemistry, University of Southampton, Southampton, UK; ²Health Sciences, University of Southampton, Southampton, UK; ³Waters Corporation, Wilmslow, UK
- TP 609 **Method Development for the Determination of 24S-Hydroxycholesterol in Human Plasma by LC/APCI-MS/MS;** Hiroshi Sugimoto; Masaaki Kakehi; Yoshinori Satomi; Hidenori Kamiguchi; Fumihiko Jinno; Takeda Pharmaceutical Company Limited, Fujisawa, Japan
- TP 610 **Rapid and Selective Determination of 3-Nitrotyrosine in Human Blood Plasma;** Oleg Timofeev¹; Jin Ji²; ¹Zintro Consulting, Monmouth Jct, NJ; ²Brunswick Laboratories, Inc., Southborough, MA
- TP 611 **Quantification of Heparan Sulphate in Mucopolysaccharidoses Patient Urines using Novel Butanolysis Depolymerisation/Desulphation Sample Work-Up;** Paul Trim; John Hopwood; Marten Snel; South Australian Health & Medical Research Inst., Adelaide, AUSTRALIA
- TP 612 **A Sensitive LC-MS/MS Method for Quantitation of 7 α -hydroxy-4-cholesten-3-one in Human Plasma;** Dawei Zhou; Xingye Yang; Manik Desai; Jinn Wu; Xinping Fang; XenoBiotic Laboratories, Inc., WuXi AppTec, Inc., Plainsboro, NJ
- TP 613 **Noninvasive Measurement of Aristolochic Acid-DNA Adducts in Urine Samples from Rats by Liquid Chromatography Coupled Electrospray Ionization Tandem Mass Spectrometry;** Elvis Leung; HKUST, Hong Kong, China

- TP 614 **Determination of Endogenous Cortisol in Human Plasma Using LC-MS/MS Techniques with A Combined Calibration Curve and Standard Addition Methods;** Yansheng Liu¹; Yu-Hui Fu¹; David Winburn¹; Rodney Boughner¹; Stephen Wanaski²; Daniel Selness³; Gene Ray¹; ¹KCAS LLC, Shawnee, KS; ²Marathon Pharmaceuticals, LLC, Northbrook, IL; ³Spaulding Clinical Research, West Bend, WI
- TP 615 **Aspects of Electrospray Ionization of 25 Hydroxy Vitamin D. Lessons Learned;** Eduard Rogatsky; Daniel Stein; *Albert Einstein College of Medicine, Bronx, NY*
- TP 616 **LC-MS/MS Bioanalytical Support of Mouse Serial Microsampling Studies via Extraction of Sub-Microliter Volumes: Examples Including the Biomarker S-Adenosylmethionine;** Bao Hoang; Eric Britton; Casey Bonner; Danielle Pessolano; Sean Maki; Rick Luzietti; Angela Qi Shen; Steven Wiltshire; *Agilux Laboratories, Worcester, MA*
- TP 617 **Using HILIC to Improve LC-MS Sensitivity for the Detection of DNA Adducts Derived from Tobacco Specific N-Nitrosamines;** Lucie Loukotkova; Lei Guo; Frederick Beland; Goncalo Gamboa Da Costa; *NCTR, US FDA, Jefferson, AR*
- TP 618 **The Ratio of 8-iso-prostaglandin F2 α to Prostaglandin F2 α Distinguishes Enzymatic from Nonenzymatic Isoprostane Formation;** Fred Bjorn Lih; Thomas J. van 't Erve; Thomas E. Eling; Maria B. Kadiiska; Ronald P. Mason; Leesa J. Deterding; *NIEHS / NIH, RTP, NC*
- TP 619 **Measurement of Flame Retardant Metabolites in Human Urine by Solid Phase Extraction- Ultra High Performance Liquid Chromatography-Tandem Mass Spectrometry;** Nayana K. Jayatilaka; Paula Restrepo; Antonia M. Calafat; Liza Valentín-Blasini; *Centers for Disease Control and Prevention, Atlanta, GA*
- TP 620 **Development of a High-Sensitivity Micro LC/MS Method for Estradiol Quantification in Human Plasma;** Angela Doneanu¹; James Murphy²; ¹Waters, Milford, MA; ²Waters Corporation, Milford, MA
- TP 621 **A Robust and Efficient Approach to Quantitation of Organic Acids in Biological Matrices;** Vikki Tsefrikas; Kyle Goodsell; Dylan Bennett; Allysen Meymaris; *Agilux Laboratories, Worcester, MA*
- TP 622 **Quantification of Monohydroxy-Polycyclic Aromatic Hydrocarbons (OH-PAHs) in Urine by Online SPE-HPLC-MS/MS;** Yuesong Wang; Lei Meng; Erin Pittman; Alisha Etheredge; Kendra Hubbard; Debra Trinidad; Kayoko Kato; Xiaoyun Ye; Antonia Calafat; *CDC, Atlanta, GA*
- TP 623 **A SWATH-MS Approach to the Secretome under Oxidative Stress Conditions: Proteins and Metabolites Unravelling;** Sandra Anjo^{1,2}; Vera Mendes¹; Mário Grãos¹; Bruno Manadas¹; ¹Center for Neuroscience and Cell Biology, Cantanhede, Portugal; ²Faculty of Sciences and Technology, Coimbra, Portugal
- TP 624 **A Multi-Marker Panel for Measuring Oxidative Stress in Tissue Samples Using LC/MS/MS;** Hideji Fujiwara; Christopher Holley; David Scherrer; Rohini Sidhu; Daniel Ory; Jean Schaffer; *Washington University School of Medicine, St. Louis, MO*
- TP 625 **High-Throughput Intracellular Pteridinic Profiling by Liquid Chromatography – Quadrupole Time-of-Flight Mass Spectrometry;** Casey Burton¹; Rui Weng²; Li Yang²; Yu Bai²; Huwei Liu²; Yinfa Ma¹; ¹Missouri University of Science and Technology, Rolla, Missouri; ²Peking University, Beijing, China
- TP 626 **Quantification of Quorum Sensing Molecules and their Interaction with Polymixin-B Hemoperfusion in Human Plasma by LC-HRMS;** Claudio Medana; Federica Dal Bello; Valentina Santoro; Chiara Martano; Davide Medica; Alessandro Quercia; Vincenzo Cantaluppi; *University of Turin, Torino, Italy*
- TP 627 **Measurement of Catecholamines in Rat and Mini-pig Plasma and Urine by Liquid Chromatography-Tandem Mass Spectrometry Coupled with Solid Phase Extraction;** Huaibing He; Ester Carballo-Jane; Xinchun Tong; Lucinda Cohen; *Merck & Co., Inc., Rahway, NJ*
- TP 628 **Towards a Multi-Analyte, High Dynamic Range, High Throughput LC/MS/MS Smoker Screening Method;** Vincent Pagnotti; June Feng; Lanqing Wang; Benjamin Blount; *U.S. Centers for Disease Control and Prevention, Atlanta, GA*
- TP 629 **Analysis of Radiation-Induced Injury by Targeted High-Throughput Metabolomics;** Jace W. Jones¹; Claire L Carter¹; Gregory Tudor²; Alexander Bennett¹; Ann Farese¹; Isabel L Jackson¹; Zeljko Vujaskovic¹; Catherine Booth²; Thomas J MacVittie¹; Maureen A Kane¹; ¹University of Maryland, Baltimore, MD; ²Epistem, Ltd., Manchester, UK

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- TP 630 **Defining Molecular Mechanisms for the Anti-Colon Cancer Activity of Anthocyanin-containing Purple-fleshed Potato: A Shotgun Proteomic Approach;** Jairam Vanamala^{1,2}; Venkata Charepalli¹; Sridhar Radhakrishnan¹; Vadiraja Bhat³; Lavanya Reddivari¹; ¹Pennsylvania State University, University Park, PA; ²The Penn State Hershey Cancer Institute, Hershey, PA; ³Agilent Technologies, Wilmington, DE
- TP 631 **From Metabolomic Phenotyping Data to Clinical Signatures;** Guido Krebich; Guido Dallmann; Therese Koal; Wulf Fischer-Knuppertz; *Biocrates Life Sciences AG, Innsbruck, Austria*
- TP 632 **Proteomics Profiling and Potential Biomarker Detection in Sjogren's Syndrome after Ultrasound-Assisted Gene Transfer of IL-17R:Fc Chimera;** Changgong Wu¹; Zhimin Wang¹; Lee Zourelis¹; Hiteshi Thakker²; Michael Passineau¹; ¹Allegheny General Hospital, Pittsburgh, PA; ²Greentree Medical Associates, Pittsburgh, PA
- TP 633 **Mass Spectrometry Based Proteomics for Absolute Quantification of Proteins from Tumor Cells;** Hong Wang; Sam Hanash; *MD Anderson Cancer Center, Houston, TX*
- TP 634 **A Quantitative Proteomics Study of Cerebrospinal Fluid from Individual Niemann-Pick Disease, Type C1 Patients;** Stephanie M. Cologna¹; Brian C. Searle²; Paul S. Blank¹; Christopher A. Wassif¹; Nicole M. Yanjanin¹; Peter S. Backlund¹; Alfred L. Yergey¹; ¹National Institutes of Health, Bethesda, MD; ²Proteome Software Inc., Portland, OR
- TP 635 **Identification of Stroke Metalloprotein Biomarkers and Metal Profile in Human Blood Plasma for Specialized Treatment;** Keaton Nahan¹; Julio Landero Figueroa¹; Opeolu Adeoye²; Joseph Caruso¹; ¹Dept of Chemistry, University of Cincinnati, Cincinnati, Ohio; ²Medical Center, University of Cincinnati, Cincinnati, OH
- TP 636 **Identification of Moesin as a New Endothelial Marker in Human Sepsis Using SILAC-Based Secretomics;** Oh Kwang Kwon¹; Sae-kwang Ku²; Wonhwa Lee¹; Sunju Kim¹; Joung A Kim¹; Jin Young Kim³; Shin-Woo Kim¹; Sangkyu Lee¹; ¹Kyungpook National University, Daegu, Republic Of Korea; ²Daegu Haany University, Gyeongsan-si, Republic Of Korea; ³Korea Basic Science Institute, Ochang, Republic Of Korea
- TP 637 **Identification of Early Proteomic Biomarkers of Nonclinical Cardiotoxicity;** Li-Rong Yu; Zhijun Cao; Yuan Gao; Richard Beger; James Fuscoe; Varsha Desai; *National Center for Toxicological Research, FDA, Jefferson, AR*
- TP 638 **Revealing Pathways In COPD-Associated Lung Cancer Via Large-Scale Quantitative Multi-omic Analysis;** Brian J Sandri¹; Andy H Limper²; Pratik Jagtap³; Svetlana V Avdulov¹; Mark S Peterson¹; Carl Murie⁴; Yang Ping²; Ola Larsson⁴; Peter B Bitterman¹; Leeann Higgins³; Todd

- W Markowski³; Tim J Griffin³; Chris H Wendt^{1,5}; ¹University of Minnesota, Minneapolis, MN; ²Mayo Clinic, Rochester, MN; ³Center for Mass Spectrometry and Proteomics, UMN, St. Paul, MN; ⁴Karolinska Institute, Solna, Sweden; ⁵VA Medical Center, Minneapolis, MN
- TP 639 **NASH Mechanism Understanding Using MS Imaging: Discover New Disease State Biomarkers;** Pierre-Maxence Vaysse¹; Anita M. van den Hoek²; Gregory Hamm¹; Robert Kleemann²; Jonathan Stauber¹; Hans M.G. Princen²; ¹ImaBiotech, MS Imaging Dept., Loos, France; ²TNO, Metabolic Health Research, Leiden, The Netherlands
- TP 640 **Development of Multi-Marker Diagnostic Platforms for Early Diagnosis of Hepatocellular Carcinoma;** Areum Sohn; , Seoul, South Korea
- TP 641 **Proteomic Identification of Head and Neck Cancer Patients with Persistent Human Papillomavirus Infections Associated with Improved Survival;** Nicolas Schlecht¹; Nicole Kawachi¹; Yanhua Wang^{1,3}; Thomas Harris¹; Thomas Belbin¹; Peicheng Du²; Richard Smith³; Ruth Angeletti¹; Michael Prystowsky¹; Jihyeon Lim¹; ¹Albert Einstein College of Medicine, Bronx, NY; ²Rutgers University, Newark, NJ; ³Montefiore Medical Center, Bronx, NY
- TP 642 **A Simple and Sensitive Method for the Analysis of Sphingolipid Glycosylation Enables the Differentiation of Ovarian Cancer Sub-Types;** Arun Everest-Dass; Merrina Anugraham; Nicolle Packer; Macquarie University, Sydney, Australia
- TP 643 **Determination of Polyp & Cancer-free Resection Margins in Colonoscopy, Complex Pelvic and Colonic Surgery using Rapid Evaporative Ionization Mass Spectrometry;** James L Alexander¹; Julia Balog^{1,2}; Alasdair J Scott¹; Abigail VM Speller¹; Laura J Muirhead¹; James Kinross¹; Julian P Teare¹; Zoltan Takats¹; ¹Imperial College London, London, UK; ²Waters Corporation, Wilmslow, UK
- TP 644 **Development of a MS Assay to Identify Breast Cancer Candidate Biomarkers from Formalin-Fixed Paraffin Embedded (FFPE) Tissue;** Ten-Yang Yen; Moe Thein; Roger Yen; Leslie Timpe; Bruce Macher; San Francisco State University, San Francisco, CA
- TP 645 **Protein Profile of Schistosoma mekongi using GeLC-MS/MS Based Proteomics;** Onrapak Reamtong¹; Polkit Sangvanich²; Supaporn Supaporn Nuamtanong¹; Phiphool Chusongsang¹; Poom Adisakwattana¹; ¹Mahidol University, Bangkok, Thailand; ²Chulalongkorn University, Bangkok, Thailand
- TP 646 **Diagnosis of Lung Tumor Types Based on Metabolomic Profiles in Lymph Node Aspirates;** Daniel Sappington; , Little Rock, AR
- TP 647 **Proteomic and Transcriptomic Profiling of an Inducible Model of Acute Myeloid Leukemia Reveals Novel Insights into Leukemogenesis;** Jarrod Sandow; Gabriella Brumatti; Giuseppe Infusini; Paul Ekert; Andrew Webb; The Walter & Eliza Hall Institute, Parkville, Australia
- TP 648 **The Oxidized Proteome of Peripheral Blood Mononuclear Cells: A Valuable Repository for Clinical Proteomics;** Daniel Lopez Ferrer; Xiaolei Xie; Xiaoyue Jiang; Andreas Huhmer; Thermo Fisher Scientific, San Jose, CA
- TP 649 **Method for the Analysis of Neurosteroids in Human Serum to a LLOQ of 5 pg/mL;** Vince Windisch¹; John Slemmon²; John Masucci²; Allan Xu¹; ¹Keystone Bioanalytical, Inc., North Wales, PA; ²Janssen Research and Development, Spring House, PA
- TP 650 **The Quantitation of Glucosylsphingosine in Mouse Models of Gaucher Disease by Liquid Chromatography-Tandem Mass Spectrometry;** Rick Hamler¹; Nastry Brignol¹; Sean Morrison¹; Angela Sanders²; Leo Dungan¹; Hui Hwa Chang¹; Kenneth J. Valenzano¹; Robert E. Boyd¹; Chau Dang¹; Lorne A. Clarke²; Sean W. Clark¹; Elfrida R. Benjamin¹; ¹Amicus Therapeutics, Cranbury, NJ; ²Dept of Medical Genetics, Univ of British Columbia, British Columbia, Canada
- TP 651 **Accurate Quantitation of Plasma Globotriaosylsphingosine (lyso-Gb3) in Healthy Individuals and Fabry Patients by Liquid Chromatography-Tandem Mass Spectrometry (LC-MS/MS);** Rick Hamler¹; Nastry Brignol¹; Robert Boyd¹; Daniel G. Bichet²; Dominique P. Germain³; Roberto Giugliani⁴; Derralyn A. Hughes⁵; Raphael Schiffmann⁶; William R. Wilcox⁷; Hadis N. Williams¹; Julie Yu¹; Jay Barth¹; Jeff Castelli¹; Kenneth J. Valenzano¹; Jeff Castelli¹; Elfrida R. Benjamin¹; ¹AMICUS Therapeutics, Paoli, PA; ²Hôpital du Sacré-Coeur, Montreal, Quebec, Canada; ³Hôpital Raymond Poincaré, University of Versailles, Garches, France; ⁴Medical Genetics Service, HCPA/UFRGS, Porto Alegre, Brazil; ⁵Royal Free Campus, University College London, London, UK; ⁶Baylor Research Institute, Dallas, Texas, TX; ⁷Department of Human Genetics, Emory University, Atlanta, GA
- TP 652 **Absolute Quantitation of Apolipoprotein E3 and E4 Isoforms from Human Cerebrospinal Fluid and Brain;** Alaina Baker-Nigh¹; Kwasi Mawuenyega¹; Vitaliy Ovod¹; Hamideh Zakeri¹; Tom Kasten¹; Randall Bateman^{1,2}; ¹Washington University School of Medicine, Saint Louis, MO; ²Knight Alzheimer's Disease Research Center, St. Louis, MO
- TP 653 **SWATH Analysis of Patient-Derived iPSC to Motor Neurons for the Discovery of Protein Network Perturbations that Underlie Motor Neuron Diseases;** Andrea Matlock; Loren Ornelas; Ronald Holewinski; Berhan Mandefro; Lindsay Lenaeus; Anais Sahabian; Clive Svendsen; Dhruv Sareen; Jennifer E. Van Eyk; Cedars-Sinai, Los Angeles, CA
- TP 654 **Detection of Breast Cancer Recurrence Using LC-MS/MS Targeted Metabolic Profiling;** Jiangjiang Zhu¹; Lingli Deng^{1,3}; Danijel Djukovic¹; Haiwei Gu¹; Daniel Rafferty^{1,2}; ¹University of Washington, Seattle, WA; ²Fred Hutchinson Cancer Research Center, Seattle, WA; ³Xiamen University, Xiamen, China
- IMAGING MS: PHARMACEUTICAL APPLICATIONS**
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- TP 655 **Utility of High Resolution MALDI Imaging in Drug Discovery: Histological Distribution of Gentamicin in Proximal Renal Tubules of Rats;** Hidefumi Kaji¹; Hiroyuki Hashimoto¹; Masayoshi Saito¹; Takushi Yamamoto²; Noriyuki Ojima²; ¹Mitsubishi Tanabe Pharma Corporation, Saitama, Japan; ²Shimadzu Corporation, Kyoto, Japan
- TP 656 **MALDI-Imaging Mass Spectrometry for Pharmacokinetics of Transcutaneous Medicine;** Eishi Imoto; Osaka University, Suita City, Japan
- TP 657 **Blocking NMDA Mediated DYN Neurotoxicity influences Brain Lipids Profile in Traumatic Brain Injury;** Amina S. Woods¹; Shelley N Jackson¹; Aurelie Roux¹; Ludovic Muller¹; J Albert Schultz²; Brian M Cox^{3,4}; Carey Balaban⁵; ¹NIDA-IRP, NIH, Baltimore, MD; ²Ionwerks, Inc., Houston, TX; ³Uniformed Services University, Bethesda, MD; ⁴Center for Neuroscience and Regenerative Medicine, Rockville, MD; ⁵University of Pittsburgh, Pittsburgh, PA
- TP 658 **Visualizing Brimonidine Distribution in Pig Optic Nerve Tissue by Imaging Mass Spectrometry;** Michelle Reyzer; Chad Chumbley; Michael DeLisi; Louise Mawn; Eva Harth; Robert Galloway; Richard Caprioli; Vanderbilt University, Nashville, TN
- TP 659 **Small Molecule Analysis in Single Hair Strands for Evaluation of Drug Adherence with IR-MALDESI MS;** Elias Rosen¹; Corbin Thompson²; Mark Bokhart¹; Heather



- Prince²; Craig Sykes²; Angela DM Kashuba²; David C. Muddiman¹; ¹North Carolina State University, Raleigh, NC; ²University of North Carolina, Chapel Hill, NC
- TP 660 **Mass Spectrometry Imaging of the Fly Brain;** Andrew Ewing^{1,2}; Nhu Phan²; John Fletcher¹; ¹Chalmers University, Gothenburg, Sweden; ²University of Gothenburg, Gothenburg, Sweden
- TP 661 **Under the skin: Biomarkers of Cutaneous Defenses to Vaccines using Mass Spectrometry Imaging;** Juliette Masure¹; H el ene Perrin²; Gregory Hamm¹; Maxence Wisztorski⁴; Melody Dufoss e²; Charlotte Primard³; Jean-Pierre Both⁵; Michel Salzet⁴; Isabelle Fournier⁴; Anthony Larue⁵; Jonathan Stauber¹; B ehazine Combadi ere²; ¹ImaBiotech, MS Imaging Dept., Loos, France; ²INSERM U1135-Cimi-Paris, Paris, France; ³Adjuvatis, Lyon, Lyon; ⁴PRISM Lab. INSERM U1192, Univ. Lille1, Villeneuve d'Ascq, France; ⁵CEA-List, Gif-sur-Yvette, France
- TP 662 **Distribution of Newly Coordinated ⁵⁷Fe-heme by MALDI FT-ICR MS Imaging Proved the Efficacy of Epoetin Beta Pegol (C.E.R.A.);** Makoto Kihara; Mariko Noguchi-Sasaki; Yukari Matsuo-Tezuka; Keigo Yorozu; Mitsue Kurasawa; Hideyuki Yasuno; Yasushi Shimonaka; Chugai Pharmaceutical Co., Ltd, Kamakura, Japan
- TP 663 **Blood-Brain Barrier Drug Targeting by Mass Spectrometry Imaging in Early Adme Profiling;** Theodosia Vallianatou¹; Henrik Loden¹; Anna Nilsson¹; Mohammadreza Shariatgorji¹; Marcela Pereira²; Per Svenningsson²; Maria Karlgren¹; Per E. Andren¹; ¹Uppsala University, Uppsala, Sweden; ²Karolinska Institute, Stockholm, Sweden
- TP 664 **MALDI-IMS-MSI for the Analysis of 3D Tissue-Engineered Psoriatic Skin Models;** Amanda Harvey¹; Laura Cole¹; John Warwick²; Richard Bojar²; David Smith¹; Neil Cross¹; Malcolm Clench¹; ¹Sheffield Hallam University, BMRC, Sheffield, UK; ²Innovenn, York, UK
- TP 665 **Mass Spectrometry Imaging of Drug Related Crystal-Like Structures in Frozen and Paraffin Embedded Rabbit Kidney Tissue Sections;** Anne L. Bruinen^{1,2}; Ronald de Vries³; Marjolein van Heerden³; Rob J. Vreeken³; Filip Cuyckens³; Ron M.A. Heeren^{1,2}; ¹FOM Institute AMOLF, Amsterdam, Netherlands; ²M4I, Maastricht University, Maastricht, NL; ³Janssen Pharmaceutica, Beerse, Be
- TP 666 **Validating Quantitative Imaging Mass Spectrometry of Pharmaceuticals in Tissue Sections;** Chad Chumbley¹; Michelle Reyzer¹; Gwendolyn Marriner²; Laura Via²; Clifton Barry III²; Richard Caprioli¹; ¹Vanderbilt University, Nashville, TN; ²NIH/NIAID, Bethesda, MD
- TP 667 **A Nanostructured Matrices Assessment to Study Drugs Distribution in Solid Tumor Tissues by Mass Spectrometry Imaging;** Silvia Giordano¹; Lavinia Morosi¹; Roberta Pastorelli¹; Massimo Zucchetti¹; Luigi Falciola²; Giuseppe Cappelletti²; Valentina Pifferi²; Melinda Morelli²; Sonja Visentin³; Enrico Davoli¹; ¹IRCCS Istituto Mario Negri, Milano, Italy; ²Chemistry Dept., University of Milan, Milano, Italy; ³Mol. Biotec. and Health Dept., University of Torino, Torino, Italy
- IMAGING MS: DISEASE MARKERS**
668-694
- TP 668 **Imaging Mass Spectrometry Reveals the Decrease of Cardiolipin on Kidney of NASH Model Mouse;** Takahiro Hayasaka; Hirotoshi Fuda; Shu-Ping Hui; Hitoshi Chiba; Hokkaido University, Sapporo, Japan
- TP 669 **Using MALDI Mass Spectrometry Imaging to Uncover the Role of Ganglioside Metabolism in Neurodegeneration;** Sarah Caughlin; Kristina Jurcic; Ken Yeung; David Cechetto; Shawn Whitehead; Western University, London, Canada
- TP 670 **Functional Metabolic Multimodality Imaging by Dynamic Nuclear Polarization-Magnetic Resonance Imaging and Mass Spectrometry Imaging;** Daisuke Miura; Fuminori Hyodo; Yoshinori Fujimura; ICMRN, Kyushu University, Fukuoka, Japan
- TP 671 **MCAEF (Matrix Coating Assisted by an Electric Field): a Novel Technique for Enhanced Imaging of Biomarker Candidates for Prostate Cancer;** Xiaodong Wang¹; Jun Han¹; Juncong Yang¹; Jingxi Pan¹; Christoph Borchers^{1,2}; ¹University of Victoria-Genome BC Proteomics Centre, Victoria, BC, Canada; ²Dept. of Biochem. & Microbiol., Univ. of Victoria, Victoria, BC, Canada
- TP 672 **Multimodal Mass Spectrometric Imaging for Targeted Metabolomics of Ovarian Cancer;** Martin R. L. Paine¹; Rachel V. Bennett¹; Jaeyeon Kim²; L. DeEtte Walker¹; John McDonald¹; Martin M. Matzuk²; Facundo M. Fern andez¹; ¹Georgia Institute of Technology, Atlanta, GA; ²Baylor College of Medicine, Houston, TX
- TP 673 **Imaging Mass Spectrometry in Prostate Cancer – Looking Beyond Histology;** Kristina Schwamborn^{1,2}; Roopika Menon³; Sven Perner³; Richard Caprioli²; ¹Technical University Munich, Munich, Germany; ²Vanderbilt University, Nashville, TN; ³Institute of Pathology, Bonn, Germany
- TP 674 **Histological Examination of FFPE Pancreas Tumor Sections Combined with Imaging Mass Spectrometry Analysis at High Speed and Spatial Resolution;** J org Kriegsmann^{1,4}; Mark Kriegsmann²; Michael Becker³; Soeren-Oliver Deininger³; Mike Otto^{1,4}; Rita Casadonte⁴; ¹Center for Histology, Cytology and Molecular Diagn, Trier, Germany; ²University of Heidelberg, Heidelberg, Germany; ³Bruker Daltonik GmbH, Bremen, Germany; ⁴Proteopath GmbH, Trier, Germany
- TP 675 **Tumor Classification Using Mass Spectrometry and Microarrays;** Jone Garate¹; Roberto Fern andez¹; Sergio Lage¹; Arantza P erez-Valle²; Tarson Tolentino-Cortez²; Aintzane Asurmendi¹; Egoitz Astigarraga²; Mar a D. Boyano¹; Gabriel Barreda-G omez²; Jos e A. Fern andez¹; ¹University of Basque Country, Leioa, Spain; ²IMG Pharma Biotech, Zamudio, Spain
- TP 676 **Imaging Mass Spectrometry of Liver Regeneration after Partial Hepatectomy in Mice Targeting Primary Bile Acids and Nucleotides;** Kohta Iguchi¹; Yudai Tsuji²; Taisuke Nakamura²; Tomoyuki Nakamura³; Etsuro Hatano¹; Shinji Uemoto¹; Masaya Ikegawa²; ¹Kyoto University, Kyoto, Japan; ²Doshisha University, Kyoto, Japan; ³Kansai Medical University, Hirakata, Japan
- TP 677 **Molecular Imaging of Lipid Alteration and Blood-Brain Barrier Disruption in a Mouse Model of Impact Concussive Traumatic Brain Injury;** Bo Yan¹; Yi Pu¹; Andrew M. Fisher^{1,2}; Chad A. Tagge^{1,2}; Lee E. Goldstein^{1,3}; Mark E. McComb¹; Catherine E. Costello¹; ¹Boston University School of Medicine, Boston, MA; ²College of Engineering, Boston University, Boston, MA; ³Boston University Photonics Center, Boston, MA
- TP 678 **3-Dimensional Molecular Imaging of the Optic Chiasm Glioma Microenvironment;** David M. Anderson¹; Anne Solga²; David Gutmann²; Shannon Cornett³; Kristie Rose¹; Kevin Schey¹; Richard Caprioli¹; ¹Vanderbilt University School of Medicine, Nashville, TN; ²Washington University School of Medicine, St. Louis, MO; ³Bruker Daltonics Inc., Billerica, MA
- TP 679 **Identification of Lipid Biomarkers of Human Colon Cancer Using Imaging Mass Spectrometry;** Jone Garate¹; Joan Bestard-Escalas²; Roberto Fernandez¹; Daniel H. Lopez²; Sergio Lage¹; Rebeca Reigada²; Sam Khorrani^{2,3}; Jose Reyes^{2,4}; Isabel Amengual^{2,5}; Gwendolyn Barcelo-Coblijn²; Jose A. Fernandez¹; ¹Universidad del Pais Vasco, Leioa, SPAIN; ²Research Unit, Hospital

- Universitari Son Espases, Palma, Spain; ³Gastroenterology Unit, Hospital Universitari Son E, Palma, Spain; ⁴Gastroenterology Unit, Hospital Comarcal de Inca, Inca, Spain; ⁵Anatomy Unit, Hospital Universitari Son Espases, Palma, Spain
- TP 680 **Nutrient Sequestration at the Pathogen-Human Host Interface: Imaging Mass Spectrometry reveals Bacterial Subpopulations in Biofilms;** Jessica Moore¹; Catherine Wakeman²; Michael Noto²; Boone Prentice¹; Jeffrey Spraggins¹; Michael Becker³; Jeremy L. Norris¹; Eric Skaar²; Richard Caprioli¹; ¹Vanderbilt University MSRC, Nashville, TN; ²Vanderbilt University School of Medicine, Nashville, TN; ³Bruker Daltonik GmbH, Bremen, Germany
- TP 681 **Proteomic Mass Imaging of Pancreas from Type 2 Diabetes (T2D) Rat Model;** Noriyuki Iwasaki¹; Kei Masuyama²; Hiroshi Wakazono²; Takashi Nirasawa¹; Hirofumi Fujigaya²; Masumi Higashiyama²; Daisuke Hibi²; Mayu Shukutani³; Yuki Kuzuhara³; Hiroyuki Yanagi²; Masaya Ikegawa³; ¹Bruker Daltonics K.K., Kanagawa, Japan; ²Ono Pharmaceutical Co., Ltd., Osaka, Japan; ³Doshisha University, Kyoto, Japan
- TP 682 **A MALDI-MS Imaging Study of Changes in Cardiolipin Distribution in Rat Model of Non-Alcoholic Steatosis;** Hay-Yan J. Wang^{1,2}; Hsuan-Wen Wu¹; Kuan-Lun Su¹; Zhi-Fu Zheng¹; ¹National Sun Yat-Sen University, Kaohsiung, Taiwan; ²Kaohsiung Medical University, Kaohsiung, Taiwan
- TP 683 **Visceral Leishmaniasis Biomarkers Discovery by MALDI Imaging Mass Spectrometry;** Daniele F. O. Rocha¹; Vanessa G. Santos¹; Caroline Jaegger¹; Katia Roberta A. Belaz¹; Anna Maria A. P. Fernandes A. P. Fernandes¹; Selma Giorgio²; Marcos N. Eberlin¹; ¹ThOMSon Lab., Chemistry Institute, UNICAMP, Campinas, Brazil; ²Biology Institute, UNICAMP, Campinas, Brazil
- TP 684 **MALDI Imaging Mass Spectrometry Reveals Age-Related Deamidation and Truncation of Human Lens Insoluble Proteins;** Jamie L Wenke; Kristie L Rose; Jeffrey Spraggins; Kevin L. Schey; ¹Vanderbilt University, Nashville, TN
- TP 685 **MALDI-MS Lipid Imaging and [11C] Acetate PET of Tumour Heterogeneity in Non-Small-Cell Lung Cancer;** Fiona Henderson¹; David Lewis²; Philippa Hart³; Kevin Brindle²; Dmitry Soloviev²; Kaye Williams¹; Adam McMahon¹; ¹University of Manchester, Manchester, UK; ²CRUK-Cambridge Institute, University of Cambridge, Cambridge, UK; ³Shimadzu, Manchester, UK
- TP 686 **Large-Scale Mass Spectrometry Imaging Investigation of Cortical Spreading Depression in a Mouse Model of Migraine;** Ricardo Carreira¹; Benjamin Balluff¹; Walid Abdelmoula¹; Jouke Dijkstra¹; Michel Ferrari¹; Else Tolner¹; Arn van den Maagdenberg¹; Liam McDonnell²; ¹LUMC, Leiden, NL; ²LUMC & PSF, Pisa, Italy
- TP 687 **Investigation of Biomarkers of Laser-Induced Retinal Damage Using Mass Spectrometric Imaging;** Richard F. Reich; Joseph M. Champaign; ¹US Air Force, Usaf Academy, Colorado [CO]
- TP 688 **Proteomic Imaging of amyloids in Brains from Amyloid Precursor Protein (APP) Transgenic Mice in comparison with Human Alzheimer Amyloid;** Masaya Ikegawa¹; Tomohiro Miyasaka¹; Noriyuki Iwasaki²; Takashi Nirasawa²; Hiroyuki Sumikura³; Shigeo Murayama³; Yasuo Ihara⁴; ¹Doshisha University, Kyoto, Japan; ²Bruker Daltonics K.K., Yokohama, Japan; ³Tokyo Metropolitan Geriatric Hospital and Inst., Tokyo, Japan; ⁴Doshisha University, Graduate School of Brain Scie, Kyoto, Japan
- TP 689 **Multimodal Imaging of Rat Brain, 1-3 Months Post Stroke: A MALDI MS Insight into Long Term Molecular Expression;** Philippa Hart¹; Fiona Henderson²; Luis Mancera¹; Omar Belgacem¹; Herve Boutin²; Adam McMahon²; ¹Shimadzu, Manchester, UK; ²Wolfson Molecular Imaging Centre, Manchester, UK
- TP 690 **Studies of Diabetic Myocardial Infarction: In Situ Hydrogel-Mediated Protein Digestion Augments the Identification of Protein Changes Detected by MALDI IMS;** Audra Judd; Salisha Hill; Jeremy L. Norris; Michelle Reyzer; Jeffrey Spraggins; Kristie L. Rose; Michael F. Hill; Richard Caprioli; ¹Vanderbilt University School of Medicine, Nashville, TN
- TP 691 **Glycopathology Characterization of an N-Glycan Biomarker Panel for Pancreatic Cancer Tissues Using MALDI Imaging Mass Spectrometry and Other Methods;** Thomas W. Powers¹; Benjamin A. Neely¹; Huiyuan Tang²; Huarong Xu¹; Peng Gao¹; Anand S. Mehta³; Brian H. Haab²; Richard R. Drake¹; ¹Medical University of South Carolina, Charleston, SC; ²Van Andel Institute, Grand Rapids, MI; ³Drexel University, Doylestown, PA
- TP 692 **Polarity Switching Mass Spectrometry Imaging of Lipids Using Infrared Matrix-Assisted Laser Desorption Electrospray Ionization (IR-MALDESI) Coupled to a Q-Exactive Plus;** Milad Nazari; Elias Rosen; David C. Muddiman; ¹North Carolina State University, Raleigh, NC
- TP 693 **Visualizing Lipid Inflammatory Pathways in Advanced Pulmonary Tuberculosis Lesion Development by MALDI-MSI and Immunohistochemistry;** Brendan Prideaux; Pei-Yu Chen; Nancy Ruel; Matt Zimmerman; Eliseo Eugenin; Véronique Dartois; ¹PHRI, New Jersey Medical School, Rutgers, Newark, NJ
- TP 694 **Ion Mobility Mass Spectrometry Imaging of the Human Intraocular Malignancy, Uveal Melanoma;** Laura M Cole¹; Hardeep S Mudhar²; Karen Sisley²; Malcolm R Clench¹; ¹Sheffield Hallam University, Sheffield, UK; ²Royal Hallamshire Hospital, Sheffield, UK





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|---|-------------------------------|---|---------|
| 7:30 – 8:00 am..... | Set up all Wednesday posters | Biomarkers: Quantitative Analysis..... | 297-308 |
| 10:30 am – 1:00 pm..... | Odd-numbered posters present | Informatics: SRM and DIA..... | 309-318 |
| 12:00 – 2:30 pm..... | Even-numbered posters present | Informatics: Peptide ID and Quantification..... | 319-339 |
| 7:30 – 8:00 pm..... | Remove all Wednesday posters | Proteomics: Quantitative - Targeted Protein Quantification..... | 340-362 |
| Elemental Analysis: General..... | 001-022 | Peptides: Quantitative Analysis I..... | 363-382 |
| Nanomaterials..... | 023-034 | Peptides: PTM Identification..... | 383-417 |
| Energy: Biofuel and Minor Fuel Components..... | 035-047 | Ionization Mechanisms..... | 418-429 |
| Food Safety..... | 048-082 | Ambient Ionization: Instrumentation..... | 430-456 |
| Food "omics": MS Characterization of Food and Nutritional Supplements..... | 083-105 | Nanoscale and Microfluidic Separations and MS..... | 457-467 |
| Small Molecules: Quantitative Analysis..... | 106-138 | Instrumentation: New Concepts..... | 468-491 |
| Drug Metabolism: Quantitative Analysis..... | 139-161 | LC-MS: Sample Preparation..... | 492-517 |
| Nucleic Acids..... | 162-183 | Imagng MS: Sample Preparation..... | 518-532 |
| Epigenetic Modifications..... | 184-199 | Imaging MS: Method Development I..... | 533-554 |
| Metabolomics: Clinical Applications..... | 200-219 | Ion Mobility: Structures..... | 555-575 |
| Carbohydrates II..... | 220-242 | Ion Mobility: Non-covalent Complexes..... | 576-586 |
| Lipids: Quantitative Analysis..... | 243-255 | Proteins: Non-covalent Interactions..... | 587-604 |
| Lipids: ID and Structural Analysis..... | 256-271 | Structural Biology..... | 605-617 |
| Biomarkers: Discovery..... | 272-296 | H/D Exchange: Protein Structure/Function I..... | 618-647 |
| | | Proteins: Conformation Analysis..... | 648-658 |
| | | Antibodies and Antibody: Drug Conjugates I..... | 659-687 |

ELEMENTAL ANALYSIS: GENERAL 001-022

- WP 001 **A Polar Reversed-Phase UPLC/Ultrahigh-Resolution MS Method for Molecular Profiling and Quantitation of Naphthenic Acids in Oil Sands Process Water;** Jun Han¹; Karen Lin¹; Yi Yi²; John Gibson²; Christoph Borchers^{1,3}; ¹University of Victoria-Genome BC Proteomics Centre, Victoria, BC, Canada; ²Alberta Innovates – Technology Futures, Victoria, BC, Canada; ³Dept. of Biochem & Microbiol., Univ. of Victoria, Victoria, BC, Canada
- WP 002 **Development of a μ -SPE-direct Sample Analysis Mass Spectrometry Method for the Identification and Quantification of Disinfection By-Products;** Lydon Alexandrou¹; Oliver Jones¹; Andrew Minett²; ¹ACROSS, School of Applied Sciences, RMIT University, Melbourne, VIC, Australia; ²EPREP Pty Ltd, Mulgrave, VIC, Australia
- WP 003 **Determination of As, Se and Zn in Superalloy by Dynamic Reaction Cell of Inductively Coupled Plasma Mass Spectrometry;** Jingyu Hu; Yanxia Hou; Guowu Yang; Mei Han; Lixia Yang; , Beijing, BEIJING
- WP 004 **High Performance Liquid Chromatography - Mass Spectrometry Identification of Tobacco-Specific Nitrosamines in Drinking Water;** Xing-Fang Li¹; Beibei Chen²; Yichao Qian¹; ¹University of Alberta, Edmonton, Canada; ²Wuhan University, Wuhan, CN
- WP 005 **GC/MS Analysis of Volatile Water Pollutants with Rapid On-Site Sample Preparation;** Olga Polyakova¹; Viatcheslav Artaev²; Albert T. Lebedev¹; ¹Moscow State University, Moscow, Russian Federation; ²LECO Corporation, St Joseph, MI
- WP 006 **GC-APLI for Trace Analysis of PAHs in Particulate Matter from Ambient Air;** Masha Pitiranggon¹; Thomas Arthen-Engeland²; Verena Tellstroem²; Beizhan Yan¹; Carsten Baessmann²; ¹Lamont-Doherty Earth Observatory of Columbia Univ., Palisades, NY; ²Bruker Daltonik GmbH, Bremen, Germany
- WP 007 **Experimental and Theoretical Insights into H₂O Activation by Th⁺: The Spin-Orbit Effect;** Richard Cox¹; Peter Armentrout²; ¹Department of Chemistry, University of Utah, Salt Lake City, UT; ²University of Utah, Salt Lake City, UT
- WP 008 **Development of a Rapid Ion Chromatography-Tandem Mass Spectrometry Method for Simultaneous Analysis of Haloacetic Acids and Related Halogen Compounds;** Runmiao Xue^{1,2}; Honglan Shi^{1,2}; John Yang³; Enos Inniss⁴; ¹Missouri University of Science and Technology, Rolla, MO; ²Center for CS3M, Rolla, MO; ³Lincoln University of Missouri, Jefferson City, MO; ⁴University of Missouri-Columbia, Columbia, MO
- WP 009 **Fragmentation Trees for Automated *de novo* Interpretation of Impure Electron Ionization Spectra from Gas Chromatographic Complex Mixture Analysis: Chemical Deconvolution;** Kevin Siek¹; Vasily Makarov²; Viatcheslav Artaev¹; Dmitry Mazur³; Albert T. Lebedev³; ¹LECO Corporation, Saint Joseph, MI; ²Mass Spectrometry Consulting Ltd., Bar, Montenegro; ³Moscow State University, Moscow, Russian Federation
- WP 010 **Novel Approach for *in vivo* Metabolic and Contaminant Profiling of Underwater Ecosystems by LC-HRMS using Solid Phase Microextraction as a Sampling Tool;** Barbara Bojko^{1,2}; Ezel Boyaci¹; Krzysztof Goryński^{1,2}; Thanos Dailianis³; Evangelina Yiantzi⁴; Eleftheria Psillakis⁴; Janusz Pawliszyn¹; ¹University of Waterloo, Waterloo, Canada; ²Collegium Medicum, Nicolaus Copernicus University, Torun, Poland; ³Hellenic Centre for Marine Research, Heraklion, Crete, Greece; ⁴Technical University of Crete, Chania, Greece
- WP 011 **Determination of BMAA, DAB, AEG and Three Alkaloid Cyanotoxins in Lake Water using Dansyl Chloride Derivatization and UHPLC-HESI-HRMS Detection;** Audrey Roy-Lachapelle; Morgan Sollic; Sébastien Sauvé; Université de Montréal, Montréal, Canada
- WP 012 **Non-targeted Approach for the Evaluation of Concentration Fluctuations in the Effluent of Different Wastewater Treatment Plants;** Matthias Ruff; Rahel Comte; Martin Loos; Heinz Singer; Eawag, Duebendorf, Switzerland
- WP 013 **Thermal Desorption - Gas Chromatography - High Resolution Time-of-Flight Mass Spectrometry (TD-GC- HRT MS) for Analysis of Geochemical Biomarkers;** Giovana Bataglion¹; Clécio Klitzke²; Joe Binkley²; Jeffrey Patrick²; Marcos Eberlin¹; ¹Unicamp, Campinas, SP-Brazil; ²LECO Corporation, St. Joseph, MI
- WP 014 **Detection of Toxic Substances in Environmental Samples by Liquid Chromatography-Tandem Mass Spectrometry and Metabolomics;** Sam Li; Wenlin Zhang; Si Ni Lee; Le Rong; Thawatchai Maneerung; Chi-Hwa Wang; Koon Gee Neoh; National University of Singapore, Singapore, Singapore
- WP 015 **Accurate Mass Quantification of Brominated Flame Retardants in Milk by Q-TOF Based;** Xin Ma; Zheng-xiang Zhang; Tao Bo; Agilent Technologies, Beijing, China

- WP 016 **Screening Lake Trout for Perfluorinated and Polyfluorinated Compounds in Lake Trout Using UPLC-QToF in Mse Mode;** Sadjad Fakouri Baygi; Bernard Crimmins; Thomas Holsten; *Clarkson University, Potsdam, NY*
- WP 017 **The Detection of Trace Organic Pollutes by the Ion-Molecular Reaction of Arylnitrenium Ions in Gas Phase via Mass Spectrometry;** Lei Yue¹; Chuanfan Ding²; Yuanjiang Pan¹; ¹*Department of chemistry, Zhejiang University, Hang Zhou, China*; ²*Department of chemistry, Fudan University, Shang Hai, China*
- WP 018 **Method Optimization for the Separation and Quantification of Key Metabolites in *Daphnia magna* tissues;** Philippe Venne¹; Viviane Yargeau²; Pedro A. Segura¹; ¹*University of Sherbrooke, Sherbrooke, Canada*; ²*McGill University, Montreal, Canada*
- WP 019 **Determination of Phthalates in Environmental Matrices;** Oihana Ros Ibarretxe¹; Grazina Pacepavicius²; Tommy Bisbicos²; Ailette Prieto Sobrino¹; Asier Vallejo Ruiz¹; Mehran Alaei²; ¹*University of the Basque Country (UPV/EHU), Bilbao, Spain*; ²*Environment Canada, Burlington, Canada*
- WP 020 **Uranium Quantification in Ores by Microwave Plasma Torch Tandem Mass Spectrometry;** Meiling Yang; Eric Handberg; Juchao Liang; Huanwen Chen; *East China Institute of Tech., Nanchang, China*
- WP 021 **Orbitrap Mass Spectrometry Characterization of Water Samples Derived from Athabasca Lean Oil Sands and Mixed Surficial Materials;** John Headley¹; Kerry M. Peru¹; Chris Swyngedouw²; Ian Fleming³; ¹*Environment Canada, Saskatoon, Canada*; ²*Exova, Calgary, Canada*; ³*University of Saskatchewan, Saskatoon, Canada*
- WP 022 **Soil Humic Acids- A Potential Common Source and Formation Process Elucidated by ESI-FTICR-MS;** Nicole DiDonato; Hongmei Chen; Derek Waggoner; Patrick Hatcher; *Old Dominion University, Norfolk, VA*
- NANOMATERIALS**
023-034
- WP 023 **The Evaluation of Amine Core Dendrimers as Calibrants for Electrospray Ionization (ESI) and Matrix-Assisted Laser Desorption/Ionization (MALDI) Mass Spectrometry;** Brittany K. Casey; Scott M. Grayson; *Tulane University, New Orleans, LA*
- WP 024 **Single Particle Inductively Coupled Plasma-Mass Spectrometry Analysis of Nanoparticles Uptake by Crops;** Yongbo Dan^{2,3}; Honglan Shi²; Xingmao Ma^{1,3}; Weilan Zhang¹; Runmiao Xue²; Chady Stephan⁴; ¹*Southern Illinois University, Carbondale, IL*; ²*Missouri University of Science and Technology, Rolla, MO*; ³*CS3M center at Missouri University of Sci&Tech, Rolla, MO*; ⁴*PerkinElmer Inc, Woodbridge, On*
- WP 025 **Investigation of Substrate-Assisted Laser Desorption for Gold Nanoparticle Analysis with ICP MS;** Iva Benešová¹; Kristýna Dlabková¹; Tomáš Vaculovič^{1,2}; Viktor Kanický^{1,2}; Jan Preisler^{1,2}; ¹*Masaryk University, Brno, Czech Republic*; ²*CEITEC MU, Brno, Czech Republic*
- WP 026 **A Novel Carrier Based on TiO₂ Suitable for Isolation of His-tagged Recombinant Proteins and Peptides;** Rudolf Kupcik; Jan Macak; Pavla Krulisova; Pavel Rehulka; Zuzana Bilkova; *University of Pardubice, Pardubice, Czech Republic*
- WP 027 **Surface Characterization of Nanometer-Thick Organic Layers on Nanomaterials using Ambient Ionization Mass Spectrometry;** Sharanya Reddy; Chady Stephan; Craig Whitehouse; *PerkinElmer, Shelton, CT*
- WP 028 **Enhanced LDI-MS Detection of Gold Nanoparticles in Biological Samples using the Synergy between Added Matrix and the Gold Core;** Alyssa Marsico; Sukru Gokhan Elci; Daniel Moyano; Gulen Yesilbag Tonga; Bradley Duncan; Ryan Landis; Vincent M. Rotello; Richard Vachet; *University of Massachusetts Amherst, Amherst, MA*
- WP 029 **Polyppyrrrole/Multi-walled Carbon Nanotube Composites Combined with GC-MS/MS for Determination of Ultraviolet Filters and its Metabolites in River Water and Urine;** Yu-Chen Liao; Yu-Min Liu; Maw-Rong Lee; *National Chung-Hsing University, Taichung, Taiwan*
- WP 030 **Solid Matrices for the Small Molecule Analysis using MALDI-TOF Mass Spectrometry;** Jo-Il Kim; Jae-Chul Pyun; *Yonsei University, Seoul, South Korea*
- WP 031 **The Use of Ion Mobility Spectrometry-Mass Spectrometry (IMS-MS) to Elucidate Arm-Dispersity within Star Polymers;** Scott M. Grayson¹; Casey D. Foley²; Boyu Zhang¹; Sarah Trimpin²; ¹*Tulane University, New Orleans, LA*; ²*Wayne State University, Detroit, MI*
- WP 032 **Quantitative Analysis of Drug Loading on Nanoparticle-based Cancer Therapeutics using Scanning Particle Mobility Mass Spectrometry;** Sherrie Elzey¹; De-Hao Tsai²; Tae Joon Cho²; Julien Gigault²; Vincent Hackley²; ¹*TSI Incorporated, Shoreview, MN*; ²*National Institute of Standards and Technology, Gaithersburg, MD*
- WP 033 **Binding Selectivity of Cucurbit[5]uril (CB5) and Substituted Cucurbit[5]uril For Anions in the Gas Phase;** Jiewen Shen; David V. Dearden; *Brigham Young University, Provo, UT*
- WP 034 **9.4 T FT-ICR Mass Spectrometer with Cluster Ion Source for Analysis of Formation and Structure of Metallofullerenes and Other Nanomaterials;** Paul W. Dunk^{1,2}; Nathan K. Kaiser²; Alan G. Marshall^{1,2}; Harold W. Kroto¹; ¹*Florida State University, Tallahassee, FL*; ²*National High Magnetic Field Laboratory, Tallahassee, FL*
- ENERGY: BIOFUEL AND MINOR FUEL COMPONENTS**
035-047
- WP 035 **Quantification of an Anionic Surfactant in Brine Using Solvent Extraction Followed by Spectrophotometry, Evaporative Light Scattering Detection, and Mass Spectrometry;** Mark Romanczyk; Xueming Dong; Ravikiran Yerabolu; Hilka Kenttamaa; *Purdue University, West Lafayette, IN*
- WP 036 **Chemical Fingerprinting of Fast and Slow Pyrolysis Oils with Fourier Transform Ion Cyclotron Resonance Mass Spectrometry;** Janne Janis; *University of Eastern Finland, Joensuu, Finland*
- WP 037 **Screening of Ligands as Copper Sequestering Agent by Electrospray Mass Spectrometry (ESI-MS): A Clue for Addition of Diesel Fuel;** Cécile Perret¹; Hélène Nierengarten³; Amandine Racaud⁴; Géraldine Papin⁴; Aziz Jouaiti²; Mir Wais Hosseini²; Emmanuelle Leize-Wagner¹; ¹*LSMIS - UMR 7140 CNRS/University of Strasbourg, Strasbourg, France*; ²*LTM - UMR 7140 CNRS/University of Strasbourg, Strasbourg, France*; ³*Service de Spectrométrie de Masse - UMR 7177, Strasbourg, France*; ⁴*CReS - TOTAL, Solaize, France*
- WP 038 **Field-portable GC/MS for the Direct Analysis of Fuel Tracers;** Philip Tackett; Cynthia Liu; Leonard Rorrer; Mitch Wells; Dennis Barket, Jr; *FLIR Systems, West Lafayette, IN*
- WP 039 **Structural Effects on the Ionization Response of Lignin Model Compounds during Electrospray Ionization;** Fan Huang; Bert C. Lynn; *University of Kentucky, Lexington, KY*
- WP 040 **Biomarker Identification in Crude Oil by using Gas Chromatography/ High-Resolution Mass Spectrometry with Electron Ionization and Field Ionization;** Masaaki Ubukata; A. John Dane; Robert B. Cody; *JEOL USA, INC., Peabody, MA*
- WP 041 **Thin-film Pyrolysis High Resolution Mass Spectrometry of Glucose-based Carbohydrates: Real-time Monitoring of Products and Their Thermal Profiles;** Daniel Cole; Carolyn Hutchinson; Young Jin Lee; *Iowa State Univ Chemistry Dept, Ames, IA*
- WP 042 **Analysis of Biodiesel Contamination In Jet Fuel using Supercritical Fluid Chromatography-Electrospray Ionisation Mass Spectrometry (SFC-ESI-MS);** Waraporn

- Ratsameepakai¹; Julie Herniman¹; Tim Jenkins²; G John Langley¹; ¹University of Southampton, Southampton, UK; ²Waters Corporation, Wilmslow, UK
- WP 043 **Molecular Level Characterization of Solid Graphite Pitches by High Resolution MALDI Ion Mobility Mass Spectrometry**; Wen Zhang; Hans Joachim Räder; Klaus Müllen; *MPI for Polymer Research, Mainz, Germany*
- WP 044 **The Carbon Isotopic (¹³C/¹²C) Signature of Sugar Cane Bioethanol: Certifying the Major Source of Renewable Fuel from Brazil**; Laura A. Neves¹; Gabriel F. Sarmanho¹; Valnei. S. Cunha¹; Romeu J. Daroda¹; Marcos N. Eberlin²; Maira Fasciotti^{1,2}; ¹INMETRO, Duque De Caxias, Brazil; ²University of Campinas, UNICAMP, Campinas, Brazil
- WP 045 **Fragmentation of Deprotonated Model Compounds with Lignin – Carbohydrate Linkages upon Collision – Activated Dissociation (CAD)**; Christopher Marcum; Weijuan Tang; Huaming Sheng; Tiffany Jarrell; Hilka Kenttämää; *Purdue University, West Lafayette, IN*
- WP 046 **Characterization of a Municipal Solid Waste Pyrolysis Oil by Electrospray Ionization FT-ICR Mass Spectrometry**; Rebecca Beasley¹; Alan G. Marshall^{1,2}; Ryan P. Rodgers^{1,3}; ¹The Florida State University, Tallahassee, FL; ²Ion Cyclotron Resonance Prog, Tallahassee, FL; ³Future Fuels Institute, Tallahassee, FL
- WP 047 **Exploring Mechanisms of Fast Pyrolysis of Lignin via Tandem Mass Spectrometry and Quantum Chemical Calculations: A Synthetic Model Compound Study**; Priya Murria; Jinshan Gao; John C. Degenstein; Huaming Sheng; Matthew R. Hurt; John J. Nash; Hilka I. Kenttämää; *Purdue University, West Lafayette, U.S.*
- FOOD SAFETY**
048-082
- WP 048 **Improved Analysis of Veterinary Drug Residues in Biological Tissues by UHPLC-MS/MS**; ; Alan Lightfield; *U.S. Dept. of Agriculture, Wyndmoor, PA*
- WP 049 **Applications of Liquid Chromatography-High Resolution Mass Spectrometry for the Analysis of Pesticides in Fresh Produce and Teas**; Kelli Simon¹; Jon Wong¹; Alexander Krynskiy¹; Zhengwei Jia²; Jian Wang³; James Wittenberg¹; Hoon Park¹; ¹FDA, College Park, MD; ²Shanghai Institute for Food and Drug Control, Shanghai, China; ³Canadian Food Inspection Agency, Calgary AB, Canada
- WP 050 **Determination of Pesticides in Foods using Dopant-optimized Gas Chromatography-Atmospheric Pressure Chemical Ionization Quadrupole-Time-of-Flight Mass Spectrometry**; Kyung Hoon Cha^{1,2}; Shin-Kwon Kang²; Sawyen Ow²; Jong Hwa Lee³; Jung-Hak Lee¹; Jeong-Han Kim¹; Dong-Ho Kim³; ¹Seoul National University, Seoul, Korea; ²Braker Korea Ltd., Seongnam-Si, Korea; ³Experimental Research Institute, NAQS, Gimcheon-si, Korea
- WP 051 **The Use of Silica Plate Laminating for Molecular Trapping Followed by Laser Desorption Ionization Mass Spectrometry**; Diogo Noin De Oliveira; Mônica Ferreira; Rodrigo Catharino; *Innovare Biomarkers Laboratory - UNICAMP, Campinas, Brazil*
- WP 052 **New Analytical Tools to Tackle an Old Problem: Strategies for the Screening and Identification of Mycotoxins in Food by UHPLC/QTOF/MS**; Elisabeth Varga¹; Emma Rennie²; Thomas Glauner³; Michael Sulyok¹; Maria Vandamme²; Rudolf Krška¹; Franz Berthiller¹; ¹Univ of Natural Resources and Life Sciences, Vienna (BOKU), Austria; ²Agilent Technologies Inc, Santa Clara, CA; ³Agilent Technologies Sales&Services GmbH, Waldbronn, Germany
- WP 053 **Fast GC-MS/MS Analysis of Multicomponent Pesticides Residues (360) in Food Matrices using UFMS Technology**; Hendrik J. Schulte¹; Hans-Ulrich Baier¹; Stéphane Moreau¹; Klaus Bollig²; ¹SHIMADZU Europa Gmbh, Duisburg, Germany; ²Shimadzu, Duisburg, N/A
- WP 054 **A Comparative Study of Targeted Screening Method by LC/MS/MS and Un-targeted Screening Method by LC-TOF in Residual Pesticides Analysis**; Zhaoqi Zhan; Jie Xing; Zhe Sun; Zhi Wei Ting; Yin Ling Chew; *Customer Support Centre, Shimadzu (Asia Pacific), Pte Ltd, Singapore*
- WP 055 **Applying 'Fast GC-MS/MS' using Triple Quadrupole Technology to Increase Productivity for Pesticide Residue Analysis in QuEChERS Extracts**; Cristian Cojocariu¹; Mike Hetmanski²; Richard Fussell²; Dominic Roberts¹; Paul Silcock¹; Sergio Guazzotti³; Jason Cole³; ¹Thermo Fisher Scientific, Runcorn, UK; ²Food and Environment Research Agency, York, UK; ³Thermo Fisher Scientific, Austin, TX
- WP 056 **Quantitative and Qualitative Confirmation of Pesticides in Beet Extract Using High Resolution Accurate Mass (HRAM) Mass Spectrometry**; Charles T. Yang²; Dipankar Ghosh²; Olaf Scheibner¹; ¹Thermo Fisher Scientific, Bremen, Germany; ²Thermo Fisher Scientific, San Jose, CA
- WP 057 **A Sensitive and Repeatable Method for Characterization of Sulfonamides and Trimethoprim in Honey in QuEChERS Extracts with Liquid-Chromatography-Tandem Mass Spectrometry**; Hernando Escobar; Jeffrey H. Dahl; Eddie Medina; Christopher T. Gilles; *Shimadzu Scientific Instruments, Columbia, MD*
- WP 058 **Analysis of QuEChERS Extracts of a Variety of Foods for Pesticide Residues using Automated SPE Coupled to GC/MS/MS and LC/MS/MS**; Mark J. Hayward¹; Jonathan Ho²; Peter Ratsep²; Rick Youngblood¹; Kim Gamble¹; ¹ITSP Solutions, Hartwell, GA; ²Shimadzu, Somerset, NJ
- WP 059 **Reducing Matrix Effects in Multi-Residue Pesticide Analysis by Sample Dilution using a Newly Developed Triple Quadrupole MS with Enhanced Sensitivity**; Mark Sartain¹; Thomas Glauner²; Anabel Fandino¹; Na Pi Parra¹; ¹Agilent Technologies, Santa Clara, CA; ²Agilent Technologies GmbH, Waldbronn, Germany
- WP 060 **Reduced Cost for Pesticides Residues Analysis by GC/MS/MS Using Mini-QuEChERS and an Ultra-Efficient Ionization Source**; Melissa Churley¹; Joan Stevens²; ¹Agilent Technologies, Santa Clara, CA; ²Agilent Technologies, Wilmington, DE
- WP 061 **Validation of a Method for the Quantitation of Multiple Pyrrolizidine Alkaloids in Herbal Teas and Honey by UHPLC/MS/MS**; Christina Gottert¹; Melinda Bittner¹; Franziska Spitzbarth¹; Angelika Oltmanns¹; Thomas Glauner²; Na Pi Parra³; Steve Royce³; Guenther Kempe¹; ¹LUA Saxony, Pharmacologically Active Compounds, Chemnitz, Germany; ²Agilent Technologies Sales & Services GmbH, Waldbronn, Germany; ³Agilent Technologies, Inc., Santa Clara, CA
- WP 062 **Pesticides Target Screening with an Atmospheric Pressure Chemical Ionisation GC Coupled to High-Resolution Q-TOF-MS**; Thomas Arthen-Engeland; Petra Decker; Karin Wendt; Oliver Raether; Verena Tellstroem; Carsten Baessmann; *Braker Daltonik GmbH, Bremen, Germany*
- WP 063 **Development of an MS/HRMS Library for Rapid Quantitation, Confirmation and Dereplication of Marine Toxins using All-Ion High Resolution Tandem Mass Spectrometry (Q-TOF) Coupled to Ultra-High Performance Liquid Chromatography (UHPLC)**; Manoella Sibati¹; Zita Zengong¹; Véronique Séchet¹; Christine Herrenknecht²; Zouher Amzili¹; Philipp Hess¹; ¹Ifremer, Laboratoire Phycotoxines, Nantes, France; ²LUNAM, Université de Nantes, Nantes, France
- WP 064 **Examination of Pesticides in Wine, Beer and Their Constituent Products using High-Throughput Techniques to Maximize Extraction & Efficiency**; Patricia Atkins; *Spex Certiprep, Metuchen, NJ*

- WP 065 **Development of an Analytical Method for Screening and Confirmation of Multi-Class Veterinary Drug Residues in Fish by LC-MS/MS;** Junghyun Kim; Hyun-Deok Cho; Won Jae Kang; Unyong Kim; Han Young Eom; Joon Hyuk Suh; Sang Beom Han; *Chung-Ang University, Seoul, South Korea*
- WP 066 **Application of UHPLC and Quadrupole Orbitrap High-Resolution Mass Spectrometer for Determination of 111 Pesticides Residues in Wines;** Niusheng Xu; *Shanghai, China*
- WP 067 **Evaluation of Variable Data Independent Acquisition (vDIA) Approach for Non-target Screening of Veterinary Drug in Animal Feed;** Zhe Zhou; Zheng Jiang; *Thermo Fisher Scientific, Shanghai, China*
- WP 068 **Optimisation and Validation of a Multi-class, Multi-residue Method for Veterinary Drug Confirmation in Animal Derived Food by UHPLC-MS/MS;** David Baker¹; Neil J Loftus¹; Laetitia Fages²; Eric Capodanno²; Mikael Levi³; ¹Shimadzu, Manchester, UK; ²Phytocontrol, Nimes, France; ³Shimadzu France, Marne-La-Vallée, France
- WP 069 **Identification of Contaminants in Dog Food by LC Time of Flight Mass Spectrometry with Fragment Ion Confirmation;** Sue Dantonio¹; Lynne Marshall²; Tes Ingbritsen³; Stephanie Morgenstern⁴; Joni Stevens⁵; ¹Agilent Technologies, Cedar Creek, TX; ²Agilent Technologies, Toledo, OH; ³Royal Standard Poodles, Staples, MN; ⁴DePaul University, Chicago, IL; ⁵Agilent Technologies, Little Falls, DE
- WP 070 **A Sensitive and Selective LC-MS/MS Detection and Quantitation of Highly Polar Aminoglycosides Antibiotics in Honey Matrix;** Neha Bhasin¹; Prasanth Joseph¹; Praveen Sharma¹; Manoj Pillai¹; Jianru Stahl-Zeng²; ¹Sciex, 121, Udyog Vihar, Gurgaon, India; ²Sciex, Darmstadt, Germany
- WP 071 **Trace Analysis of Dioxins and Dioxin-Like PCBs utilizing GC/MS/MS with a New High Efficiency Source;** Jessica Westland; *Agilent Technologies, Wilmington, Delaware*
- WP 072 **Targeted Multi Residue LC-MS/MS Method for Sulfonamides and Nitroimidazoles Antibiotics in Honey with LC-MS/MS;** Neha Bhasin¹; Prasanth Joseph¹; Praveen Sharma¹; Manoj Pillai¹; Jens Dahlmann²; ¹Sciex, 121, Udyog Vihar, Phase IV, Gurgaon, Haryana, India; ²Sciex, Darmstadt, Germany
- WP 073 **Method Development for Fake Lamb Meat Detection using LC-MS/MS system;** Lihai Guo; Haiyan Cheng; Wenhai Jin; Huaifen Liu; *AB SCIEX, Beijing, China*
- WP 074 **A High Sensitivity LC/MS/MS Method with QuEChERS Sample Pre-treatment for Analysis of Aflatoxin in Peanut Butter Samples;** Yin Ling Chew¹; Jie Xing¹; Zhi Wei Ting¹; Jun Xiang Lee²; Zhaoqi Zhan¹; ¹Customer Support Centre, Shimadzu (Asia Pacific), Pte Ltd, Singapore; ²School of Physical & Mathematical Sciences, Nanyang Technological University, Singapore
- WP 075 **Screening for Pesticide Residues in Fruits and Vegetables by GC/Q-TOF with an Exact Mass Library;** Philip L. Wylie; Joni Stevens; Kumi Shiota Ozawa; Joerg Riener; Wen-wen Wang; Jennifer Gushue; *Agilent Technologies, Wilmington, DE*
- WP 076 **Fast Screening, Identification and Quantification of Pesticide Residues in Baby Food using GC Orbitrap MS Technology;** Cristian Cococariu¹; Richard J. Fussell³; Mike Hetmanski³; Dominic Roberts¹; Jason Cole²; Paul Silcock¹; ¹Thermo Fisher Scientific, Runcorn, UK; ²Thermo Fisher Scientific, Austin, TX; ³Food and Environment Research Agency, York, UK
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- Indore, MP, India; ²PREMIER Biosoft, Palo Alto, CA; ³Agilent Technologies, Santa Clara, CA, USA
- WP 266 **Shot-gun Analysis of Rough-Type Lipopolysaccharides using UVPD and a Custom Suite of Fragment Assignment Tools;** Dustin Klein; W. Ryan Parker; Alexander Boulgakov; Jennifer Brodbelt; *University of Texas at Austin, Austin, TX*
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- WP 269 **Specific Dissociations of Protonated N-acyl Amino Acid Mono Ethyl Esters under Resonant and Non-Resonant Excitation Conditions in FT/MS;** Toufik Toaalibi Boukerche¹; Sandra Alves²; Mohamed Bouchekara³; Mohammed Belbachir⁴; Jean-Claude Tabet²; ¹*Université d'Oran BP 1524, Oran, Algeria*; ²*University Paris VI (UPMC) case 45 UMR 8232 CNRS, Paris Cedex 05, France*; ³*L'COMM Université de Mascara, BP 763, Mascara, Algeria*; ⁴*Université d'Oran ES-SENIA, Oran, Algeria*
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Pocock⁴; Malcolm Ward¹; ¹Proteome Sciences, Cobham, UK; ²University of Eastern Finland, Kuopio, Finland; ³The Sahlgrenska Academy, University of Gothenburg, Gothenburg, Sweden; ⁴UCL Institute of Neurology, London, UK

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- WP 343 **A Single, Rapid Integrated Method to Quantify the Anti-Inflammatory Protein, TSG-6, by On-Column Proteolytic Digestion Followed by LC/ESI-MSMS;** Joshua Emory²; Benjamin Oyler¹; Timothy Varney²; Kathleen Housman²; Jonathan Oyler²; ¹*University of Maryland, Baltimore, Whiteford, MD*; ²*USA Medical Research Institute of Chemical Defense, Aberdeen Proving Ground, MD*
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- WP 345 **Absolute Quantification of Key Pathway Proteins Reveals SOS1 as the Bottleneck of ERK Response in the Ras-MAPK Pathway;** Tujin Shi¹; Mario Niepel²; Carrie D. Nicora¹; Yuqian Gao¹; Thomas L. Fillmore³; William B. Chrisler¹; Matthew J. Gaffrey¹; Ronald J. Moore¹; Tao Liu¹; David G. Camp II¹; Richard D. Smith¹; Karin D. Rodland¹; Peter K. Sorger²; H. Steven Wiley³; Wei-Jun Qian¹; ¹*PNNL, Richland, WA*; ²*Harvard Medical School, Boston, MA*; ³*EMSL, PNNL, Richland, WA*
- WP 346 **Gaining Insight into Complex Biology During the Drug Discovery Process Using Quantitative Immunocapture MicroFlow LC-MS/MS;** Eugene F. Ciccimaro; Bogdan Slecza; Yongxin Zhu; John T. Mehl; Bryan Parks; Susan Kuklennyik; David M. Schieltz; Michael Gardner; Jon Rees; McWilliams Lisa; Yulanda Williamson; John R. Barr; *Centers for Disease Control and Prevention, Atlanta, GA*
- WP 347 **Automating MRM-Based Protein Quantification using the Bravo AssayMAP Platform;** Martin Uhrbom¹; Andrew J. Percy²; Christoph H. Borchers²; Tasso Miliotis¹; ¹*AstraZeneca R&D Molndal, Molndal, Sweden*; ²*UVic - Genome British Columbia Proteomics Centre, Vancouver, Canada*
- WP 348 **A Novel Method of 18O/Metal Isobaric Labeling Combined with MRM Mass Spectrometry for the Absolute Quantification of Drug Metabolic Enzymes;** Yangjun Zhang^{1,2}; Hui Yan^{1,2}; Feiran Hao^{1,2}; Xiaohong Qian^{1,2}; ¹*Beijing Proteome Research Ctr, Beijing, China*; ²*Beijing Institute of Radiation Medicine, Beijing, China*
- WP 349 **MRM Quantitation of a Broad Panel of Candidate Disease-linked Proteins in Mouse Plasma and Multiple Tissues;** Sarah Michaud¹; Andrew Percy¹; Juncong Yang¹; Suping Zhang¹; Christoph Borchers^{1,2}; ¹*University of Victoria-Genome BC Proteomics Centre, Victoria, BC, Canada*; ²*Univ. of Victoria, Victoria, BC, Canada*
- WP 350 **Quantitative Analysis of AKT/mTOR Pathway using Immunoprecipitation and Targeted Mass Spectrometry;** Bhavin Patel; Suzanne Smith; Alex Behling; Leigh Conner; Kay Opperman; Ryan Bomgarden; Barbara Kaboord; John C. Rogers; *Thermo Fisher Scientific, Rockford, IL*
- WP 351 **High-Throughput sMRM Based Quantitation of PTMs in Monoclonal Antibodies and Antibody Drug Conjugates with a Qtrap 6500;** Qing Xie; *South San Francisco, CA*
- WP 352 **A Quantitative Analysis of Central Metabolic Enzymes in Microbial Cell Factories using Nano LC-Ultra-Fast Mass Spectrometry;** Fumio Matsuda¹; Tairo Ogura²; Yoshihiro Toya¹; Natsuki Hiasa¹; Katsunori Yoshikawa¹; Atsumi Tomita¹; Ichiro Hirano²; Hiroshi Shimizu¹; ¹*Osaka University, Suita, Japan*; ²*Shimadzu Corporation, Kyoto, Japan*
- WP 353 **Validation Studies of a Proteomics Normalization Standard Consisting of 1,000 Stable Isotope Labeled Peptides;** Christopher Colangelo¹; Craig Dufresne²; Alexander R. Ivanov³; Gordana Ivosev⁴; David Hawke⁵; Antonius Koller⁶; Brendan Maclean⁷; Brett Phinney⁸; Kristie Rose⁹; Paul Rudnick¹⁰; Brian Searle¹¹; Scott A. Shaffer¹²; ¹*Primary Ion, Old Lyme, CT*; ²*Thermo Fisher Scientific, West Palm Beach, FL*; ³*Barnett Inst., Northeastern Univ., Boston, MA*; ⁴*Sciex, Concord, Canada*; ⁵*UT- M.D. Anderson Cancer Center, Houston, TX*; ⁶*Columbia Univ., New York, NY*; ⁷*Univ of Washington, Seattle, WA*; ⁸*Univ. of CA, Davis, CA*; ⁹*Vanderbilt University, Nashville, TN*; ¹⁰*Spectragen Informatics, Rockville, MD*; ¹¹*Proteome Software Inc., Portland, OR*; ¹²*Univ. of Massachusetts Medical School, Worcester, MA*
- WP 354 **Characterization of Adiponectin Multimers in Bottlenose Dolphin by Mass Spectrometry.;** Philip Sobolesky¹; John Arthur²; Stephanie Venn-Watson³; Michael Janech¹; ¹*Medical University of South Carolina, Charleston, SC*; ²*Department of Veterans Affairs Medical Center, Charleston, SC*; ³*The National Marine Mammal Foundation, San Diego, CA*
- WP 355 **Development of Multiplex LC-MS/MS Strategies for the Quantitation of Plant-Expressed Proteins;** Trent Oman; Cong Wu; Barry Schafer; *Dow AgroSciences, Indianapolis, IN*
- WP 356 **Precise MRM Quantitation of Candidate Protein Biomarkers in Control and Patient Urine Samples using Internal Standards and Advanced Methodology;** Andrew Percy¹; Juncong Yang¹; Darryl Hardie¹; Andrew Chambers¹; Jessica Tamura-Wells¹; Christoph Borchers^{1,2}; ¹*Univ. of Victoria-Genome BC Proteomics Centre, Victoria, BC, CANADA*; ²*Dept. of Biochem. & Microbiol., Univ. of Victoria, Victoria, BC, Canada*
- WP 357 **Quantitative Characterization of Protein Content from HDL and LDL Size Fractions;** Bryan Parks; Susan Kuklennyik; David M. Schieltz; Michael Gardner; Jon Rees; McWilliams Lisa; Yulanda Williamson; John R. Barr; *Centers for Disease Control and Prevention, Atlanta, GA*
- WP 358 **Multiplexed Mass Spectrometry Analysis of Metabolic Reprogramming in Colorectal Cancer Cells;** Josiah Hutton¹; Lisa Zimmerman^{1,2}; Robert Slebos^{1,2}; Daniel Liebler^{1,2}; ¹*Vanderbilt University Medical Center, Nashville, TN*; ²*Jim Ayers Institute, Nashville, TN*

- WP 359 **Evaluating Challenges Associated with Fast Quantitation of Multiple Proteins using a UHPLC-triple Quadrupole Electrospray Ionization Mass Spectrometer (LC-QQQ ESI-MS);** Rohana Liyanage¹; Jennifer Gidden¹; Jeremy Post²; David Colquhoun²; Ben Figard³; Jackson O. Lay Jr.¹; ¹University of Arkansas, Fayetteville, AR; ²Shimadzu Scientific Instruments, Columbia, MD; ³Shimadzu Scientific, Houston, TX
- WP 360 **A Complete Solution for the Reproducible and Standardized Evaluation of Candidate CVD Protein Biomarkers in Human Plasma;** Andrew Percy¹; Juncong Yang¹; Darryl Hardie¹; Nicole Sessler¹; Yassene Mohammed^{1,2}; Christoph Borchers^{1,3}; ¹University of Victoria-Genome BC Proteomics Centre, Victoria, BC, Canada; ²Center for Proteomics & Metabolom., Leiden UMedCtr, Leiden, The Netherlands; ³Dept. of Biochem. & Microbiol., Univ. of Victoria, Victoria, BC, Canada
- WP 361 **Toward the Development of Scheduled MRM Analysis for Proteome-Wide Profiling of GTP-binding Proteins;** Ming Huang; Yongsheng Xiao; Yinsheng Wang; University of California - Riverside, Riverside, CA
- WP 362 **Affinity Tag- and in vitro Expression-Based Synthesis of Stable Isotope-Labeled Peptides for Quantitative Proteomics;** Feng Xian^{1,2}; Quanhui Wang^{1,2}; Haidan Sun¹; Xiaomin Lou¹; Jin Zi²; Guixue Hou^{1,2}; Lin Wu¹; Siqi Liu^{1,2}; ¹Beijing Institute of Genomics, CAS, Beijing, China; ²BGI-Shenzhen, Shenzhen, China
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- WP 363 **Natural Flanking Sequences for Peptides Included in Quantification Concatamer Internal Standard;** Crystal Cheung¹; Kyle Anderson²; Meiyao Wang¹; Illarion Turko²; ¹IBBR, Rockville, Maryland; ²NIST, Gaithersburg, MD
- WP 364 **Quantification of Histone Post-Translational Modifications by Mass Spectrometry;** Zuo-Fei Yuan¹; Shu Lin¹; Rosalynn C. Molden²; Xing-Jun Cao¹; Natarajan V. Bhanu¹; Xiaoshi Wang¹; Simone Sidoli¹; Shichong Liu¹; Benjamin A. Garcia¹; ¹University of Pennsylvania, Philadelphia, PA; ²Princeton University, Princeton, NJ
- WP 365 **Ultrafast and Robust Optimization of Peptide MRMs Using a Fast-Scanning Triple Quadrupole Mass Spectrometer;** Jeff Dahl; David Colquhoun; Shimadzu Scientific Instruments, Columbia, MD
- WP 366 **Generation of Reproducible Mass Spectra by MALDI and Its Application to Quantification of Peptides and Proteins;** Sung Hee Ahn¹; Jeong Hee Moon²; Seong Hoon Lee¹; Myung Soo Kim¹; ¹Seoul National University, Seoul, Korea; ²Medical Proteomics Research Center, KRIBB, Daejeon, Korea
- WP 367 **Bioanalysis of Therapeutic Peptides by LC/MS/MS: Challenges and Strategies;** Eric Ma; Moucun Yuan; William Mylott; Bruce Hidy; Rand Jenkins; PPD, Richmond, VA
- WP 368 **On-line Preservation for in vivo Microdialysis with MS³ Quantification and Dynamic Monitoring of Endogenous Opioids in the Anterior Cingulate Cortex;** Nicholas Laude¹; Diana Meske¹; Kramer Catherine¹; Eric Lemister¹; Edita Navratilova¹; Frank Porreca^{1,2}; ¹The University of Arizona, Tucson, AZ; ²Mayo Clinic, Phoenix, AZ
- WP 369 **Efficient Micro-Scale Basic Reverse Phase Peptide Fractionation for Global and Targeted Proteomics;** Hyoung Joo Lee; Hye-Jung Kim; Daniel C. Liebler; Department of Biochemistry, Vanderbilt University, Nashville, TN
- WP 370 **Application of a Fluorescent Peptide Assay to the Optimization of Peptide Generation from Patient-derived Breast Cancer Xenografts;** Yiling Mi¹; Petra Erdmann-Gilmore¹; Rose Connors¹; Matthew R. Meyer¹; Shunqiang Li¹; Sherri R. Davies¹; Matthew J. Ellis²; R. Reid Townsend¹; ¹Washington University School of Medicine, St. Louis, MO; ²Baylor College of Medicine, Houston, TX
- WP 371 **Identification and Characterization of Impurities in a VLP-Peptide Conjugate Vaccine by LC-MS;** Melissa Thompson; Barbara Kelly; Kevin Bullock; John Amery; Pfizer Inc., Chesterfield, MO
- WP 372 **Absolute Quantification of Flavin-containing Monooxygenases (FMOs) in Human Liver Microsomes by UPLC-MS/MS-based Targeted Quantitative Proteomic Approach;** Yao Chen; Michael Zhuo Wang; Pharmaceutical Chemistry, University of Kansas, Lawrence, KS
- WP 373 **Higher Isobaric Multiplexing for Discovery Proteomics of Genomically-Characterized Patient-Derived Breast Cancer Xenografts;** Xuya Wang³; Petra Erdmann-Gilmore¹; Alan E. Davis¹; Henry W. Rohrs¹; Shunqiang Li¹; Sherri R. Davies¹; Matthew J. Ellis¹; Ryan Bomgarden⁴; Rosa Viner²; John C. Rogers⁴; David Fenyo³; Jason M. Held¹; R. Reid Townsend¹; ¹Washington University, St. Louis, MO; ²Thermo Fisher Scientific, San Jose, CA; ³New York University, New York, NY; ⁴Thermo Fisher Scientific, Rockford, IL
- WP 374 **Using Mass Spectrometry in Protein Quantification for Influenza Vaccine Quality Control: To Label or Not to Label?** Terry D. Cyr; Daryl G.S. Smith; Lisa Walrond; Marybeth Creskey; Genevieve Gingras; Yves Aubin; Health Canada, Ottawa, Canada
- WP 375 **Fast, Sensitive, Robust SPE-LC-MS/MS Method for Quantitation of Insulin Analogues in Clinical Studies;** Lei Xiong¹; Witold Woroniecki¹; Rahul Baghla²; Suma Ramagiri³; Gary Impey³; Hua-Fen Liu¹; ¹AB SCIEX, Redwood City, California; ²AB SCIEX, Gurgaon, India; ³AB SCIEX, Concord, ON
- WP 376 **LC/MS/MS Analysis of Oxytocin and ARG-Vasopressin in Human Plasma/Serum using Strata™-X-CW Solid Phase Extraction and a Luna PFP(2) HPLC Column;** Xianrong (Jenny) Wei; Sean Orłowicz; Phenomenex, Torrance, CA
- WP 377 **Development of the Ultra-Sensitive Liquid Chromatography-Tandem Mass Spectrometry Method for Insulin Lispro;** Xiaodong Zhu; Thomas Lloyd; Jingguo Hou; Jerry Gardella; Edward Wells; Steve Unger; Worldwide Clinical Trials Drug Development Solution, Austin, TX
- WP 378 **LC-MS/MS Quantification of SOM230 (Pasireotide), a Cyclic Peptide, in Monkey Plasma;** Yunlin Fu; Wenkui Li; Jimmy Flarakos; Francis Tse; Novartis Institutes for Biomedical Research, East Hanover, NJ
- WP 379 **High Throughput Quantitation of 46 Histone PTMs through Unscheduled SRM-based Method Development on a Nano-HPLC Triple Quadrupole Platform;** Jenny Chen¹; Tommy Cheung²; David Arnott²; Yan Chen¹; Keith Waddell¹; Cindy Lai¹; ¹ThermoFisher Scientific Inc., San Jose, CA; ²Genentech, South San Francisco, CA
- WP 380 **MRM Analysis together with ATP Affinity Probes for the Quantitative Discovery of Target Kinases of MM-3-51 in Du-145 Cells;** Weili Miao; Lei Guo; Yinsheng Wang; Riverside, CA
- WP 381 **Impact of Mobile Phase Modifiers and Supercharging Reagents on Charge State Distribution and Sensitivity of Therapeutic Peptides by LC-HRMS;** Jean-Nicholas Mess; Daniel Villeneuve; Fabio Garofolo; Algorithme Pharma Inc., Laval, Canada
- WP 382 **Development of an LC-MS/MS Method for Variagin Quantitation: Application to Pre-Clinical Pharmacokinetic Studies;** Norrapat Shih^{1,2}; R. Manjunatha Kini^{1,2}; ¹Dept. of Biological Sciences, National University of Singapore, Singapore; ²NUS Graduate School for Integrative Sciences, & Engineering, Singapore
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- WP 383 **Outfoxing Phosphohistidine: New Strategies for Global Phosphohistidinomics Reveal Old and New Targets Among Enzymes of Central Metabolism;** Rob Oslund¹;



- Jung-Min Kee¹; Anthony Couvillon²; Vivek Bhatia³; Tom Muir¹; [David H. Perlman](#)¹; ¹Princeton University, Princeton, NJ; ²Cell Signalling Technologies, Danvers, MA; ³Heartflow, Inc, Redwood City, CA
- WP 384 **Concomitant Analysis of Phosphoproteome and N-linked Sialoproteome by Stepwise Metal Oxide Chromatography**; [Miao-Hsia Lin](#); Chia-Feng Tsai; Wei-Ting Lai; Pei-Yi Lin; Yu-Ju Chen; *Academia Sinica, Taipei, Taiwan*
- WP 385 **Determining the Binding Sites of β -Cyclodextrin and Peptides by Electron-Capture Dissociation Tandem Mass Spectrometry**; [Yulin Qi](#); Dietrich Volmer; *Saarland University, Saarbrücken, Germany*
- WP 386 **Development and Application of a Modified Biotin Switch Assay to Quantify Sulfenic Acid Modification of Proteins**; [Ru Li](#); Shujun Lin; Juergen Kast; *The Biomedical Research Centre, UBC, Vancouver, Canada*
- WP 387 **A Chemical Derivatization Strategy for Profiling Protein Methylation**; [Zhibin Ning](#); Alexandra Star; Anna Mierzwa; Sylvain Lanouette; Janice Mayne; Jean-Francois Couture; Daniel Figeys; *Ottawa Institute of Systems Biology, Ottawa, Canada*
- WP 388 **Characterizing Growth Phase-Dependent Changes in the *Bacillus subtilis* Acetylome and Proteome using Label-Free Quantification**; [Todd M. Greco](#)¹; Valerie J. Carabetta²; David Dubnau²; Ileana M. Cristea¹; ¹Princeton University, Princeton, NJ; ²New Jersey Medical School, Rutgers University, Newark, NJ
- WP 389 **Towards Global Sulfation Analysis: Integrating Weak Anion Exchange and Ultraviolet Photodissociation Mass Spectrometry with Strategic Modulation of Peptide Basicity**; [Michelle Robinson](#)¹; Jennifer Brodbelt²; ¹University of Texas at Austin, Austin, TX; ²The University of Texas, Austin, TX
- WP 390 **In-depth Mouse Muscle Ubiquitylome Characterization using diGly Enrichment Followed by MudPIT**; Punitee Garyali; Whitney Smith-Kinnaman; Peter Roach; [Amber Mosley](#); *Indiana University SOM, Department of Biochemistry, Indianapolis, IN*
- WP 391 **Analysis Of Alexa-594 Modified Peptides By Electrospray – Ionization Mass Spectrometry And Electron-Transfer Dissociation**; [Julian Whitelegge](#)¹; Joseph Capri¹; Piotr Ruchala¹; Marcella Gilmore²; Don Laudicina²; ¹University of California LA, Los Angeles, CA; ²Allergan Inc., Irvine, CA
- WP 392 **Single-probe Ionization Device: Application to the Detection of Sulfated Peptides and Sugars**; [Rachel Vowcicefski](#); Ning Pan; Zhibo Yang; *University of Oklahoma, Norman, OK*
- WP 393 **Glycopeptidomics: Characterizing Global Glycoprotein and Site Heterogeneity**; [Robert J. Chalkley](#)¹; Shouling Xu^{1,2}; Peter R. Baker¹; Katalin F. Medzihradzky¹; ¹UCSF, San Francisco, CA; ²Carnegie Institution for Science, Stanford, CA
- WP 394 **Characterization of Glycopeptides by Hot Electron Capture Dissociation**; Kshitij Khatri¹; Yi Pu²; Deborah R. Leon¹; Catherine E. Costello²; Joseph Zaia¹; [Cheng Lin](#)¹; ¹Boston University School of Medicine, Boston, MA; ²Boston University, Boston, MA
- WP 395 **Discovery and Characterization of Post-Translationally Modified Peptides with No Mass Shifts**; [Erik T. Jansson](#); Itamar Livnat; Hua-Chia Tai; Stanislav S. Rubakhin; Jonathan V. Sweedler; *University of Illinois at Urbana-Champaign, Urbana, IL*
- WP 396 **Integrated Proteomic and Glycoproteomic Analyses of Prostate Cancer Cells**; [Punit Shah](#); Xiangchun Wang; Weiming Yang; Shadi Toghi Eshghi; Shisheng Sun; Naser Hoti; Jered Pasay; Abigail Rubin; Hui Zhang; *Johns Hopkins University, Baltimore, MD*
- WP 397 **Multi-acylation of Melittin by lysophosphatidylcholines (lysoPCs) and diacylphosphatidylcholines (diacylPCs) and the Enhanced Reactivity of Melittin Towards lysoPCs**; [Vian S. Ismail](#); John M. Sanderson; Jackie A. Mosely; *Durham University, Durham, UK*
- WP 398 **Identification of S-Glutathionylated Cysteine Residues in Murine Hepatic Proteins by nLC-CID-ETD MS/MS following Immunoaffinity Enrichment**; [Susana Comte-Walters](#); Tiffany Ancrum; Danyelle Townsend; Lauren Ball; *Medical Univ of S Carolina, Charleston, SC*
- WP 399 **Ultra-Low Flow Capillary Electrophoresis - Mass Spectrometry for Proteome Wide PTM Identification and Quantification**; Klaus Faserl; [Herbert H. Lindner](#); *Biocenter, Division of Clinical Biochemistry, Innsbruck, Austria*
- WP 400 **pGlyco: A Novel Pipeline for the Identification of Intact Glycopeptides**; [Wen-Feng Zeng](#)¹; Mingqi Liu²; Yang Zhang²; Jianqiang Wu¹; Pan Fang²; Weiqian Chao²; Chao Liu¹; Hao Chi¹; Ruixiang Sun¹; Si-Min He¹; Pengyuan Yang²; ¹ICT, Chinese Academy of Sciences, Beijing, China; ²Institutes of Biomedical Sciences, Fudan University, Shanghai, China
- WP 401 **PARP9 Inhibits ADP-ribosylation of STAT1 by PARP14**; [Iwao Yamada](#)^{1,2}; Hideo Yoshida^{1,2}; Hiroshi Iwata¹; Masanori Aikawa¹; Sasha A. Singh¹; ¹Brigham and Women's Hospital, Boston, MA; ²Kowa Company, Ltd., Tokyo, Japan
- WP 402 **ETD Fragmentation Improves the Global Analysis of Ubiquitylated Proteins**; [Tanya Porras-Yakushi](#); Michael J Sweredoski; Sonja Hess; *Caltech, Pasadena, CA*
- WP 403 **An Improved Strategy for Characterizing Arginine Methylation using Off-Line High-pH Reversed-Phase Fractionation and Q-Exactive HF Analysis**; [Kathrine B. Sylvestersen](#); Sara C. Larsen; Michael L. Nielsen; *NNF Center for Protein Research, Copenhagen N, Denmark*
- WP 404 **Characterization of Polyubiquitin Chains: Linear and Branched Ubiquitin Trimers**; [Amanda Lee](#); Yeji Kim; Emma K. Dixon; Tanuja R. Kashyap; Yan Wang; David Fushman; Catherine Fenselau; *University of Maryland, College Park, MD*
- WP 405 **Global Analysis of Arginine Methylation and *in vivo* CARM1 Substrates via IAP-MS**; [Evgenia Shishkova](#)¹; Lu Wang²; Alexander H. Hebert¹; Michael S. Westphall³; Wei Xu²; Joshua J. Coon¹; ¹Department of Biomolecular Chemistry, Madison, WI; ²Department of Oncology, Madison, WI; ³Univ of Wisconsin, Madison, WI
- WP 406 **Comparison and Combination of Search Engines to Discover and Characterize PTM Signatures in Biology**; Xiaoyue Jiang¹; [Keith Waddell](#)¹; Michael Blank¹; Kai Fritzscheier²; Bernard Delanghe²; Rosa Viner¹; Andreas FR Huhmer¹; ¹Thermo Fisher Scientific, San Jose, CA; ²Thermo Fisher Scientific, Bremen, Germany
- WP 407 **Data Independent Acquisition Dependent Acquisition**; [Richard S. Johnson](#); Han-Yin Yang; Michael J. Maccoss; *University of Washington, Seattle, WA*
- WP 408 **Improved Strategy for Identification of ATM/ATR Substrates on a Q Exactive HF Platform**; [Sara C. Larsen](#); Kathrine B. Sylvestersen; Dorte B. Bekker-Jensen; Michael L. Nielsen; *NNF Center for Protein Research, Copenhagen, Denmark*
- WP 409 **A D-Amino Acid-Containing Neuropeptide Discovery Funnel**; [Itamar Livnat](#); Hua-Chia Tai; Erik Jansson; Stanislav Rubakhin; Jonathan Sweedler; *University of Illinois at Urbana-Champaign, Urbana, IL*
- WP 410 **Identification of Amadori Products on Proteins from Roasted Peanut Extracts using MS3 Approaches and Novel Computational Methods**; [Katina L. Johnson](#)¹; Geoffrey A. Mueller¹; Soheila J. Maleki²; Anna Pomes³; Jason G. Williams¹; ¹National Institute of Environmental Health Science, Research Triangle Park, NC; ²US Department of Agriculture, New Orleans, LA; ³Indoor Biotechnologies, Charlottesville, VA

- WP 411 **Characterization of Product Related Impurities of an IgG by LC-MS/MS and Middle-Down MS/MS;** Chunyan Gu¹; Deyun Wang²; Huijuan Li¹; Mohammed Shameem¹; Yan-Hui Liu¹; ¹Merck, Kenilworth, NJ; ²Lancaster Labs, Lancaster, PA
- WP 412 **SUMOylation Dynamics in Response to Replication Stress Reveals Novel SUMO Target Proteins and SUMO Sites Relevant for Genomic Stability;** Zhenyu Xiao¹; Jer-gung Chang¹; Ivo Hendriks¹; Jón Sigurðsson²; Jesper Olsen²; Alfred Vertegaal¹; ¹Leiden University Medical Center, Leiden, Netherlands; ²Novo Nordisk Foundation Center for Protein Research, Copenhagen, Denmark
- WP 413 **Determination of the Disulfide Linkages Present in Synthetic Ssm6a, a Novel Na_{1.7} Inhibitory Peptide from Centipede Venom by Partial Reduction;** John Hui; John Robinson; Chris Spahr; Justin Murray; Stone D.-H. Shi; *Therapeutic Discovery, Amgen Inc, Thousand Oaks, CA*
- WP 414 **Deep, Quantitative Coverage of the Lysine Acetylome using Novel Anti-Acetyl-Lysine Antibodies and an Optimized Proteomic Workflow;** Tanya Svinkina¹; Hongbo Gu²; Jeffrey C. Silva²; Philipp Mertins¹; Jana Qiao¹; Shaunt Fereshetian¹; Jacob D. Jaffe¹; Eric Kuhn¹; Namrata D. Udeshi¹; Steven A. Carr¹; ¹Broad Institute of MIT and Harvard, Cambridge, MA; ²Cell Signaling Technology, Inc., Danvers, MA
- WP 415 **Isocyanic acid Neutral Loss Ion Reduce False Positive Identification of Arginine Citrullination in Database Searches of LC-MS/MS Data;** Tatiana N. Boronina¹; Raghothama Chaerkady²; Maximilian Konig¹; Felipe Andrade¹; Robert O'meally¹; Lauren DeVine¹; Robert Cole¹; ¹Johns Hopkins School of Medicine, Baltimore, MD; ²Johns Hopkins University, Baltimore, MD
- WP 416 **CESI-MS Analysis of Asparagine Deamidation and Aspartate Isomerization in Polypeptides;** Bettina Sarg; Klaus Faserl; Herbert H. Lindner; *Div. of Clin. Biochemistry, Biocenter Innsbruck, Innsbruck, Austria*
- WP 417 **Glycopeptides Automatically Assigned Using ESI-MS/MS Exact Mass Data and the MASSPEC Algorithm;** Marshall M. Siegel¹; Gary Walker¹; Kim Alving²; ¹MS Mass Spec Consultants, Fair Lawn, NJ; ²Genzyme, Waltham, MA
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- WP 418 **Correlation of Matrix Excited State Dynamics with Morphology and MALDI Performance;** Kris Kirmess¹; Richard Knochenmuss²; Gary Blanchard³; Gary R. Kinsel¹; ¹Southern Illinois University Carbondale, Carbondale, Illinois; ²Tofwerk, Seftigen, N/A; ³Michigan State University, East Lansing, MI
- WP 419 **Thermally Induced Dissolution of Salts in Matrix-Assisted Laser Desorption/Ionization;** Chuping Lee; I-Chung Lu; Yuan Tseh Lee; Chi-Kung Ni; *Academia Sinica, Taipei, Taiwan*
- WP 420 **The Effect of Ultra-Low Flow on the Ionization of Biotherapeutics;** Andras Guttman; *AB Sciex, San Diego, CA*
- WP 421 **Supermetallization of Peptides and Proteins during Electrospray Ionization;** Maria Indeykina^{1,2}; Yury Kostyukovich^{2,4}; Marina Rodchenkova^{1,2}; Alexey Kononikhin^{1,2}; Igor Popov^{2,3}; Eugene Nikolaev^{2,4}; ¹Institute for Biochemical Physics, Moscow, Russian Federation; ²Institute for Energy Problems of Chemical Physics, Moscow, Russian Federation; ³Moscow Institute of Physics and Technology, Dolgoprudny, Russian Federation; ⁴Skolkovo Institute of Science and Technology, Skolkovo, Russian Federation
- WP 422 **Protonation in Electrospray Ionization Mass Spectrometry;** Yixin Zou¹; Georgia Dolios²; Yukui Zhang³; Rong Wang²; ¹Zhejiang Haochuang Biotech Co., Ltd, Hangzhou, China; ²Mount Sinai School of Med, New York, NY; ³Dalian Institute Chemical Physics, CAS, Dalian, China
- WP 423 **On the Ionization Mechanism in Atmospheric Pressure Negative Ion Mass Spectrometry – The Role of Ozone and CO₂ –;** Valerie Derpmann¹; Florian Stappert²; Hendrik Kersten²; Thorsten Benter²; ¹Carl Zeiss SMT GmbH, Oberkochen, Germany; ²University of Wuppertal, Wuppertal, Germany
- WP 424 **Time of Ionization Spectrometry of Charged Droplets;** Carina Minardi; Arjuna Subramanian; Kaveh Jorabchi; *Georgetown University, Washington, DC*
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- WP 426 **Stereoselectivity of ESI-dependent Electrochemical Reactions;** Ashraf Madian¹; Samantha Kaiser¹; Samantha Leidner¹; Denise Hayward²; Dave Loffredo²; Andrew Thiel²; Daniel Copeland¹; ¹One2One® Pharmaceutical R&D, Hospira Inc., Lake Forest, IL; ²Global Pharmaceutical R&D, Hospira Inc., Lake Forest, IL
- WP 427 **Generation and Evolution of Electronically Excited Species in Spark Discharge Plasmas - A Time and Mass Resolved Study;** Sebastian Klopotoski; Hendrik Kersten; Thorsten Benter; *University of Wuppertal, Wuppertal, Germany*
- WP 428 **Formate Actuated Reduction of Organic Molecules During Electrospray Ionization;** Peifeng Hu; Manorama Tummala; *Baxter Healthcare, Round Lake, IL*
- WP 429 **Influence of Transfer Capillary Temperature on Adduct Formation in AP-MALDI MS;** Anna Schultheis; Bernhard Spengler; *Analytical Chemistry, Giessen, Germany*
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- WP 431 **Metabolic Analysis of Single Human Cells by Capillary Microsampling Electrospray Ionization Mass Spectrometry and Stable Isotope Labeling;** Linwen Zhang¹; Linda L. Allworth²; Akos Vertes¹; ¹the George Washington University, Washington, DC; ²Thomas Jefferson HS for Science and Technology, Alexandria, VA
- WP 432 **Single-Step Elution and Nib-Based Electrospray Ionization from Noviplex Sample Collection Cards;** Steven L. Reeber; Gary L. Glish; *University of North Carolina at Chapel Hill, Chapel Hill, NC*
- WP 433 **Study of Biological Samples with a Home-Built Low-Temperature-Plasma Mass Spectrometry Imaging (LTP-MSI) System;** Abigail Moreno Pedraza; Robert Winkler; *CINVESTAV Unidad Irapuato, Irapuato, Mexico*
- WP 434 **Comparison of Air and Nitrogen Gas Sources for DART Mass Spectrometry;** William A. Harris; Douglas B. Henderson; Johnny K. Ho; Danielle N. Dickinson; *Northrop Grumman, Linthicum Heights, MD*
- WP 435 **Improved Spatial Resolution for Mid-IR Laser Ablation Electrospray Ionization Mass Spectrometry in Transmission Geometry;** Richard Thurston; Rachelle Jacobson; Akos Vertes; *George Washington University, Washington, District of Columbia*
- WP 436 **Direct Tissue Analysis And Characterization Of Unsaturated Lipids Using a Miniature Mass Spectrometer;** Ran Zou; Yuan Su; Xiao Wang; Leelyn Chong; Yu Xia; Zheng Ouyang; *Purdue University, West Lafayette, IN*
- WP 437 **Co-registered Topographical, Band-Excitation Nanomechanical and Mass Spectral Imaging using a Combined Atomic Force Microscopy/Mass Spectrometry Platform;** Olga Ovchinnikova; Tamin Tai; Vera Bocharova; Mahmut Baris Okatan; Alex Belianinov;



- Vilmos Kertesz; Stephen Jesse; Gary J. Van Berkel; Oak Ridge National Laboratory, Oak Ridge, TN
- WP 438 **Gas Assisted AC Pipette Tip Electrospray Source;** Yunqing Huang; Gong-Yu Jiang; Chao Gao; Qiao Jin; Wenjian Sun; Shimadzu Research Laboratory(Shanghai) Co.,Ltd., Shanghai, China
- WP 439 **Cross-platform Applicability of DESI-MSI – Effect of Ion Source Setups and MS Analysers on Performance and Information Recovery;** Jocelyn Tillner¹; Emrys Jones¹; Steve Pringle²; Tamas Karancsi³; James L Walsh⁴; Ian Gilmore⁵; Josephine Bunch⁶; Zoltan Takats¹; ¹Imperial College London, London, UK; ²Waters Corporation, Wilmslow, UK; ³Waters Research Centre, Budapest, Hungary; ⁴University of Liverpool, Liverpool, UK; ⁵National Physical Laboratory, Teddington, UK
- WP 440 **On-line Planar Chromatography/Mass Spectrometry using Spray Ionization;** Michael Wei; Elizabeth Dhummakupt; Richard A. Yost; University of Florida, Gainesville, FL
- WP 441 **Mass Spectrometry on the Go;** Christopher Pulliam¹; Ryan Bain¹; Joshua Wiley²; R. Graham Cooks¹; ¹Purdue University, West Lafayette, IN; ²California Institute of Technology, Pasadena, CA
- WP 442 **Comparative Study of LC-MS Analysis of Peptide Mixtures by Thermal Ionization under Ambient Conditions and ESI;** Evgeny Kukaev^{1,2}; Alexey Kononikhin^{1,3}; Igor Popov^{1,2}; Eugene Nikolaev^{1,3}; ¹Moscow Institute of Physics and Technology, Moscow, Russia; ²Emanuel Institute of Biochemical Physics, Moscow, Russia; ³Institute for Energy Problems of Chemical Physics, Moscow, Russia
- WP 443 **Study of Spray Ionization and Ion Transfer for Miniature Mass Spectrometers;** Xiao Wang; Yue Ren; Xiaoyu Zhou; Zheng Ouyang; Purdue University, West Lafayette, IN
- WP 444 **The Microwave Plasma Torch as a Combined Molecular and Atomic Ambient Ionization Source;** Kenyon Evans-Nguyen¹; Ashley Windom¹; Colleen Quinn¹; Hilary Brown²; Spiros Manolakos³; Theresa Evans-Nguyen³; ¹University of Tampa, Tampa, FL; ²Purdue University, West Lafayette, IN; ³The Charles Stark Draper Laboratory, Inc., Tampa, FL
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- WP 446 **Direct Coupling of Solid Phase Microextraction (SPME) to Mass Spectrometry: Applications in the Clinical Lab;** German Augusto Gomez-Rios; Barbara Bojko; Janusz Pawliszyn; University of Waterloo, Waterloo, Canada
- WP 447 **Multimodal Vacuum-assisted Laser Ablation/ Transmission Plasma Ion Source for Real-time Reaction Monitoring;** Joel Keelor¹; Chris Butch¹; Charles Liotta¹; Paul Farnsworth²; Facundo Fernandez¹; ¹Georgia Institute of Technology, Atlanta, GA; ²Brigham Young University, Provo, UT
- WP 448 **Desorption Capillary Photoionization;** Markus Haapala; Jaakko Teppo; Elisa Ollikainen; Iiro Kiiski; Anu Vaikkinen; Tiina J Kauppila; Risto Kostianen; University of Helsinki, Helsinki, Finland
- WP 449 **Development and Application of Hot-Gas-Assisted Desorption Atmospheric Pressure Chemical Ionization for Fast, Ambient Analysis of Milk;** ZhiHao Wang¹; Jiang Wang¹; Kun Liu¹; Eric Handberg¹; ShuiPing Yang²; Huanwen Chen¹; ¹East China Institute of Tech., Nanchang, China; ²East China Institute of Tech., Fuzhou, China
- WP 450 **Ultrasonic Acoustic Wave Nebulization-Mass Spectrometry (UltraAWN-MS) for Unconventional Explosives Characterization;** Benjamin Oyler¹; Alexander MacKerell¹; Kellie Hom¹; Joseph Chipuk²; Richard Lareau³; Shivangi Awasthi¹; Sung Hwan Yoon¹; David Goodlett¹; David Kilgour¹; ¹University of Maryland, Baltimore, Baltimore, MD; ²Signature Science, Alexandria, VA; ³Dept. of Homeland Security, S&T Directorate, Atlantic City, NJ
- WP 451 **Membrane Electrospray Ionization for Direct Ultrasensitive Biomarker Quantitation in Biofluids Using Mass Spectrometry;** Mei Zhang^{1,2}; Fankai Lin¹; Jianguo Xu²; Wei Xu¹; ¹Beijing Institute of Technology, Beijing, China; ²Chinese Center for Disease Control and Prevention, Beijing, China
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- WP 459 **Microfluidic Isoelectric Focusing Combined with MALDI- and nano-ESI-MS;** Saara Mikkonen¹; Wolfgang Thormann²; Åsa Emmer¹; ¹KTH Royal Institute of Technology, Stockholm, Sweden; ²University of Bern, Bern, Switzerland
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- WP 469 **A Novel Quadrupole Mass Spectrometer Detection System;** Raman Mathur; Michael G. Konicek; Rexford T. Heller; John Smith; Alan Schoen; *Thermo Fisher Scientific, San Jose, CA*
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- WP 542 **An Integrated and High Throughput Approach for *in situ* Protein Digestion, Peptide Imaging and Sequence Verification;** Fengfei Ma; Jingxin Wang; Lingjun Li; *Univ of Wisconsin-Madison, Madison, WI*

- WP 543 **De novo Discovery of Tumor Clones Linked to Metastasis and Poor Prognosis Using MALDI Imaging Mass Spectrometry**; Benjamin Balluff¹; Walid Abdelmoula¹; Jouke Dijkstra¹; Axel Walch²; Liam McDonnell³; ¹LUMC, Leiden, NL; ²Helmholtz Zentrum München, Munich, DE; ³LUMC & PSF, Pisa, Italy
- WP 544 **Contrast-Enhanced Mass Spectrometry Imaging Reveals Tumour Heterogeneity and Boundaries**; Alessandra Tata^{1,2}; Jinzi Zheng²; Howard Ginsberg³; David Jaffray^{2,4}; Demian Ifa¹; Arash Zarrine Afsar^{2,3}; ¹Department of Chemistry, CRMS, York University, Toronto, Canada; ²Techna, University Health Network, Toronto, Canada; ³Dept. of Surgery, University of Toronto, Toronto, Canada; ⁴Dept. Medical Biophysics, University of Toronto, Toronto, Canada
- WP 545 **New Biomarkers Discovery Approach based on Morphological Evaluation of Mass Spectrometry Imaging (MSI) Dataset: A Case Study**; Gael Picard de Muller; Gregory Hamm; Fabien Pamelard; David Bonnel; Kevin Lorgouilloux; Jonathan Stauber; *ImaBiotech, MS Imaging Dept., Loos, France*
- WP 546 **Mass Spectrometry Imaging of Proteins after On-Tissue Digestion: Approaching Cellular Resolution in Fresh-Frozen and FFPE Tissue**; Andreas Roempp; Katharina Huber; Pegah Khamehghir-Silz; Bernhard Spengler; *Justus Liebig University, Giessen, Germany*
- WP 547 **In situ Assaying the Activity of Ammonia Lyase Mutants Demonstrated by a Bi-Substrate Model Reaction with DESI IM MS Imaging**; Cunyu Yan¹; Fabio Parmeggiani¹; Jason Schmidberger¹; Emrys Jones²; Emmanuelle Claude²; Nicholas J. Turner¹; Sabine L. Flitsch¹; Perdita Barran¹; ¹University of Manchester, Manchester, UK; ²Waters MS Technologies Centre, Wilmslow, UK
- WP 548 **Examination of Plasmodium berghei Oocysts in the Mosquito using MALDI Fourier Transform Imaging Mass Spectrometry**; Berin Boughton¹; Daniel Sarabia²; Dean Goodman²; Mark Condina³; Geoff McFadden²; Ute Roessner²; ¹Metabolomics Australia, University of Melbourne, Parkville, Australia; ²School of Biosciences, The University of Melbourne, Parkville, VIC, Australia; ³Bruker Pty Ltd, Melbourne, VIC, Australia
- WP 549 **An Investigation into Multi-Model Tissue Imaging on a Single Section by DESI and MALDI TOF Mass Spectrometry**; Mark Towers¹; Emrys Jones¹; Anna Mroz²; Zoltan Takats²; Emmanuelle Claude¹; Jim Langridge¹; ¹Waters Corporation, Wilmslow, UK; ²Imperial College London, London, UK
- WP 550 **Visualization of Lipids Involved in the Growth of Pseudomonas putida Biofilm using Matrix-Assisted Laser Desorption Ionization Mass Spectrometry Imaging**; Bin Li¹; Sage Dunham¹; Travis King²; Kensey R. Amaya²; Jonathan Sweedler¹; ¹University of Illinois at Urbana-Champaign, Urbana, IL; ²ERDC-CERL, Environmental Chemistry Laboratory, Champaign, IL
- WP 551 **A Comprehensive Study of the Brain Lipidome Using Silver Nanoparticles (Colloidal and Implanted)**; Ludovic Muller¹; Aurelie Roux¹; Shelley N Jackson¹; J. Albert Schultz²; Amina S. Woods¹; ¹NIH/NIDA-IRP, Baltimore, MD; ²Ionwerks, Houston, TX
- WP 552 **Enhancing in situ Biomolecule Identification by Novel Combination of Multiplexed Mass Spectrometric Imaging with DDA on a MALDI Orbitrap Platform**; Chuanzi OuYang¹; Bingming Chen²; Lingjun Li^{1,2}; ¹Department of Chemistry, UW-Madison, Madison, WI; ²School of Pharmacy, UW-Madison, Madison, WI
- WP 553 **Advanced Multi-modal Mass Spectrometry Applied to the Complexity of Lipid Imaging Analysis**; Katherine Kellersberger; Shannon Cornett; Michael Easterling; *Bruker Daltonics, Billerica, MA*
- WP 554 **Molecular Mapping of Alzheimer's Disease – Imaging Mass Spectrometry**; Andrea Kelley¹; George Perry¹; Rudolph J. Castellani²; Stephan Bach¹; ¹University of Texas at San Antonio, San Antonio, Tx; ²University of Maryland School of Medicine, Baltimore, MD
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- WP 555 **Understanding the Roles of Electronic and Steric Effects in Separating Isomers using Differential Mobility Spectrometry**; Chris J. Lock¹; J. Larry Campbell¹; Chang Liu¹; J.C. Yves Leblanc¹; Jefry Shields²; John Janiszewski²; Christian Ieritano³; Gene Ye³; Gillian Hawes³; Moaraj Hasan³; W. Scott Hopkins³; ¹SCIEX, Concord, ON, Canada; ²Pfizer, Groton, CT; ³University of Waterloo, Waterloo, ON, Canada
- WP 556 **Characterizing Biomolecular Ion Structure using Ion Mobility Spectrometry Coupled with Gas-Phase Hydrogen Deuterium Exchange And Tandem Mass Spectrometry**; Stephen Valentine; Mahdiar Khakinejad; Samaneh Ghassabi-Kondalaji; Gregory Donohoe; Jim Arndt; *West Virginia University, Morgantown, WV*
- WP 557 **Ion Mobility Spectrometry of Foldamers: Characterization of the Folding State**; Frederic Rosu^{1,2}; Xuesong Li^{1,3}; Victor Maurizot^{1,3}; Ivan Huc^{1,3}; Valerie Gabelica^{1,4}; ¹Univ. Bordeaux, IECB, Bordeaux, France; ²CNRS UMS 3033, IECB, Pessac, France; ³CNRS UMR 5284, CBMN, Pessac, France; ⁴INSERM, U869, ARNA Laboratory, Bordeaux, France
- WP 558 **Effect of Temperature, Charge, and Time on the Electrical Mobility of Minimally Perturbed Electrospayed Protein Ions in the Gas Phase**; Michel Attoui¹; Juan Fernandez de la Mora²; ¹Physics Department, University of Paris 12, Paris, France; ²Yale University - Mechanical Engineering Department, New Haven, CT
- WP 559 **What Happens to DNA Duplexes in the Gas Phase? Massimiliano Porrini**^{1,2}; Frederic Rosu³; Valerie Gabelica^{1,2}; ¹University of Bordeaux, IECB, Pessac, France; ²INSERM, U869, ARNA laboratory, Bordeaux, France; ³CNRS, UMS 3033, IECB, University of Bordeaux, Pessac, France
- WP 560 **Ion Mobility Quadrupole Time-of-Flight (IM Q-TOF) Mass Spectrometric Applications of Monoclonal Antibody and its Derivatives**; David Wong; *Agilent Technologies, Inc., Santa Clara, CA*
- WP 561 **The Influence of Lipid Bilayer Physicochemical Properties on the Conformer Preferences of the Model Ion Channel Gramicidin A**; John Patrick^{1,2}; David H. Russell^{1,2}; ¹Texas A&M University, College Station, TX; ²Texas A&M University, College Station, TX
- WP 562 **Conformational Landscapes of Model Proteins Measured on a Commercial Drift Tube Ion Mobility-Mass Spectrometer**; Ewa Jurmeczeko¹; Jody C. May¹; George C. Stafford²; John C. Fjeldsted²; John A. McLean¹; ¹Vanderbilt University, Nashville, Tennessee; ²Agilent Technologies, Santa Clara, CA
- WP 563 **On the Role of Penultimate Proline Isomerizations in Neuropeptide Conformations**; Matthew Glover; David Clemmer; *Indiana University, Bloomington, IN*
- WP 564 **Ion Mobility Mass Spectrometry as a Tool to Perform Structural Characterization of Peptides Bearing Disulfide Bond(s)**; Philippe Massonnet¹; Gregory Uper²; Michel Degueldre¹; Denis Morsa¹; Nicolas Smargiasso¹; Nicolas Gilles²; Loic Quinton¹; Edwin De Pauw¹; ¹Laboratory of Mass Spectrometry - Ulg, Liège, Belgium; ²CEA/DSV/iBiTec-S/SIMOPRO, Gif sur Yvette, France
- WP 565 **Extracting Collision Cross-sections of Ion Mobility Unresolved Isomers Using Tandem Mass Spectrometry and Chemometric Deconvolution**; Brett Harper; Elizabeth Neumann; Touradj Solouki; *Baylor University, Waco, TX*
- WP 566 **The Role of Inter- and Intramolecular Interactions on the Conformer Preferences of Biomolecules during Electrospray Ionization**; Kelly Servage¹; Joshua Silveira²; Kyle Fort³; David H. Russell¹; ¹Texas A&M University,

- College Station, TX; ²Bruker Daltonics, Billerica, MA; ³Utrecht University, CH Utrecht, The Netherlands
- WP 567 **Correlating Ion-Neutral Collision Cross Sections to Protein Native Conformation and Energy Folding Landscape**; Shu-Hua Chen; David H. Russell; Texas A&M University, College Station, TX
- WP 568 **Investigation of Ion Mobility Mass Spectrometry Analysis of Electrochemically Generated Oxidation Products of Opiates and Comparison with Theoretical CCS Values**; Cris Laphorn¹; Frank Pullen¹; Susana da Silva Torres²; Mark R. Taylor²; Russell Mortishire-Smith³; Jayne Kirk³; Andrew Baker⁴; ¹University of Greenwich, Chatham Maritime, UK; ²Pfizer, Sandwich, UK; ³Waters Corp, Manchester, UK; ⁴Waters, Inc., Pleasanton, CA
- WP 569 **Ion Mobility - Mass Spectrometry for Structural Analysis of Protein Therapeutics**; Carly Ferguson; Michael Boyne; Ashley Gucinski; Food and Drug Administration, St. Louis, MO
- WP 570 **Changes in Drift Spectra Intensity Distribution of Cyclodextrin Negative Ions with Solution pH**; Paul S. Blank¹; Christian Klein²; Julie Wight³; Ruwan Kurulugama²; Stephanie Cologna¹; Peter S. Backlund¹; Alfred L. Yergey¹; ¹NICHD, NIH, Bethesda, MD; ²Agilent Technologies, Santa Clara, CA; ³Agilent Technologies, Poolesville, MD
- WP 571 **Protein Structure Collapse in the Gas-phase Revealed by Ion Mobility and Molecular Dynamics**; Iain D G Campuzano¹; Morgan Lawrenz¹; Carlos Larriba Andaluz²; ¹Amgen Inc., Thousand Oaks, CA; ²University of Minnesota, Bloomington, IN
- WP 572 **Probing Solution-Related Structures of Disordered Peptide Indolicidin with IMS-MS and IMS-IMS-MS Techniques**; Neelam Khanal; Maissa M. Gaye; David E. Clemmer; Department of Chemistry, Indiana University, Bloomington, IN
- WP 573 **Electrospray Ionization of Proteins: Conformations Versus Aggregates Probed by Ion Mobility/Mass Spectrometry**; Kent Gillig; Chung-Hsuan Chen; Academia Sinica, Taipei, Taiwan
- WP 574 **Effect of beta-Cyclodextrin on Protein Structure Investigated by Ion Mobility-Mass Spectrometry**; Yinjuan Chen¹; Xinhua Dai²; Peng Xiao²; Xiang Fang²; Chuan-Fan Ding¹; ¹Fudan University, Shanghai, China; ²National Institute of Metrology, Beijing, China
- WP 575 **Evidence for Differential Structural Preferences of the Leu7Pro Mutant Neuropeptide Y Signal Peptide Probed by Ion Mobility-Mass Spectrometry**; Zhengwei Chen; Christopher Lietz; Lingjun Li; University of Wisconsin-Madison, Madison, WI
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- WP 576 **Investigating Changes in the Gas-Phase Conformation of Heparin/HS binding Proteins Using Traveling Wave Ion Mobility Spectrometry (TWIMS)**; Yuejie Zhao¹; Lingyun Li²; Robert Linhardt²; Yongmei Xu³; Jian Liu³; Arunima Singh¹; Robert Woods¹; Jon Amster¹; ¹University of Georgia, Athens, GA; ²Rensselaer Polytechnic University, Troy, NY; ³University of North Carolina, Chapel Hill, NC
- WP 577 **Utilizing High Throughput IMS-MS Measurements to Study Noncovalent Protein/Ligand Interactions Kinetics**; Daniel J. Orton¹; Ryan T. Kelly²; Yehia M. Ibrahim¹; Xing Zhang¹; Tridib Ghosh²; John R. Cort¹; Richard D. Smith¹; Erin S. Baker¹; ¹Pacific Northwest National Laboratory, Richland, WA; ²Environmental Molecular Sciences Laboratory PNNL, Richland, WA
- WP 578 **Application of Ion Mobility Mass Spectrometry for the Analysis of Ruthenium-Arene Complexes**; Izabella Czerwinska; Johann Far; Christopher Kune; Nicolas Smargiasso; Denis Morsa; Edwin De Pauw; Mass Spectrometry Laboratory, GIGA-R, University of Liege, Belgium
- WP 579 **Evaluating Ion Mobility-Mass Spectrometry as a Tool for Discovering Conformationally-Selective Src Kinase Inhibitors**; Jessica Rabuck-Gibbons; Matthew Soellner; Brandon Ruotolo; University of Michigan, Ann Arbor, MI
- WP 580 **Mass and Mobility Distributions of Labile Metal Complexes of Uranium, Barium, Cesium and Lanthanum**; Austen Davis; Brian H. Clowers; Washington State University, Pullman, WA
- WP 581 **Ion Mobility-Mass Spectrometry for Screening Libraries of Rationally-designed Bifunctional Small Molecule Libraries Capable of Chemical and Structural Amyloid Modulation**; Richard A. Kerr¹; Younwoo Nam²; Michael Beck¹; Mi Hee Lim²; Brandon T. Ruotolo¹; ¹University of Michigan, Ann Arbor, MI; ²Ulsan National Institute of Science and Technology, Ulsan, South Korea
- WP 582 **Ion Mobility Mass Spectrometry: A New Approach for Polymer Drug Carrier and Delivery Characterization**; Jean R. N. Haler^{1,2}; Denis Morsa¹; Johann Far¹; Philippe Lecomte²; Christine Jérôme²; Edwin De Pauw¹; ¹Mass Spectrometry Laboratory, University of Liège, Liège, Belgium; ²CERM, University of Liège, Liège, Belgium
- WP 583 **Neuropeptide Inspired Alzheimer's Disease Therapeutic Discovery Utilizing Ion Mobility - Mass Spectrometry**; Molly Soper; Brandon Ruotolo; University Of Michigan, Ann Arbor, MI
- WP 584 **A Collision Induced Unfolding Assay for differentiating ATP-competitive and Allosteric Protein Tyrosine Kinase Inhibitors**; James Keating; Jessica Rabuck-Gibbons; Brandon Ruotolo; University of Michigan, Department of Chemistry, Ann Arbor, MI
- WP 585 **Ion Mobility-Mass Spectrometry Reveals the Early Assembly of Amyloid β -protein: The effects of Familial Mutations A2T and A2V**; Xueyun Zheng¹; Robin Roychaudhuri²; David Teplow²; Michael T. Bowers¹; ¹University of California, Santa Barbara, CA; ²University of California, Los Angeles, CA
- WP 586 **Effect of Glycosaminoglycan Disaccharide Binding on the Structural Heterogeneity and Dynamics of the Chemokine CCL5**; Hiroki Sakai; Christian Bleiholder; Florida State University, Tallahassee, FL
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- WP 587 **Monitoring Protein Stabilization by Multiple Analytical Techniques**; Krishnamoorthy Kuppannan¹; Margaret Covington¹; Florin Dan¹; Yujing Tan¹; Yongfu Li¹; David Meunier¹; Danielle Dodge¹; Joshua Katz²; ¹The Dow Chemical Company, Midland, MI; ²The Dow Chemical Company, Collegeville, PA
- WP 588 **Multisubunit Protein Interactions and Protein-Ligand Binding Sites Revealed By Surface Induced Dissociation Ion Mobility-Mass Spectrometry**; Yue Ju; Royston Quintyn; Vicki Wysocki; The Ohio State University, Columbus, Ohio
- WP 589 **Screening Glycolipids Against Proteins using Electrospray Ionization Mass Spectrometry and Picodiscs**; Jun Li; Elena Kitova; John Klassen; University of Alberta, Edmonton, Canada
- WP 590 **The GFP Interactome: Implications for Assessing GFP-tagged Protein Interactions using Immunoaffinity Purification-Mass Spectrometry Analysis**; Tara Nash; Kevin Blackburn; Steven Clouse; Michael Goshe; North Carolina State University, Raleigh, NC
- WP 591 **Native nano-ESI-MS Application in Fragment Based Drug Discovery: Investigating Antagonism of Protein-Protein Interactions**; Agni Faviola Mika Gavriilidou¹; Finn Holding²; Renato Zenobi¹; ¹ETH, Department of Chemistry & Applied Biosciences, Zurich, Switzerland; ²Astex Pharmaceuticals, Cambridge, UK


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- WP 592 **Enhanced I-DIRT (eI-DIRT): Improved Identification of Specific Protein-Protein Interactions in Cellular Milieux by Glutaraldehyde Stabilization and Stable Isotope Labeling MS;** Roman Subbotin; Julio Padovan; Brian Chait; *The Rockefeller University, New York, NY*
- WP 593 **Quantifying Protein-Glycolipid Interactions in Different Lipid Environments using Electrospray Ionization Mass Spectrometry;** Ling Han; Elena Kitova; John Klassen; *University of Alberta, Edmonton, Canada*
- WP 594 **Protein-Protein Interaction (PPI) In Lectin Affinity Chromatography;** Jihoon Shin¹; Youngwon Jung²; Wonryeon Cho¹; ¹Wonkwang University, Iksan, Republic of Korea; ²Yonsei University, Seoul, Republic of Korea
- WP 595 **Use of Native Mass Spectrometry for Quantification of Protein Complex;** Wenjing Li; Bao Tran; Sung Hwan Yoon; Keely Pierzchalski; Jianshi Yu; David R Goodlett; Maureen A Kane; *University of Maryland, Baltimore, MD*
- WP 596 **Mutual Stabilization of Helix Structures in the Three-Helix Bundle Protein KIX Studied by Electron Capture Dissociation;** Eva-Maria Schneeberger; Moritz Schennach; Kathrin Breuker; *University of Innsbruck, Innsbruck, Austria*
- WP 597 **Epitope Mapping of West Nile Virus Envelope Protein Bound to a Therapeutic Antibody by FPOP and HDX: Method Development;** Yining Huang¹; Manolo Plasencia¹; Melissa A. Edeling²; Christopher A. Nelson²; Don L. Rempel¹; Henry W. Rohrs¹; Daved H. Fremont²; Michael L. Gross¹; ¹Washington University in St. Louis, St. Louis, MO; ²Washington University School of Medicine, St. Louis, MO
- WP 598 **193nm UVPD of Natively Ionized DHFR for Elucidation of Protein-Ligand Interactions and Conformational Movements upon Inhibition by Methotrexate;** Michael Cammarata; Ross Thyer; Jennifer Brodbelt; *The University of Texas, Austin, TX*
- WP 599 **Epitope Mapping of WNV Envelope Protein Bound to a Therapeutic Antibody by FPOP: Correlation of Interface Dynamics and Oxidative Labeling;** Manolo Plasencia¹; Yining Huang¹; Melissa A. Edeling²; Christopher A. Nelson²; Don L. Rempel¹; Henry W. Rohrs¹; Daved H. Fremont²; Michael L. Gross¹; ¹Washington University in St. Louis, St. Louis, MO; ²Washington University School of Medicine, St. Louis, MO
- WP 600 **Tannins (Procyanidins) Binding to a Salivary Peptide (Histatin 5) Studied using Electrospray Ionization Tandem Mass Spectrometry (ESI-MS/MS) and Molecular Simulations;** Joshua M. Shraberg¹; Steven W. Rick¹; Nalaka Rannulu¹; Richard B. Cole^{1,2}; ¹Dept. Of Chemistry, U. Of New Orleans, New Orleans, LA; ²Univ. P. et M. Curie (Paris 6), Paris Cedex 05, France
- WP 601 **Determining the Cooperativity and Structural Effects of Copper Binding to the Homotetramer CsoR;** Alexander D. Jacobs¹; Feng-Ming Chang¹; Lindsay J. Morrison²; Jonathan M. Dilger¹; Vicki H. Wysocki²; David P. Giedroc¹; David E. Clemmer¹; ¹Indiana University, Bloomington, IN; ²Ohio State University, Columbus, OH
- WP 602 **Drugging the Undruggable: IM-MS Functional Binding Assay for Small Molecule Inhibitors of Conformationally Dynamic Proteins;** Chris Nortcliffe¹; Giovanna Zinzalla²; Perdita Barran¹; ¹University of Manchester, Manchester, UK; ²Karolinska Institutet, Stockholm, Sweden
- WP 603 **Protein Interaction Partners of Protein Phosphatase 2A Catalytic Subunit in Rat β -Islet cells Using Quantitative Mass Spectrometry;** Divyasri Damacharla; xiangmin Zhang; Danjun Ma; Yue Qi; Anjaneyulu Kowluru; Zhengping Yi; *Wayne State University, Detroit, MI*
- WP 604 **Combining Native MS and IM-MS for Structural Elucidation of the yeast mRNA 3'-end Maturation Complex CFIA;** Johann Stojko¹; Adrien Dupin²; Sébastien Fribourg²; Alain Van Dorsselaer¹; Sarah Cianférani¹; ¹LSMBO, DSA, IPHC, Strasbourg, France; ²INSERM, U869, IECB, Bordeaux, France
- WP 605 **Allosteric Activation of Tumor Suppressor PP2A by a Small Molecule Activator Series Revealed using Hydroxyl Radical Footprinting;** Janna Kiselar¹; Giri Gokulrangan²; David Kastrinsky³; Nilesh Zaware³; Michael Ohlmeyer³; Mark R Chance¹; Goutham Narla¹; ¹Case Western Reserve Univ, Cleveland, OH; ²Pfizer Biotherapeutics WRD, Andover, MA; ³Mount Sinai Hospital, NY, NY
- WP 606 **Structural and Biochemical Characterisation of Oligomeric Alpha-Synuclein by Ion Mobility Spectrometry - Mass Spectrometry;** Eva Illes-Toth²; Mafalda Ramos²; Roberto Cappai¹; Caroline Dalton²; David Smith²; ¹University of Melbourne, Melbourne, VIC; ²Sheffield Hallam University, Sheffield, UK
- WP 607 **Probing Ligand Interactions of the Chemokine Receptor CXCR7 by Mass Spectrometry;** Liwen Wang¹; Martin Gustavsson²; Tracy Handel²; Mark R. Chance¹; ¹Case Western Reserve Univ, Cleveland, OH; ²University of California, San Diego, San Diego, CA
- WP 608 **Charge Detection Mass Spectrometry Measures DNA Packaging in Bacteriophage P22 above 50 MDa and Resolves Four Morphologies in Mutant P22;** David Keifer; Kevin Bond; Martin Jarrold; *Indiana University, Bloomington, IN*
- WP 609 **A Hybrid MS-based Strategy Provides Structural Insights into Transient Protein Assemblies;** Argyris Politis; *King's College London, London, UK*
- WP 610 **Exploring the Protein-Protein Chemical Crosslinking of a Highly Non-Iso-Stoichiometric Protein Complex;** Yeva Mirzakhanyan; Tuan ngo; Paul Gershon; *UC-Irvine, Irvine, CA*
- WP 611 **Molecular Architecture of the Yeast Mediator Complex;** Michael Trnka¹; Philip Robinson²; Riccardo Pellarin¹; Sali Andrej¹; Roger Kornberg²; AL Burlingame¹; ¹University of California, San Francisco, San Francisco, CA; ²Stanford University, Stanford, CA
- WP 612 **A Structural Proteomics Study of High-Density Lipoprotein (HDL);** Jason Serpa¹; Teddy Chan²; Gordon Francis²; Evgeniy Petrotchenko¹; Christoph Borchers^{1,3}; ¹University of Victoria-Genome BC Proteomics Centre, Victoria, BC, Canada; ²Ctr. for Heart Lung Innov., UBC & St. Paul's Hosp., Vancouver, BC, Canada; ³Dept. of Biochem. & Microbiol., Univ. of Victoria, Victoria, BC, Canada
- WP 613 **Probing Intact Red Cell Membranes using Zero-length Chemical Cross-linking and Mass Spectrometry (CX-MS);** Roland Rivera-Santiago^{1,2}; Sandra Harper²; Sira Sriswasdi³; David Speicher²; ¹University of Pennsylvania, Philadelphia, PA; ²The Wistar Institute, Philadelphia, PA; ³University of Tokyo, Tokyo, Japan
- WP 614 **Structural Proteomics Study of Native α -synuclein in Solution;** Nicholas Brodie¹; Evgeniy Petrotchenko¹; Christoph Borchers^{1,2}; ¹University of Victoria-Genome BC Proteomics Centre, Victoria, BC, Canada; ²Dept. of Biochem. & Microbiol., Univ. of Victoria, Victoria, BC, Canada
- WP 615 **Use of Ion Mobility and Cross Linking Mass Spectrometry with Hybrid Modelling to Delineate the Structure of CbpA;** Konstantinos Thalassinou; Harpal Sahota; Adam Cryar; Maya Topf; *Institute of Structural and Molecular Biology, London, UK*
- WP 616 **Fragmentation and Aggregation of Physiological and Parkinson- Synucleins Revealed by Ion Mobility- MS and HDX- MS;** Michael Przybylski¹; Kathrin Lindner¹; Nicolas Pierson²; Ying Zhang³; Brindusa-Alina Petre¹; Stefan Schildknecht¹; Michael Gross³; David Clemmer²; ¹Steinbeis Centre Biopolymer Analysis, Konstanz, Germany; ²Indiana University Dept. Chemistry, Bloomington, IN; ³Washington University St.Louis, St. Louis, MO

- WP 617 **HDL Particle Size Versus the HDL Proteome**; David Schieltz; Jon Rees; Zsuzsanna Kuklennyik; Bryan Parks; Michael Gardner; Lisa McWilliams; Yulanda Williamson; John R Barr; *Centers For Disease Control and Prevention, Atlanta, GA*
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- WP 618 **Discovering a Connection between Structural Sensitivity to pH & Interaction with FcRn in IgG1 Molecules**; Benjamin Walters¹; Pernille F. Jensen³; Vincent Larraillet⁴; Tom Patapoff²; Kasper Rand³; Jennifer Zhang¹; ¹*Protein Analytical Chemistry, Genentech, South San Francisco, California*; ²*Early Stage Pharmaceutical Development, Genentech, South San Francisco, California*; ³*Dept. of Pharmacy, U. of Copenhagen, Copenhagen, Denmark*; ⁴*pRed, Roche Innovation Center, Penzberg, Germany*
- WP 619 **New Model for Prediction and Comparison of Per-residue Deuterium Uptake Level and Structure of Peptides Ion on the Gas Phase**; Samaneh Ghassabi Kondalaji¹; Mahdiar Khakinejad¹; Stephen Valentine²; ¹*Morgantown, WV*; ²*West Virginia University, Morgantown, WV*
- WP 620 **HDX-MS Characterization of New Class of Multimerization Selective Inhibitors of HIV-1 Integrase**; Venkatasubramanian Dharmarajan¹; Matthew Plumb²; Matthew Gibson²; Mamuka Kvaratskhelia²; Patrick R. Griffin¹; ¹*The Scripps Research Institute, Jupiter, FL*; ²*The Ohio State University, Columbus, OH*
- WP 621 **Effects of Class II and III UAB Reginoids on the Dynamics of Nuclear Receptors by Hydrogen Deuterium Exchange Mass Spectrometry**; Amanda Proper; Emily Cowart; Donald Muccio; Matthew Renfrow; *University of Alabama at Birmingham, Birmingham, AL*
- WP 622 **Examining Liposome Association and Small Molecule Inhibition of Fatty Acid Amide Hydrolase (FAAH) by Hydrogen/Deuterium Exchange Mass Spectrometry**; Brent Kochert; Alexandros Makriyannis; John Engen; *Northeastern University, Boston, MA*
- WP 623 **Characterization of the Conformation of Therapeutic Antibody Oxidation Variants with Optimized Hydrogen/Deuterium Exchange Mass Spectrometry**; Terry Zhang¹; David Horn¹; Shanhua Lin²; Xiaodong Liu²; Jonathan Joseph¹; ¹*ThermoFisher, San Jose, CA*; ²*ThermoFisher, Sunnyvale, CA*
- WP 624 **Assessment of HOS of IgG2 Monoclonal Antibodies using Two Proteases in a Single Column Approach to Enhance the Sequence Coverage**; Sasidhar N Nirudodhi¹; Justin Sperry¹; Jason Rouse²; James A. Carroll¹; ¹*Pfizer, Chesterfield, MO*; ²*Pfizer, Inc., Andover, MA*
- WP 625 **Hydrogen/Deuterium Exchange - Mass Spectrometry Reveals Conformational Changes between Human Phosphatase PP2C α and a Catalytically Inactive Metal Binding Site Mutant**; Elyssia S. Gallagher^{1,2}; Subrata Debnath³; Sharlyn J. Mazur³; Lisa M. Miller Jenkins³; Stewart R. Durell³; Ettore Appella³; Jeffrey W. Hudgens^{1,2}; ¹*National Institute of Standards and Technology, Rockville, MD*; ²*Institute for Bioscience & Biotechnology Research, Rockville, MD*; ³*National Cancer Institute, NIH, Bethesda, MD*
- WP 626 **Mapping Protein-Protein Interaction Sites and Protein Dynamics using HDXMS: How Binding to CK Stabilizes the Ankyrin Repeat Domain of ASB9**; Deepa Balasubramaniam; *UCSD, La Jolla, CA*
- WP 627 **Impact of Unpaired Cysteines on the Conformation and Antigen Binding of Two Different Monoclonal Antibodies by Hydrogen/Deuterium Exchange Mass Spectrometry**; Hui-Min Zhang; Jin Li; Ben Walters; Jennifer Zhang; Yung-Hsiang Kao; *Genentech, South San Francisco, CA*
- WP 628 **Stepwise Sequential Protein Folding by a Hydrogen Exchange – Mass Spectrometry Method**; Wenbing Hu; Zhongyuan Kan; Benjamin Walters; Leland Mayne; S. Walter Englander; *University of Pennsylvania, Philadelphia, PA*
- WP 629 **Hydrogen/deuterium Exchange Mass Spectrometry Reveals Soybean Lipoygenase Conformational Flexibility**; Anthony T. Iavarone; Adam R. Offenbacher; Judith P. Klinman; *UC Berkeley, Berkeley, CA*
- WP 630 **Local Folding Energies/Rates of Wild-Type Staphylococcal Nuclease Determined by Protein Equilibrium Population Snapshot H/D Exchange Electrospray Ionization Mass Spectrometry (PEPS-HDX-ESI-MS)**; Rohana Liyanage; Hayden Pacl; Julie Rhee; Jennifer Gidden; Wesley Stites; Jackson O Lay Jr; *University of Arkansas, Fayetteville, AR*
- WP 631 **Profiling Protein Dynamics in SET Domain Containing Proteins**; Kristian E. Teichert^{1,2}; Roxana E. Iacob¹; Thomas E. Wales¹; Roodolph St. Pierre²; Mette Ishoey²; Sixun Chen³; Joshia Paulk²; James E. Bradner²; John R. Engen¹; ¹*Northeastern University, Boston, MA*; ²*Dana Farber Cancer Institute, Boston, MA*; ³*Broad Institute, Cambridge, MA*
- WP 632 **Biophysical Analysis of the C-Terminal Tail of EGF Receptor Tyrosine Kinase using HDX-MS and Small-angle X-ray Scattering**; Theodore Keppel; Kwabena Sarpong; John Monsey; Jian Zhu; Ron Bose; *Washington University, St. Louis, MO*
- WP 633 **Probing the Interface between the Sulfite Reductase Subunits, Hemoprotein and Flavoprotein, by H/D Exchange monitored by FT-ICR MS**; Yeqing Tao¹; Isabel Askenasy³; Nicolas L. Young²; M. Elizabeth Stroube³; Alan G. Marshall^{1,2}; ¹*Department of Chemistry and Biochemistry, Tallahassee, FL*; ²*NHMFL, Tallahassee, FL*; ³*Department of Biological Science and Institute, Tallahassee, FL*
- WP 634 **Hydrogen Exchange Mass Spectrometry (HDX-MS) Reveals Local Structural Perturbations in Mutant Forms of Apolipoprotein A-I**; Christopher Wilson¹; Madhurima Das²; Xiaohu Mei²; Olga Gursky²; John R. Engen¹; ¹*Northeastern University, Boston, MA*; ²*Boston University School of Medicine, Boston, MA*
- WP 635 **Investigation of Protein-Protein Interactions in the Human Pyruvate Dehydrogenase Complex by Hydrogen/Deuterium Exchange Mass Spectrometry**; Junjie Wang¹; Jieyu Zhou¹; Natalia S. Nemeria¹; Mulchand S. Patel²; Frank Jordan¹; ¹*Rutgers, the State University of New Jersey, Newark, NJ*; ²*University at Buffalo, Buffalo, NY*
- WP 636 **Unraveling Dynamic Interactions within the Peripheral Stalk of F₁F₀ ATP Synthase by HDX-MS**; Courtney Fast; Siavash Vahidi; Carla Busnello; Yumin Bi; Stanley Dunn; Lars Konermann; *Univ. of Western Ontario, London, ON*
- WP 637 **A Key Tryptophan in the Tec-family Tyrosine Kinase Btk Allosterically Regulates Kinase Activation**; Thomas E. Wales¹; Raji E. Joseph²; Amy H. Andreotti²; Amy H. Andreotti²; John R. Engen¹; ¹*Northeastern University, Boston, MA*; ²*Iowa State University, Ames, IA*
- WP 638 **How Well Do We Understand Protein HDX Protection Patterns? A Molecular Dynamics Simulation Study**; Robert McAllister; Lars Konermann; *Univ. of Western Ontario, London, ON*
- WP 639 **Ligand-Induced Changes in Structure and Dynamics of the Dihydrodipicolinate (DHDPs) Synthase Enzyme Complex Studied by HDX-MS**; Modupeola Sowole¹; Sarah Simpson²; Yulia Skovpen²; David Palmer²; Lars Konermann¹; ¹*University of Western Ontario, London, Canada*; ²*University of Saskatchewan, Saskatoon, Canada*
- WP 640 **Structural Analysis of SynGAP by HDX-MS**; Quinlin Hanson; Eric Underbakke; *Iowa State University, Ames, IA*



- WP 641 **Combining Native MS, IM-MS and HDX-MS for Structural Characterization of Bcd1p/Rtt106p complex involved in the box C/D snoRNPs Assembly Machinery;** Guillaume Terral¹; Benoit Bragantini²; Jean-Michel Saliou¹; Alain Van Dorsselaer¹; Xavier Manival²; Bruno Charpentier²; Sarah Cianféroni¹; ¹Laboratoire de Spectrométrie de Masse BioOrganique, Strasbourg, France; ²Ing. Moléculaire et Physiopathologie Articulaire, Vandoeuvre-lès-Nancy, France
- WP 642 **Gas-phase Hydrogen/Deuterium Exchange can be Used to Detect Conformational Differences in Protein Structure and Distinguish between Conformational Families;** Helen S Beeston¹; James R Ault¹; Henry C Fisher¹; Steven D Pringle²; Jeffrey M Brown²; Alison E Ashcroft¹; ¹University of Leeds, Leeds, UK; ²Waters Corporation, Wilmslow, UK
- WP 643 **Protein Structural Dynamics at the Gas/Water Interface Examined by Hydrogen Exchange Mass Spectrometry;** Yiming Xiao¹; Lars Konermann²; ¹University of Western Ontario, London, Canada; ²Univ. of Western Ontario, London, ON
- WP 644 **Lipid Packing Density Alters the Conformation of Membrane-Associated HIV-1 Nef;** Gregory F. Pirrone¹; Michael S. Kent²; John R. Engen¹; ¹Northwestern University, Boston, MA; ²Sandia National Laboratories, Albuquerque, NM
- WP 645 **Tryptophan289 Single Point Mutation Modulates the Dynamic Properties of Human Monoacylglycerol Lipase: A Hydrogen Deuterium Exchange Mass Spectrometry Study;** ioannis karageorgos^{1,2}; Elyssia S. Gallagher^{1,2}; Nikolai Zvonok³; Alexandros Makriyannis³; Jeffrey W. Hudgens^{1,2}; ¹National Institute of Standards and Technology, Rockville, MD; ²Institute for Bioscience & Biotechnology Research, Rockville, MD; ³Center for Drug Discovery, Northeastern University, Boston, MA
- WP 646 **Millisecond HX-MS to Detect Residual Helicity in a Disordered Protein using a Denatured State Reference;** Mohammed Al-Naqshabandi^{1,2}; David D. Weis¹; ¹University of Kansas, Lawrence, KS; ²Soran University, Erbil, Iraq
- PROTEINS: CONFORMATION ANALYSIS**
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- WP 648 **Influence of Lipid Environment on Gramicidin A Dimer Conformation Probed using Nanodiscs and ESI-IMS-MS;** Emma-Dune Leriche; Xuxin Fan; Elena N. Kitova; John S. Klassen; ¹University of Alberta, Edmonton, Canada
- WP 649 **Conformational Changes of an Allosteric Enzyme Probed in Solution and in the Gas-Phase: IM-MS, HDX-MS and AUC Studies of MtATP-phosphoribosyltransferase;** Kamila Pacholarz^{1,2}; Thomas Jowitt¹; Rebecca Burnley³; Victoria Ordsmith²; Massimiliano Porrini⁴; Gérald Larrouy-Maumus⁵; João Pisco⁵; Rachel Garlish³; Richard Taylor³; Luiz de Carvalho⁵; Perdita Barran¹; ¹University of Manchester, Manchester, UK; ²University of Edinburgh, Edinburgh, UK; ³UCB, Slough, UK; ⁴Institute Européen de Chimie et Biologie, Pessac, France; ⁵MRC National Institute for Medical Research, London, UK
- WP 650 **Probing GPCR-ligand Interaction by Chemical Crosslinking and Mass Spectrometry;** Bill Huang; Ji-Won Lee; Hee-Yong Kim; ¹NIAAA/NIH, Rockville, MD
- WP 651 **Insights into Gas-phase Protein Conformations from Matrix Assisted Ionization (MAI) using Ion Mobility Spectrometry-Mass Spectrometry;** Daniel Woodall¹; Shameemah Thawoos¹; Corinne Lutomski¹; Sarah Trimpin^{1,2}; ¹Wayne State University, Detroit, MI; ²Cardiovascular Research Institute, Detroit, MI
- WP 652 **Development of a Rapid & Sensitive Shape Selective Screen to Monitor the Folding/Assembly of Recombinant Proteins;** Owen Cornwall¹; Daniel Higazi²; Nicholas Bond²; Matthew Edgeworth¹; James Scrivens¹; ¹University of Warwick, Coventry, UK; ²MedImmune, Cambridge, UK
- WP 653 **Ion Mobility Mass Spectrometry Reveals (Non-)Structural Order in p27;** Rebecca Beveridge¹; Yongqi Huang²; Rahul Das³; Rohit Pappu³; Richard Kriwacki²; Perdita Barran¹; ¹University of Manchester, Manchester, UK; ²St. Jude Children's Research Hospital, Memphis, TN; ³Washington University, St. Louis, MO
- WP 654 **Protein Conformational Study by Selected Accumulation Ion Mobility Spectrometry-Electron Capture Dissociation Tandem Mass Spectrometry;** Yi Pu¹; Rebecca S. Glaskin²; Mark E. Ridgeway³; Melvin A. Park³; Cheng Lin²; Catherine E. Costello^{1,2}; ¹Boston University, Boston, MA; ²Boston University School of Medicine, Boston, MA; ³Bruker Daltonics, Billerica, MA
- WP 655 **Effect of Post-Translational Modifications on the Metal Binding and Conformation of Alpha-Synuclein;** Aimee Paskins; Rebecca Mason; Cathrine Duckett; Caroline Dalton; David Smith; ¹Sheffield Hallam University, Sheffield, UK
- WP 656 **Analysis of p85 α Molecular Architecture using Chemical Cross-Linking;** Evan T Brower¹; Raghothama Chaerkady¹; Qing Wang¹; Mathias Schäfer²; Andrea Sinz²; Kenneth W. Kinzler¹; Bert Vogelstein¹; L. Mario Amzel¹; Robert N. Cole¹; Sandra B. Gabelli¹; ¹Johns Hopkins University, Baltimore, MD; ²Universität zu Köln, Greinstrasse, Germany; ³Martin-Luther-Universität, Halle-Wittenberg, Germany
- WP 657 **Twisting the Twist: an Ion Mobility-Mass Spectrometry study of the p53:MDM2 interaction;** Eleanor Dickinson; ¹University of Manchester, Manchester, UK
- WP 658 **Mapping the Protein Structural Changes by Quantitative Cross-linking;** Zdenek Kukacka^{1,2}; Michal Rosulek^{1,2}; Daniel Kavan^{1,2}; Petr Pompach^{1,2}; Petr Novak^{1,2}; ¹Institute of Microbiology, Prague, Czech Republic; ²Charles University, Prague, Czech Republic
- ANTIBODIES AND ANTIBODY: DRUG CONJUGATES I**
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- WP 659 **Characterization of Host Cell Proteins in the Protein A Purification of a Variety of Monoclonal Antibodies;** Chong-Feng Xu; Zhenzhen Wang; Daniel Xu; Christina Alves; Li Zang; ¹Biogen Idec, Cambridge, MA
- WP 660 **Mass Spectrometry Characterization of SJCD3 MAb and Comparison with OKT3;** Bo Zhai¹; Aaron Shafer¹; Kevin van Cott²; Chao-Xuan Zhang¹; Michael Meagher¹; ¹St Jude Children's Research Hospital, Memphis, TN; ²University of Nebraska-Lincoln, Lincoln, NE
- WP 661 **A Universal Solution for the Pre-Clinical Bioanalysis of Humanized Therapeutic Monoclonal Antibodies in Plasma;** Kwasi Antwi; Urban Kiernan; Eric Niederkofler; ¹Thermo Fisher Scientific, Tempe, AZ
- WP 662 **In-depth Identification of Protein Images by Combining High Mass Resolution MALDI-FTICR Imaging and High Performance qTOF nLC-MS/MS;** Arnd Ingendoh¹; Matt Willetts²; Shannon Cornett²; ¹Bruker Daltonik, Bremen, Germany; ²Bruker Daltonics, Billerica, MA
- WP 663 **Comprehensive Characterization of a Representative Antibody-Drug Conjugate by CESI-MS;** Bryan Fonslow²; Eric Johansen¹; Hans Dewald²; ¹SCIEX, Redwood City, CA; ²SCIEX, Brea, CA
- WP 664 **Rapid Identification and Quantitation of Disulfide Bonds in Antibodies and Other Purified Proteins;** Wilfred H. Tang; Yong Joo Kil; Kevin L. Crowell; Marshall W. Bern; Eric Carlson; Chris Becker; ¹Protein Metrics Inc., San Carlos, CA
- WP 665 **Characterization of Monoclonal Antibodies and ADCs using a Benchtop Orbitrap Mass Spectrometer;** Xiaoxi Zhang; ¹ThermoFisher Scientific, Shanghai, China
- WP 666 **Exact de novo Sequencing of a Monoclonal Antibody with Fab Glycosylation;** Marshall W. Bern¹; David

- Morgenstern²; Beatrix Ueberheide²; Walter Bogdanoff³; Rebecca Dubois³; ¹*Protein Metrics, San Carlos, CA*; ²*New York University, New York, NY*; ³*University of California, Santa Cruz, CA*
- WP 667 **De novo Sequencing Our Polyclonal Immune Response Without B-cell Sequencing**; Adrian Guthals¹; Yutian Gan²; Wendy Sandoval²; Nuno Bandeira^{1,3}; ¹*University of California, San Diego, La Jolla, CA*; ²*Genentech, South San Francisco, CA*; ³*Skaggs School of Pharmacy, UC San Diego, La Jolla, CA*
- WP 668 **Investigation of Anti-Drug-Antibody Impact on LC-MS/MS Bioanalysis of Unconjugated Payload of Antibody Drug Conjugate in a Monkey Toxicity Study**; Hang Zeng¹; Ragu Ramanathan¹; Frank Barletta¹; Michael Giovanelli²; Rick Steenwyk¹; ¹*Pfizer, Inc., Groton, CT*; ²*DSRD, Pfizer, Inc, Groton, CT*
- WP 669 **Understanding of Critical Quality Attributes of Biopharmaceuticals In Vivo**; Yinyin Li¹; Emma Zhang²; Peter Li²; Billy Wu²; Patrick Swann¹; Yelena Lyubarskaya¹; ¹*Biogen Idec, Cambridge, MA*; ²*BioAnalytix Inc, Cambridge, MA*
- WP 670 **Characterization of Degradants of a Therapeutic Monoclonal Antibody via Combined Topdown and Bottom Up LC-MS/MS**; Antonio Triolo¹; Elisa Libralesso¹; Francesca Boscaro²; Francesca Romana Dani²; Elena Michelucci²; Giuseppe Pieraccini²; Gloriano Moneti²; ¹*Menarini Ricerche Spa, Firenze, Italy*; ²*CISM Centro di Servizi di Spettrometria di Massa, Firenze, Italy*
- WP 671 **Localizing the Conjugation Sites of Cysteine-Conjugated Antibody Drug Conjugates by Improved LC-MS Subunit Analysis for ADC Positional Isomer Identification**; Henry Shion¹; Robert Birdsall¹; Liuxi Chen¹; Ying-Qing Yu¹; Frank W. Kotch³; April Xu²; Thomas J. Porter⁴; Weibin Chen¹; ¹*Waters Biopharmaceutical Business Operations, Milford, MA*; ²*Pfizer Analytical Research & Development, Pearl River, NY*; ³*Pfizer Bioprocess Research & Development, Pearl River, NY*; ⁴*Pfizer Analytical Research & Development, Andover, MA*
- WP 672 **Rapid LC/MS Identification of mAbs Utilizing CDR Masking**; Amy Hilderbrand¹; Rashmi Jain²; Nisana Andersen¹; Benjamin Moore¹; Chenchen Wang¹; Cleo Salisbury¹; ¹*Genentech, South San Francisco, CA*; ²*University of California San Diego, San Diego, CA*
- WP 673 **Evaluation of Hemoglobin as a Carrier of Anti-HIV Drug (Adefovir) in Macrophage-targeting Drug Delivery System**; Shengsheng Xu; Igor A. Kaltashov; *University of Massachusetts-Amherst, Amherst, Massachusetts*
- WP 674 **Analysis of Antibody Drug Conjugate using High Flow HPLC Coupled to Time-of-Flight Mass Spectrometry**; Ravindra Gudihal; Sundaram M Palaniswamy; Sudha Rajagopalan; *Agilent Technologies India Pvt. Ltd, Bangalore, India*
- WP 675 **Immunocapture LC-MS/MS Hybrid Assays for Conjugated-Antibody and Total-Antibody in Antibody Drug Conjugate (ADC) Bioanalysis**; Huidong Gu; Ang Liu; Frank Zambito; Alexander Kozhich; Heather Myler; Anne-Françoise Aubry; Mark Arnold; Jian Wang; *Bristol-Myers Squibb, Princeton, NJ*
- WP 676 **Full Validation of Therapeutic Antibody Sequences by Middle-Up Mass Measurements and Middle-Down Protein Sequencing**; Anja Resemann¹; Wolfgang Jabs¹; Anja Wiechmann¹; Elsa Wagner²; Olivier Colas²; Waltraud Evers¹; Eckhard Belau¹; Lars Vorwerk¹; Catherine Evans³; Alain Beck²; Detlev Suckau¹; ¹*Bruker Daltonik GmbH, Bremen, Germany*; ²*Centre d'Immunologie Pierre-Fabre, St. Julien-en-Genevois, France*; ³*Bruker Daltonics Ltd, Coventry, UK*
- WP 677 **Enhancing Characterization Antibody-based Biologic using Differential Mobility and Mass Spectrometry**; Tanya Gamble¹; J.C. Yves Leblanc¹; Eric Johansen²; Suma Ramagiri¹; ¹*SCIEX, Concord, ON, ON*; ²*SCIEX, Redwood, CA*
- WP 678 **Comprehensive LC/MS Characterization of a Broadly Neutralizing HIV-1 mAb**; Li Cao; Vera Ivleva; Jie Liu; Deepika Gollapudi; Jonathan Cooper; Richard Schwartz; *VPP, NIAID, NIH, Gaithersburg, MD*
- WP 679 **Application of Data Independent Acquisition for Top-Down Characterization of IgG Light**; Sahana Mollah; Melanie Juba; Xu Wang; *AB SCIEX, Redwood City, CA*
- WP 680 **Mass Spectrometry Rearrangement by Collision Induced Dissociation of Cleavable ADC Linker Containing Aminobenzylcarbamate Group**; Xidong Feng; Dahui Zhou; Kenneth Dirico; Russell G Dushin; Chakrapani Subramanyam; Christopher J O'Donnell; Justin Stroh; Michael J Shapiro; *Pfizer Worldwide Research, Groton, CT*
- WP 681 **Characterization of Glycosylation and Amino Acid Sequence Features of Pig Immunoglobulins**; Paul Lopez¹; Lauren Girard¹; Andrey Oliveira¹; Edward Bodnar¹; Apolline Salama²; Jean-Paul Soullillou²; Helene Perreault¹; ¹*University of Manitoba, Winnipeg, Canada*; ²*UMR INSERM 10-64, Université de Nantes, Nantes, France*
- WP 682 **A Universal Immunocapture-LC-MS/MS Workflow for Biological Compound Quantitation in Preclinical Studies**; Lei Xiong¹; Witold Woroniecki¹; Suma Ramagiri²; Gary Impey²; Hua-Fen Liu¹; ¹*AB SCIEX, Redwood City, California*; ²*AB SCIEX, Concord, ON*
- WP 683 **Characterization of Charge Variants of Therapeutic Antibodies A (taA) in CEX Fractions by Bottom-up and Top-down MS**; Chien-Wen Hung; Benedetto Aquilino; Urs Hanke; Claudia Torella; Christoph Roesli; Florian Wolschin; Andreas Seidl; *Sandoz Biopharmaceuticals, Oberhaching, Germany*
- WP 684 **Two Approaches that Facilitate Antibody Analysis**; Nick DeGraan-Weber; James P. Reilly; *Indiana University, Bloomington, IN*
- WP 685 **Automated Affinity Capture and Rapid On-Tip Digestion to Accurately Quantitate in vivo Deamidation of Therapeutic Antibodies**; John C. Tran; Daniel Tran; Phillip Chu; Denise Krawitz; Amy Hilderbrand; Kathy Kozak; Yichin Liu; Jianyong Wang; *Genentech, South San Francisco, CA*
- WP 686 **Rapid Comprehensive Comparison of Five Versions of Bevacizumab – Avastin versus Its Biosimilars**; Chris Becker¹; Yong Kil¹; Eric Carlson¹; David Morgenstern²; Beatrix Ueberheide²; ¹*Protein Metrics Inc., San Carlos, CA*; ²*NYU School of Medicine, New York, NY*
- WP 687 **Top Down LC/MS Characterization of RP-HPLC Impurities of Monoclonal Antibody by High Energy Collision-Induced Dissociation**; Jia Zhao; flora gu; yan-hui liu; Huijuan Li; Mohammed shameem; *Merck, Kenilworth, NJ*





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

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AMBIENT IONIZATION: FUNDAMENTALS 001-019

- ThP 001 **Effect of Humidity on Ionization Efficiencies in Dopant-Assisted GC-APCI-TOF MS;** [Carolyn Hutchinson](#); Daniel Cole; Young Jin Lee; *Iowa State University, Ames, IA*
- ThP 002 **High Sensitive and Throughput Direct Analysis of Genotoxicity Acrylamide Generated by High Temperature Food Processes using DART-MS Combined with Corona++™;** [Motoshi Sakakura](#)¹; Hiroshi Hike¹; Takatomo Kawamukai¹; Teruhisa Shiota¹; Kanako Sekimoto²; Mitsuo Takayama²; ¹*AMR Inc., Meguro-Ku, Japan*; ²*Yokohama City Univ., Yokohama, Japan*
- ThP 003 **Comparison of Internal Energy Distributions of Ions Created by Electrospray Ionization and Laser Ablation-Liquid Vortex Capture/Electrospray Ionization;** [John F. Cahill](#); Vilmos Kertesz; Olga S. Ovchinnikova; Gary J. Van Berkel; *Oak Ridge National Laboratory, Oak Ridge, TN*
- ThP 004 **Particle Size Measurement from Tissue Ablation for Laser Ambient Ionization and Sampling;** [Fan Cao](#); Kermit K. Murray; *Louisiana State University, Baton Rouge, LA*
- ThP 005 **The Potential of Peptide/Protein Arrays using Desorption Electrospray Ionisation Mass Spectrometry; Sensitivity and Limit of Detection;** [Elzbieta Gurdak](#)¹; Andrew Hook²; Alexander Shard¹; Josephine Bunch¹; ¹*National Physical Laboratory, Teddington, UK*; ²*University of Nottingham, Nottingham, UK*
- ThP 006 **Comparison of Negative Ion ESI Ionization Efficiencies for a Diversity of Small Acidic Molecules with Widely Varying pK_a's;** [James Mattila](#); Shelsea Hurdle; Stephen Lucas; Christine A. Hughey; *James Madison University, Harrisonburg, VA*
- ThP 007 **Extractive Electrospray Ionization Mass Spectrometry with Metal Cationization;** [Kenneth Swanson](#); Sandra Spencer; Gary L. Glish; *Univ. of North Carolina at Chapel Hill, Chapel Hill, NC*
- ThP 008 **Corona Discharge Suppression in Negative-ion Mode Nanoelectrospray via Trifluoroethanol Addition;** [Phillip McClory](#); Kristina Hakansson; *University of Michigan, Ann Arbor, MI*
- ThP 009 **Collision Surfaces and Ambient Ionization Mechanisms; Studies Leading to the Improvement of Signal Intensities in Rapid Evaporative Ionization Mass Spectrometry;** Emrys A Jones¹; [Ottmar Golf](#)¹; Steven Pringle²; Tamas Karancsi³; Zoltan Takats¹; ¹*Imperial College London, London, UK*; ²*Waters Corporation, Manchester, UK*; ³*Waters Research Center, Budapest, Hungary*

- ThP 010 **Benzyl Carbanion Transfer in the Fragmentation of N-(phenylsulfonyl)-benzeneacetamides: A Gas-phase Intramolecular SNAr Reaction;** Shanshan Shen; Yunfeng Chai; Yaqin Liu; Chang Li; [Yuanjiang Pan](#); *Zhejiang University, Hangzhou, China*
- ThP 011 **A Study of the Gas-Phase Chemistry in a Dielectric Barrier Discharge using Argon and Hydrogen-Doped Argon as the Support Gases;** [Wade Ellis](#); Paul Farnsworth; *Brigham Young University, Provo, UT*
- ThP 012 **Contained-Electrospray: A New Spray Ionization Process for Improving Ion Yields for Complex Samples during ESI-MS Analysis;** [Dmytro Kulyk](#); Abraham Badu Tawiah; *Ohio State University, Columbus, OH*
- ThP 013 **Zero Volt Paper Spray Ionization and its Mechanism;** [Yafeng Li](#)¹; Michael Wlekinski¹; Soumabha Bag¹; Depanjan Sarkar²; Rahul Narayanan, T. Pradeep²; R. Graham Cooks^{1,2}; ¹*Purdue University, West Lafayette, Indiana*; ²*Indian Institute of Technology Madras, Chennai, India*
- ThP 014 **Generation of Multiply Charged Ions using a liquid AP MALDI Ion Source without Heated Ion Transfer Tube;** [Pavel Ryumin](#)¹; Jeff Brown^{1,2}; Rainer Cramer¹; ¹*University of Reading, Reading, UK*; ²*Waters Corporation, Wilmslow, UK*
- ThP 015 **A Comparison of Atmospheric Pressure Surface Sampling Methods: DESI, PADI, AP-MALDI and LESA;** [Tara La Roche Salter](#)¹; Rory Steven¹; Elizabeth Randall^{1,2}; Alan Race¹; Ian Gilmore¹; Josephine Bunch^{1,3}; ¹*National Physical Laboratory, Teddington, UK*; ²*University of Birmingham, Birmingham, UK*; ³*University of Nottingham, Nottingham, UK*
- ThP 016 **Hydrophobic Paper Spray Ionization Mass Spectrometry;** [Kathryn M. Davis](#); Abraham Badu-Tawiah; *The Ohio State University, Columbus, OH*
- ThP 017 **Surface-modified Wooden-tip Electrospray Ionization Mass Spectrometry for Enhanced Detection of Analytes in Complex Samples: Mechanism and Applications;** [Bin Hu](#)¹; Yun-Yun Yang²; Jie-Wei Deng^{1,3}; Zhong-Ping Yao¹; ¹*Hong Kong Polytechnic University, Hong Kong, China*; ²*China National Analytical Center Guangzhou, Guangzhou, China*; ³*Sun Yat-Sen University, Guangzhou, China*
- ThP 018 **Fundamental Studies of Atmospheric Pressure Dielectric Barrier Discharge Jet used for Depth Profiling Mass Spectrometry;** [Gerardo Gamez](#); Songyue Shi; Xiaoxia Gong; Marcel Kroschok; John Usala; *Texas Tech University, Lubbock, TX*
- ThP 019 **Toward Understanding Factors that Influence Globular Protein Ion Charge in Native Electrospray Ionization;** [Anna Susa](#); Evan Williams; *Berkeley, CA*

INSTRUMENTATION: MINI/PORTABLE/FIELDABLE MS

020-032

- ThP 020 **Development, Study and Application of Hand Portable GC/MS as a Field Investigative Tool for the First Responder**; Gareth Dobson; *Smiths Detection, Edgewood, MD*
- ThP 021 **The Research of the Scan Function About Linear Ion Trap at Low Vacuum**; Hao Lv¹; Zhanfeng Zhao¹; Eric Handberg²; Zhiquan Zhou¹; ¹*Harbin Institute of Technology at Weihai, Weihai, China*; ²*East China Institute of Tech., Nanchang, China*
- ThP 022 **Application of Sub-Ambient Pressure Gas Chromatography to the Development of a Miniature Ion-Trap GC/MS**; Conor Mullens; Daniel Debord; Corey Stedwell; Michael Spencer; David Rafferty; *1st Detect, Webster, TX*
- ThP 023 **Improvements to Membrane Inlet Interface for Subsea *in-situ* mass spectrometry**; Brian Gregson; Gary Hendrick; David Fries; *Spyglass Technologies, Inc., St. Petersburg, FL*
- ThP 024 **Evaluating Ion Trap Materials for Hand Portable, High Pressure Mass Spectrometry**; Kenion Blakeman; Tina Stacy; Craig Cavanaugh; J. Michael Ramsey; *University of North Carolina, Chapel Hill, NC*
- ThP 025 **Combining Real-Time Portable Membrane Introduction Mass Spectrometer and Whole Air Sampling Canister Data for Atmospheric Analysis of Volatile Organic Compounds**; Nicholas G. Davey^{1,4}; Ryan J. Bell^{3,4}; Isobel J. Simpson²; Donald R. Blake²; Erik T. Krogh^{1,4}; Christopher G. Gill^{1,4}; ¹*University of Victoria, Victoria, BC, Canada*; ²*UC Irvine, Irvine, CA*; ³*Beaver Creek Analytical LLC, Boulder, CO*; ⁴*Appl. Env. Res. Labs. (AERL), Nanaimo, Canada*
- ThP 026 **Optimization of the Cylindrical Ion Trap Geometry Operated at High Pressure**; Dmitriy Chernookiy; Bruno Coupier; J. Michael Ramsey; *University of North Carolina, Chapel Hill, Chapel Hill, NC*
- ThP 027 **Low Voltage RF Amplitude Scanning with Multi-Frequencies for Ion Trap Mass Spectrometry**; Seung Yong Kim¹; Jong Rok Ahn¹; Wanseop Jeong¹; Mo Yang¹; Eungnam Kim²; Jin-Young Choi²; Hyun Sik Kim¹; ¹*Korea Basic Science Institute, Ochang-Eup Cheongju-Si, South Korea*; ²*Korea University, Seoul, Korea*
- ThP 028 **Real-time Sample Analysis using Remote Sampling Probe and Miniature Mass Spectrometer**; Chien-Hsun Chen¹; Ziqing Lin¹; R. Graham Cooks²; Zheng Ouyang¹; ¹*Biomedical Engineering, Purdue University, West Lafayette, IN*; ²*Chemistry Department, Purdue University, West Lafayette, IN*
- ThP 029 **Manipulation of Trapped Ions in High Pressures in CITS and SLITs**; Andrew Hampton; J. Michael Ramsey; *UNC - Chapel Hill, Chapel Hill, NC*
- ThP 030 **Making Sense of Water Quality: A Portable MS-UV Sensing Platform for Real-Time Monitoring in Aquaculture**; Simon Maher^{1,3}; Barry Smith²; Mariya Juno³; Fred Jjunju³; Behnam Bastani^{1,3}; Lei Su³; Urszula Salaj-Kosla⁴; Liam Lewis⁴; Jean-Michel Mortz²; Dag Hammer⁶; Gyda Christophersen⁶; Pat O'Leary⁷; Allan MacMaster⁸; Stephen Taylor^{2,3}; Iain Young¹; ¹*Institute of Integrative Biology, University of Liverpool, UK*; ²*Q Technologies, Liverpool, UK*; ³*Dept. Electrical Engineering & Electronics, University of Liverpool, UK*; ⁴*Cork Institute of Technology, Cork, Ireland*; ⁵*BAMO-IER GmbH, Mannheim, Germany*; ⁶*Teknologisk Institutt as, Oslo, Norway*; ⁷*Faaltech Technologies, Cork, Ireland*; ⁸*Anglesey Aquaculture Ltd, Beaumaris, UK*
- ThP 031 **Characterization of Small Organic Molecules and Proteins by Matrix-Assisted Ionization-Portable Mass Spectrometry**; Zachary Devereaux; Sarah Trimpin; *Wayne State University, Detroit, MI*
- ThP 032 **Improvement of a Micro- Time of Flight Mass-Spectrometer based on MEMS Technologies**; Romain Mahieu²; Laurent Duraffourg²; Marc Gely²; Thomas Alava²; Charles-Marie Tasseti¹; Frederic Progent¹; ¹*CEA, DAM, DIF, F-91297 Arpajon, France*; ²*CEA LETI, Grenoble, France*

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- ThP 034 **Simultaneous Determination of 74 kinds of pesticides in Chinese Herbal Medicine Listed in Chinese Pharmacopoeia (2015) by GPC-GC-MS/MS**; Yang Huiyan; Fan Jun; Huang Taohong; Shin-ichi Kawano; Yuki Hashi; *Shimadzu, Shanghai, China*
- ThP 035 **Improved Analysis of Allergens in Cosmetics by Cold EI GC/MS**; Sharanya Reddy; Thomas Dillon; Adam Patkin; Bill Hahn; *PerkinElmer, Shelton, CT*
- ThP 036 **Determination of Chemicals in Consumer Goods, Food Commodities and Drugs in a Rapid Method with Limited Sample Prep**; Louis Maljers¹; Gordon van 't Slot²; ¹*Bruker, Fremont, Ca*; ²*Bruker, Bremen, Germany*
- ThP 037 **Volatile & Semi-Volatile Profile Comparison of Whole Versus Cracked Versus Dry Homogenized Barley Grains by Direct Thermal Extraction GC/MS**; Ronald E. Shomo, II; Christopher Baker; John Manura; *Scientific Instrument Services, Ringoes, NJ*
- ThP 038 **Assessing the Thermal Stability and Degradation Characteristics of Chemical Warfare Nerve Agents via Pyrolysis GC-MS**; Jeffrey Mcquire¹; John Carpin¹; Matthew Parrish²; ¹*US Army ECBC, Aberdeen Proving Ground, MD*; ²*LEIDOS, Gunpowder, MD*
- ThP 039 **Evaluation of Direct and Dopant-Assisted APLI in GC-MS Applications**; Faezeh Dousty¹; Hendrik Kersten²; Thorsten Benter²; Rob O'Brien³; ¹*University of British Columbia Okanagan, Kelowna, BC, Canada*; ²*University of Wuppertal, Wuppertal, Germany*; ³*Supra Res & Dev, Kelowna, BC, Canada*
- ThP 040 **High Mass Accuracy Measurements and Elemental Composition Determination of Molecular Ions and Fragments of Pesticides with Single Quadrupole GC/MS Systems**; Ming Gu; Hongliang Xu; Yongdong Wang; *Cerno Bioscience, Norwalk, CT*
- ThP 041 **Rapid Analysis of Polychlorinated Biphenyls (PCBs) in Vegetables by QuEChERS-based Extraction and GPC-GCMS**; Xizhi Wang¹; Shiheng Luo¹; Feifei Tian¹; Jun Fan²; Guixiang Yang¹; Taohong Huang²; Shin-ichi Kawano²; Yuki Hashi²; ¹*Shimadzu Global COE, Shimadzu (China) Co.,Ltd., Beijing, China*; ²*Shimadzu Global COE, Shimadzu (China) Co.,Ltd., Shanghai, China*
- ThP 042 **Characterization of Rose and Other Essential Oils and Synthetic Additives in them Using GC/MS with Cold EI Source**; Avinash Dalmia; Urs Steiner; *PerkinElmer, Shelton, CT*
- ThP 043 **Chemometric Methods for Botanical Classification of Chinese Honey According to Their Volatile Profiling by Solid-Phase Microextraction and Gas Chromatography-Mass**; Hui Chen¹; Linghe Jin²; Chunlin Fan¹; Guofang Pang¹; Wenwen Wang³; Philip L. Wylie⁴; Joerg Riener⁵; Kumi Shiota Ozawa⁶; ¹*Chinese Academy of Inspection and Quarantine, Beijing, China*; ²*Shandong Agriculture University, Tai'an, China*; ³*Agilent Technologies, Beijing, China*; ⁴*Agilent Technologies, Wilmington, DE*; ⁵*Agilent Technologies, Waldbronn, Germany*; ⁶*Agilent Technologies, Barueri, Brazil*
- ThP 044 **SIMAT: GC-SIM-MS Analysis Tool**; Mohammad R Nezami Ranjbar²; Cristina Di Poto¹; Yue Wang²; Habtom Resson¹; ¹*Georgetown University, Lombardi Cancer Center, Washington, DC*; ²*Virginia Tech, Arlington, VA*



- ThP 045 **A Spike-In Experiment for Assessment of GC-MS-based Analysis of Metabolites in Human Plasma;** Rency Varghese; Yue Luo; Cristina Di Poto; Mohammad R Nezami Ranjbar; Habtom Ressonm; *Georgetown University, Lombardi Cancer Center, Washington, DC*
- ThP 046 **Rapid Screening of Different Groups of Steroids by Multiple Selected Ion Monitoring in Biological Fluids;** Dick Bernhard; Bruno Vogt; Genevieve Escher; *Inselspital Nephrology, Hypertension, Bern, Switzerland*
- ThP 047 **New, Innovative Thermal Modulator Design for Two-Dimensional Gas Chromatography/ Mass Spectrometry Analysis;** Gaetano Stallone¹; Massimiliano Saini Fasanotti²; Ilaria Ferrante²; ¹*Volatome, Giovinazzo, Italy*; ²*DANI Instruments SpA, Cologno Monzese, Italy*
- ThP 048 **Evaluation of Methylisothiazolinone (MI) Extraction from Sunscreen using Supported Liquid Extraction prior to GC/MS Analysis;** Rhys Jones¹; Lee Williams¹; Alan Edgington¹; Helen Lodder¹; Adam Senior¹; Geoff Davies¹; Steve Jordan¹; Claire Desbrow¹; Victor vandell²; Elena Gairloch²; ¹*Biotage GB Limited, Cardiff, Mid Glamorgan*; ²*Biotage LLC, Charlotte, NC*
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- ThP 052 **A Microfabricated Chromatographic Chip Integrated with a Peak-Refocusing Cold Trap for a Multi-dimensional GC/MS Analysis;** Sanggoo Kim; Sungmin Lim; *Korea Basic Sci. Institute, Seoul, South Korea*
- ThP 053 **Two-Dimensional Comprehensive Gas Chromatography Multi-Reflection Time-Of-Flight Mass Spectrometry: A Unique Tool to Merge Accurate Mass Information with High Chromatographic Resolution;** Thomas Groeger¹; Ralf Zimmermann²; Benedikt Weggler¹; Martin Sklorz²; Aimee Sutherland¹; Juergen Wendt³; ¹*Helmholtz Zentrum Muenchen, Oberschleissheim, Germany*; ²*University of Rostock, Rostock, Germany*; ³*LECO Instrumente GmbH, Moenchengladbach, Germany*
- ThP 054 **Extending the Range of Compounds Amenable for GC-MS Analysis;** Alexander Fialkov; Tal Alon; Aviv Amirav; *Tel Aviv University, Tel Aviv, Israel*
- ThP 055 **Analysis of Metabolites in Human Plasma Using Stable Isotopes and Ultra-Fast GC-MS/MS System;** Yumi Unno²; Shuichi Kawana¹; Yukihiko Kudo¹; Takero Sakai¹; Shin Nishiumi²; Masaru Yoshida²; Noriyuki Ojima¹; ¹*Shimadzu Corporation, Kyoto, Japan*; ²*Kobe University Graduate School of Medicine, Kobe, Japan*
- ThP 056 **Automated Development of the Comprehensive Compound Database for Targeted MRM-based Metabolomics of Arabidopsis Plants using GC-MS/MS Technology;** Feroza K. Choudhury¹; Dwain Cardona²; Amith Reddy¹; Ron Mittler¹; Vladimir Shulaev¹; ¹*University of North Texas, Denton, TX*; ²*Thermo Fisher Scientific, Austin, TX*
- ThP 057 **Screening for Hundreds of Pesticide Residues Using a GC/Q-TOF with an Exact Mass Pesticide Database in Various Food Matrices;** Joerg Riener¹; Samanta Uclés²; Philip L. Wylie³; Wenwen Wang⁴; Jennifer Gushue⁵; Amadeo Fernández-Alba²; ¹*Agilent Technologies, Waldbronn, Germany*; ²*University of Almería, Almería, SPAIN*; ³*Agilent Technologies, Wilmington, DE*; ⁴*Agilent Technologies Co. Ltd, Beijing, China*; ⁵*Agilent Technologies, Santa Clara, CA*
- ThP 058 **A Comparison of ITEX Dynamic Headspace/GC/MS to Other Enrichment Techniques for Analysis of Flavoring Compounds;** Douglas Doster; *Aspen Research Corporation, New Germany, MN*
- ThP 059 **Determination of Residual Styrene Monomer in Copolymers by Headspace Solid Phase Microextraction Followed by GC/MS Using Isotope Dilution Calibration;** Dayna Turner; Andrei Stefanescu; *Novus International, Saint Charles, MO*
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- ThP 061 **Gas Chromatography Plasma-Assisted Reaction Chemical Ionization Mass Spectrometry: Quantification of Organohalogen at High Sensitivity;** Haopeng Wang¹; Carina Minardi¹; Hamid Badie²; Kaveh Kahan²; Kaveh Jorabchi¹; ¹*Georgetown University, Washington, DC*; ²*PerkinElmer Inc., Woodbridge, Canada*

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- ThP 063 **Comprehensive Extractables Analysis of Medical Grade O-ring;** Dan Ewing¹; Bill Hurley²; Andrew Feilden³; Michael Creese³; Kate Comstock⁴; Ekong Bassey⁴; John Schmelzel⁴; ¹*Parker Hannifin O-ring Division, Lexington, KY*; ²*Darcoid Nor-Cal Seal, Oakland, CA*; ³*Smithers Rapra, Shawbury, UK*; ⁴*Thermo Fisher Scientific, San Jose, CA*
- ThP 064 **Characterization of Facial Cleansers by Kendrick Mass Defect Analysis using MALDI Spiral-TOFMS;** Kanae Teramoto¹; Masaaki Ubukata²; Robert Cody²; Hiroaki Sato³; ¹*JEOL Ltd., Akishima, Japan*; ²*JEOL USA Inc., Peabody, MA*; ³*Advanced Industrial Science and Technology (AIST), Tsukuba, Japan*
- ThP 065 **Role of the Matrix in Fragile End-Group Cleavage upon MALDI of Synthetic Polymers;** Christophe Chendo; Trang N.T. Phan; Didier Gigmes; Laurence Charles; *Aix-Marseille University, Marseille, France*
- ThP 066 **Trapped Ion Mobility Mass Spectrometry for Improved Additive Detection and Polymer Identification;** Jan Jordens¹; Matthieu Besemer¹; Ynze Mengerink¹; Mark Ridgeway²; Melvin A. Park²; Maarten Honing¹; ¹*Resolve, Geleen, Netherlands*; ²*Bruker Daltonics, Inc., Billerica, MA*
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- ThP 068 **Structural Elucidation of Co-Polymer-Like Surfactants using MALDI Hi-Energy Collision Induced Dissociation;** Roberto Castangia²; Martin Resch Resch¹; Matthew Openshaw²; Omar Belgacem²; ¹*Shimadzu, Manchester, UK*; ²*Shimadzu, Kratos, Manchester, UK*
- ThP 069 **A Tandem Mass Spectrometry-Based Method to Assess the Architectural Purity of Synthetic Polymers: The Case of a Cyclic Poly lactide;** Thomas Josse¹; Julien De Winter¹; Philippe Dubois¹; Olivier Coulembier¹; Antony Memboeuf²; Pascal Gerbaux¹; ¹*University of Mons, Mons, N/A*; ²*Université de Bretagne Occidentale, Brest, France*
- ThP 070 **Mass Spectrometry Characterization of Glycopolymers with Controlled Branching;** Sahar Sallam¹; Chrys Wesdemiotis¹; Liao Walter²; Andrea Kasko²; ¹*The University of Akron, Akron, OH*; ²*University of California, Los Angeles, CA*

- ThP 071 **Matrix Assisted Laser Desorption Ionization Mass Spectrometry of Plasma Polymerized Styrene**; Lee Elliott; , *Carbondale, Illinois*
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- ThP 074 **Rapid Identification of Nylons by Temperature-Rising Direct Analysis in Real Time Mass Spectrometry (TR-DART-MS)**; Chikako Takeji¹; Kazumasa Kinoshita¹; Takao Nishiguchi¹; Haruo Shimada²; Katsuyuki Maeno²; Yasuo Shida³; ¹*BioChromato, Inc., Fujisawa, Japan*; ²*Shiseido Research Center, Yokohama, Japan*; ³*University of Yamanashi, Kofu, Japan*
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- ThP 115 **Characterization of Gas-Phase Tungsten Dithiolene Anions**; Taylor Souza; Partha Basu; Michael J. Van Stipdonk; *Duquesne University, Pittsburgh, PA*
- ThP 116 **ESI-MS/MS and DFT Computations on Negative and Positive Ions from 4-aminoalkyl-3-hydroxy-1,2,5-Oxadiazoles Featuring a Novel Heterocyclic Biomimetic of the Carboxylic Group**; J. Stuart Grossert¹; Donatella Boschi²; Marco Lolli²; Robert White¹; ¹*Dalhousie University, Department of Chemistry, Halifax, Canada*; ²*Departimento del Farmaco, Universita di Torino, Torino, Italy*
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- ThP 123 **Travelling Wave Ion Mobility Enhanced Separation of Poly-Halogenated Dioxins and Furans in Controlled Burn Samples**; Kari Organtini¹; Lauren Mullin^{2,3}; Adam Ladak³; ¹*The Pennsylvania State University, State College, PA*; ²*MTM Research Centre Örebro University, Örebro, Sweden*; ³*Waters Corporation, Milford, MA*
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- ThP 446 **MASH Suite Pro: A Comprehensive Tool for Top-down Proteomics;** Wenxuan Cai¹; Huseyin Guner¹; Santosh Valeja¹; Ying Peng¹; Xiaowen Liu²; Ying Ge¹; ¹*UW-Madison, Madison, WI*; ²*Indiana University-Purdue University, Indianapolis, IN*
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- ThP 450 **TopPIC: A Software Tool for Top-Down Mass Spectrometry-Based Proteoform Identification and Characterization;** Qiang Kou¹; Likun Xun¹; Xiaowen Liu^{1,2}; ¹*Indiana University Purdue University Indianapolis, Indianapolis, IN*; ²*Indiana University School of Medicine, Indianapolis, IN*
- ThP 451 **Large Scale Quantitation of Stable Isotope Labeled Proteomes Using Retention and Drift Time Profiling;** Andrew Collins¹; Antony McCabe¹; Ian Morns³; Johannes PC Vissers²; Andrew R Jones¹; ¹*Institute of Integrative Biology, University of Liverpool, UK*; ²*Waters Corporation, Manchester, UK*; ³*Nonlinear Dynamics Limited, Newcastle upon Tyne, UK*
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- ThP 457 **Peptide Centric Functional Enrichment for Complex Proteomics Datasets;** Vikram Mitra¹; David Britton¹; Vadim Farztdinov¹; Alberto Quaglia²; Yoh Zen³; Claire Russell¹; Malcolm Ward¹; Emma Lahert¹; Ian Pike¹; ¹*Proteome Sciences plc, Cobham, UK*; ²*Institute of Liver Studies, King's College Hospital, London, UK*; ³*University Graduate School of Medicine, Kobe, JP*
- ThP 458 **Antibody Identification from a Polyclonal Mixture using Immunoproteogenomics;** Stefano Bonissone¹; Yana Safonova^{2,3}; Eugene Kurpilyansky^{2,3}; Ekaterina Starostina²; Alla Lapidus^{2,3}; Wendy Sandoval⁴; Jennie Lill⁴; Pavel Pevzner¹; ¹*University of California at San Diego, San Diego, CA*; ²*St. Petersburg Academic University, St Petersburg, Russia*; ³*St. Petersburg State University, St. Petersburg, Russia*; ⁴*Genentech, South San Francisco, CA*
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- ThP 460 **Comprehensive Database Search Strategy for Proteogenomics**; [Harsha P. Gunawardena](#)¹; John Wrobel¹; Jonathon O'Brien¹; Ling Xie¹; Kelly Ruggles²; David Fenyo²; Sherri Davies³; Li Ding³; Reid Townsend³; Matthew Ellis⁴; Bhajat F. Qaqish¹; Xian Chen¹; ¹University of North Carolina at Chapel Hill, Chapel Hill, NC; ²NYU Langone Medical Center, New York, NY; ³Washington University School of Medicine, St. Louis, Missouri; ⁴Baylor College of Medicine, Houston, TX
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- ThP 463 **Statistical and Pathway Analysis of Protein Data**; [Stephen Madden](#)¹; Joseph C. Roark¹; Vadiraja Bhat¹; Carolina B. Livi¹; Christine A. Miller¹; Mona Al-Gizawiy²; Kathleen Schmainda²; Shama P. Mirza²; ¹Agilent Technologies, Inc., Santa Clara, CA; ²Medical College of Wisconsin, Milwaukee, WI
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- ThP 476 **Quantitative Cross-Linking for Conformational Changes Analysis**; [Luana Oliveira Dos Santos](#)¹; Marcelo Yudi Icimoto²; Alyne Marem Silva Barbosa²; Leandro Mantovani Castro³; Emer Suavinho Ferro³; Vitor Oliveira²; Fabio C. Gozzo¹; ¹University of Campinas, Campinas, SP; ²Federal University of São Paulo, São Paulo, SP; ³University of São Paulo, São Paulo, SP
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- Beijing, Beijing, China; ³Zhejiang University School of Medicine, Hangzhou, China
- ThP 481 **Structural Study of Thyroid Hormone Receptor Complexes using Chemical Crosslinking Mass Spectrometry;** Adriana Pianaro¹; Tábata Renée Doratioto²; Juliana Fattori²; Tiago Santana Balbuena³; Ana Carolina Migliorini Figueira²; Fábio César Gozzo¹; ¹Instituto de Química - UNICAMP, Campinas, Brazil; ²Laboratório Nacional de Biotecnologia, CNPEM, Campinas, São Paulo/ Brazil; ³Departamento de Tecnologia, UNESP, Jaboticabal, São Paulo/ Brazil
- ThP 482 **Structural Analyses of the Oligomerization Mechanism of Amyloid β Peptides;** Ayumi Tanaka¹; Shigeto Iwamoto¹; Takashi Saito²; Hitomi Yamaguchi¹; Sosuke Yoshinaga¹; Yoshihiko Takinami³; Sawyen Ow⁴; Jouji Seta³; Toshiyuki Kohno⁵; Takaomi C. Saido²; Hiroaki Terasawa¹; ¹Faculty of Life Sciences, Kumamoto University, Kumamoto, Japan; ²RIKEN Brain Science Institute, Wako, Saitama, Japan; ³Division of Application, Bruker Daltonics K. K., Yokohama, Japan; ⁴Application, Bruker Sdn. Bhd., Selangor, Malaysia; ⁵Kitasato University School of Medicine, Sagami-hara, Japan
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- ThP 492 **Carbenes as New Reagents for Fast Photochemical Oxidation of Proteins;** Bojie Zhang; Don L. Rempel; Ben Niu; Manolo D. Plasencia; Michael L. Gross; *Washington University, St. Louis, MO*
- ThP 493 **Mapping the Solvent Exposed Lysine Residues of Native Apolipoprotein B-100;** Parisa Pirani¹; Ujwal Patil¹; Angela Ellender¹; Casey Grimm²; Yang Cai³; Matthew Tarr¹; ¹University of New Orleans, New Orleans, LA; ²Southern Regional Research Center, New Orleans, LA; ³The Research Institute for Children, New Orleans, New Orleans, LA
- ThP 494 **Cyclization of an Amine-reactive Tag as a Tool to Probe Local Chemical Environments of Proteins;** Jake Rosenberg; Jennifer Brodbelt; *The University of Texas, Austin, TX*
- ThP 495 **Fast Photochemical Oxidation of Proteins (FPOP) and Nativespray/ECD Probe the Structural Differences Between Wild-type and Mutant SOD1;** Ben Niu¹; Hao Zhang¹; Weidong Cui¹; Jill Zitzewitz²; Sagar Kathuria²; C. Robert Matthews²; Michael L. Gross¹; ¹Washington University, Saint Louis, MO; ²University of Massachusetts Medical School, Worcester, MA
- ThP 496 **Fast Photochemical Oxidation of Proteins (FPOP) for Quantitative Residue-level Analysis of Conformational Changes in Amyloid Beta Aggregation;** Ke Li; Ying Zhang; Don Rempel; Michael Gross; *Washington University, St. Louis, MO*
- ThP 497 **Probing the Conformational Change of Cyanobacterial Orange Carotenoid Protein Photoactivation Using FPOP;** Junqing Zhang; *Washington University in St. Louis, St. Louis, MO*
- ThP 498 **Epitope Mapping of Human Interleukin 23 Interacting with Antibody by Fast Photochemical Oxidation of Proteins;** Jing Li¹; Guodong Chen²; Richard Huang²; Hui Wei²; Adrienne Tymiak²; Michael Gross¹; ¹Washington University in St. Louis, St. Louis, MO; ²Bristol-Myers Squibb, Princeton, NJ
- ThP 499 **Development of a Micro-Flow System for Single Cell Protein Footprinting Analysis;** Aimee Rinas; Lisa Jones; *Indiana University Purdue University Indianapolis, Indianapolis, IN*
- ThP 500 **Covalent Labeling Techniques for Characterizing Higher Order Structure of Monoclonal Antibodies;** Parminder Kaur^{1,2}; Janna Kiselar¹; Wuxian Shi¹; Sichun Yang¹; Mark Chance^{1,2}; ¹Case Western Reserve Univ, Cleveland, OH; ²NeoProteomics, Inc., Cleveland, OH
- ThP 501 **Finding and Identifying Large and Extensively Modified Peptides in MS Data from Footprinting Experiments;** Henry W. Rohrs; Manolo Plasencia; Jing Li; Ke Li; Michael Gross; *Washington University, St Louis, MO*
- ThP 502 **Host-pathogen Interactome Response to Type III Secretion;** Arti Navare; Devin Schwappe; Benjamin Staudinger; Pradeep Singh; James Bruce; *University of Washington, Seattle, WA*
- ThP 503 **Standardization of Hydroxyl Radical Protein Footprinting Data using a Radical Dosimeter in High Resolution Footprinting of Lysozyme;** Boer Xie; *Complex Carbohydrate Research Center, UGA, Athens, GA*
- ThP 504 **CXCL4 dimer-dimer Interface Characterization by High Resolution Hydroxyl Radical Protein Footprinting;** Zixuan Li¹; Tracy Handel²; Joshua Sharp¹; ¹University of Georgia, Athens, GA; ²University of California San Diego, San Diego, CA
- ThP 505 **Ultra-fast Photolytic Protein Labelling under Solid-Phase Conditions;** Daniel Ziemianowicz; David Schriemer; *University of Calgary, Calgary, Canada*


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- ThP 506 **Structural and Functional Characterization of Pathogenic GPI-specific Monoclonal Antibodies α GPI11H3 and α GPI46H9**; Kwabena Frimpong-Manso Oponi¹; Samuel Solomon²; Yelena Yefremova¹; Cornelia Koy¹; Harald Illges^{2,3}; Michael O. Glocker¹; ¹Proteome Center Rostock, Rostock, Germany; ²University of Konstanz, Konstanz, Germany; ³University of Applied Sciences, Bonn, Germany
- ThP 507 **Measurement of Cysteine -linked ADCs under Native Conditions using an Orbitrap Mass Analyzer**; Jing Li¹; Shujun Yang²; ¹Thermo Fisher Scientific, Shanghai, China; ²NewBio Therapeutics, Inc, Shanghai, China
- ThP 508 **Analysis of non-Deglycosylated Antibody-Drug-Conjugates by TripleTOF® High Resolution Quadrupole-Time-Of-Flight Instrument and Effective Reconstruction Software**; Milla-Riina Neffling¹; Bruno Genet²; David Bugnaze²; Eric Lacassie²; Justin Blethrow³; Eric Johansen³; ¹SCIEX, Warrington, UK; ²Sanofi-Vitry Biologics SCP/Analytics, Vitry-Sur-Seine, France; ³SCIEX, Red Wood Shores, CA
- ThP 509 **Rapid Method for Monitoring Monoclonal Antibody (mAb) Production in Biotechnological Processes using Quantitative MALDI-TOF-MS**; Robert Steinhoff¹; Jasmin Krimer¹; Martin Pabst²; Renato Zenobi¹; ¹ETH Zurich, Zurich, Switzerland; ²Polytherics, Cambridge, UK
- ThP 510 **Quantitative Analysis of Post Translation Modification of Protein Therapeutics at a Subunit Level by Spectral Deconvolution**; Ming Gu¹; Kadir Ilker Sen²; Yongdong Wang¹; Darryl Davis²; ¹Cerno Bioscience, Norwalk, CT; ²Janssen Pharmaceutical Companies of Johnson & Johnson, Springhouse, PA
- ThP 511 **High Sensitivity Native Mass Spectrometry Characterization of Antibody Fluorescent Conjugates (AFC)**; Caroline S. Chu¹; Gregory Staples¹; Andy Gieschen²; Ning Tang¹; ¹Agilent Technologies, Santa Clara, CA; ²Agilent Technologies, La Jolla, CA
- ThP 512 **Combining Top Down and Bottom Up MALDI TOF/TOF Data in the de novo Sequencing of Monoclonal Antibodies**; Andy Mahan¹; Yazen Jmeian²; Darryl Davis¹; ¹Johnson and Johnson, Spring House, PA; ²Janssen Research & Development, Radnor, PA
- ThP 513 **Application of Capillary Electrophoresis Coupled to Quadrupole Time-of-Flight Mass Spectrometry for the Analysis of Immunoconjugates**; Suresh Babu CV¹; Anne Basler²; Sina Bunzendahl²; Rainer Kneuer²; ¹Agilent Technologies, Bangalore, India; ²Novartis Institutes for Biomed. Research, Basel, Switzerland
- ThP 514 **Enhancing LC/MS Sensitivity and Spectral Quality of Reduced Antibodies and Antibody Drug Conjugates**; Wei Ding; Difei Qiu; Scott Miller; Bristol-Myers Squibb, New Brunswick, NJ
- ThP 515 **Mass Spectrometric Investigation of Maleimide Linker Hydrolysis in Antibody-drug Conjugates**; Ling Xu¹; Laura Packer¹; Yue Zhang²; Shaoxia Yu¹; Jing-Tao Wu¹; Mark Qian¹; ¹Takeda Pharmaceutical International Inc., Cambridge, MA; ²BioAnalytix Inc, Cambridge, MA
- ThP 516 **Collision Induced Unfolding of Intact Antibodies, Biotherapeutics and Biosimilars: Rapid Characterization of Disulfide Bonding Patterns and Structures**; Yuwei Tian; Linjie Han; Adam Buckner; Brandon Ruotolo; Department of Chemistry, University of Michigan, Ann Arbor, MI
- ThP 517 **Peptide Mapping of Antibody Drug Conjugate using CE-ESI-MS**; Suresh Babu Cv; Ravindra Gudihal; Palaniswamy Meenakshi-SundaR M; Nilanjan Guha; Sudha Rajagopalan; Agilent Technologies, Bangalore, India
- ThP 518 **Analysis of Herceptin Oxidation Variants Using a Supermacro Porous Reverse Phase Column Coupled with an Orbitrap Mass Spectrometer**; Shanhua Lin¹; Terry Zhang²; Hongxia (Jessica) Wang²; Jonathan L. Josephs²; Xiaodong Liu¹; ¹Thermo Fisher Scientific, Sunnyvale, CA; ²Thermo Fisher Scientific, San Jose, CA
- ThP 519 **Comprehensive Analysis of Intact Antibody Drug Conjugates using an Integrated Microfluidic HPLC-Chip MS Workflows**; Caroline S. Chu¹; Andy Gieschen²; M Sundaram Palaniswamy³; Ning Tang¹; ¹Agilent Technologies, Santa Clara, CA; ²Agilent Technologies, La Jolla, CA; ³Agilent Technologies Inc, Bangalore, India
- ThP 520 **Drug-to-Antibody Ratio Characterization of Antibody Drug Conjugate by Ion Mobility Mass Spectrometry**; Richard Huang¹; David Passmore²; Vangipuram Rangan²; Shrikant Deshpande²; Adrienne Tymiak¹; Guodong Chen¹; ¹Bristol-Myers Squibb, Princeton, NJ; ²Bristol-Myers Squibb, Redwood City, CA
- ThP 521 **Conformational Epitope Mapping of Angiopoietin-2 (ANG-2) Specific Monoclonal Antibodies (mAb) by Partial Trypsin Digestion Followed by nanoLC-MRM**; Lei Wang¹; Tetsuo Sekino²; Kenji Abe²; Mark Matijevic¹; Jesse Chow¹; Yoshiya Oda¹; ¹Eisai Inc, Andover, MA; ²EIDIA Co., Ltd., Inashiki, Japan
- ThP 522 **Overcoming Method-Related Challenges During Antibody Drug Conjugate Characterization by LC/MS**; Jacquelynn Smith¹; Paul Brown¹; Cecily Swabowski¹; Jason Rouse²; James Carroll¹; Olga Friese¹; ¹Biotherapeutics Pharm. Sci., Pfizer Inc., St. Louis, MO; ²Biotherapeutics Pharm. Sci., Pfizer Inc., Andover, MO
- ThP 523 **Characterization of Trisulfide Modifications of Recombinant Antibodies by Intact Mass Measurement and Non-Reduced Peptide Mapping**; Bianca Grünwalder; Vincent Larraillet; Oliver Popp; Annette N.D. Scharf; Maximiliane Hilger; pRED, Roche Innovation Center, Penzberg, Germany
- ThP 524 **An Optimized Approach for the Sensitive Detection of Sequence Variants in Biotherapeutic Proteins**; Paul W. Brown¹; James Carroll¹; Jason Rouse²; ¹Pfizer, St. Louis, MO; ²Pfizer, Andover, MA
- ThP 525 **Strategy for the Quantification of a Paclitaxel conjugated ADC (DAR \geq 1) in Rat Plasma by LC-HRMS**; Jean-Nicholas Mess; Fabio Garofolo; Algorithme Pharma Inc., Laval, Canada
- ThP 526 **Separation and Characterization of Intact mAb Conjugate Charge Variants via Microfluidic CE-ESI with Online MS Analysis**; Erin A. Redman¹; J. Scott Mellors²; J. Michael Ramsey¹; ¹University of North Carolina at Chapel Hill, Chapel Hill, NC; ²908 Devices Inc., Boston, MA
- ThP 527 **Quantitation of Cytotoxic Free Drug Released From an ADC into Conditioned Cell Culture Media**; Maria Christina Malinao; Josh Snyder; Julien Dugal-Tessier; Christopher Kemball; Min Wu; Brian Mendelsohn; Agensys, Inc., Santa Monica, CA
- ThP 528 **Analysis of Therapeutic Proteins Using Hydrophobic Interaction / Reversed-phase 2D-LC/MS with Multiple Heart-cutting**; Gregory Staples; Hongfeng Yin; Kevin Killeen; Agilent Technologies, Santa Clara, CA
- ThP 529 **Use of Signature Ions with Accurate Mass and Collision Induced Dissociation to Unambiguously Assign Toxin Locations for Antibody Drug Conjugates**; Michael Bacica¹; Aaron Wrobleski²; Jon Fitchett¹; Bryan Jones¹; ¹Lilly Biotech Center-San Diego, San Diego, CA; ²LRL DCRT, Indianapolis, IN
- ThP 530 **A Comprehensive Quantitative Study of Monoclonal Antibody (mAb) by Q-TOF/MS and Ion Mobility Q-TOF/MS**; Ning Tang; David L Wong; Agilent Technologies, Santa Clara, CA

- ThP 531 **Rapid Detection of Deamidation in Monoclonal Antibodies using Ultrahigh-Resolution QTOF Mass Spectrometry**; Wolfgang Jabs¹; Waltraud Evers¹; Anja Wiechmann¹; Jason Wood²; Guillaume Tremintin³; Detlev Suckau¹; Keith Johnson⁴; Heather DeGruttola⁴; Lisa Marzilli⁴; Jason Rouse⁴; ¹Bruker Daltonik GmbH, Bremen, Germany; ²Bruker Daltonics Inc, Billerica, MA; ³Bruker Daltonics Inc, Fremont, CA; ⁴Pfizer Inc, Andover, MA
- ThP 532 **Upstream Quality Control of Therapeutic Antibodies using Automated IdeS Digestion and Subunit Separation in Combination with Ultrahigh-Resolution QTOF Analysis**; Martin Hedström¹; Fredrik Olsson²; Dag Erlandsson¹; Anja Wiechmann³; Catherine Evans⁴; Guillaume Tremintin⁵; Jason Wood⁶; Detlev Suckau³; Wolfgang Jabs³; ¹CapSenze HB, Lund, Sweden; ²Genovis AB, Lund, Sweden; ³Bruker Daltonik GmbH, Bremen, Germany; ⁴Bruker Daltonics Ltd, Coventry, UK; ⁵Bruker Daltonics Inc, Fremont, CA; ⁶Bruker Daltonics Inc, Billerica, MA
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- ThP 534 **Comprehensive Profiling of Protein Lysine Acetylation in Human Esophageal Carcinoma Cell SHEEC**; Kai Zhang¹; Shanshan Tian¹; Guijin Zhai¹; Zhenchang Guo¹; Zhongyi Cheng²; ¹Tianjin Medical University, Tianjin, China; ²PTM Biolabs, Inc, Hangzhou, China
- ThP 535 **MS-based Quantitative Proteomics using SILAC Mouse Reveals the Rhythmicity of the Circadian PTMome in the Liver**; Loïc Dayon¹; Daniel Mauvoisin²; Antonio Núñez Galindo¹; Jingkui Wang³; Félix Naef³; Martin Kussmann¹; Frédéric Gachon²; ¹NIHS, Molecular Biomarkers, Lausanne, CH; ²NIHS, Circadian Rhythm Group, Lausanne, CH; ³Institute of Bioengineering, EPFL, Lausanne, CH
- ThP 536 **Proteofom Dynamics in the CNS: 3D Spatial Mapping of Myelin Basic Protein by Top Down**; Daniel Plymire; John Corbett; Steven Patrie; University of Texas Southwestern Medical Center, Dallas, TX
- ThP 537 **Identification of Liver Proteins Targeted by Reactive Metabolites using LC-MS/MS**; Makan Golizeh; André Leblanc; Lekha Sleno; UQAM, Montreal, Canada
- ThP 538 **High Sensitivity LC-MS and LC-MS/MS Peptide Mapping Method for Characterization of Post-Translational Modifications in Therapeutic Antibodies**; Jason X. Tang; Yuping Zhou; Eli Lilly & Company, Indianapolis, IN
- ThP 539 **Novel Activity Based Protein Profiling Probe Identifies Putative Denitrase in Microglia**; Harris Bell-Temin^{1,2}; Jennifer Guergues¹; Annie Carpenter¹; Christina Carlson¹; Stanley M. Stevens Jr. ¹; ¹University of South Florida, Tampa, FL; ²University of Pittsburgh, Pittsburgh, PA
- ThP 540 **Systematic Identification of the Lysine Acetylation in Rice (*Oryza sativa*)**; Yehui Xiong²; Zhongyi Cheng¹; Wende Liu²; Guo-Liang Wang³; ¹PTM Biolabs, Inc, Hangzhou, China; ²Institute of Plant Protection, Chinese Academy of, Beijing, CN; ³Ohio State University, Columbus, OH
- ThP 541 **A Chemical Proteomics Approach for Global Analysis of Lysine Mono-Methylation**; Zhixiang Wu¹; Zhongyi Cheng²; Mingwei Sun¹; Xuelian Wan¹; Ping Liu¹; Tieming He²; Minjia Tan¹; Yingming Zhao^{1,3}; ¹Shanghai Institute of Materia Medica, Shanghai, China; ²PTM BioLab (Hangzhou) Co. Ltd, Hangzhou, China; ³Ben May Department of Cancer Research, The University of Chicago, Chicago, IL
- ThP 542 **N-terminome Analysis of the Human Mitochondrial Proteome**; Alvaro Sebastian Vaca Jacome¹; Thierry Rabilloud²; Christine Schaeffer-Reiss¹; Magali Rompais¹; Daniel Ayoub¹; Lydie Lane^{3,4}; Amos Bairoch^{3,4}; Alain Van Dorsselaer¹; Christine Carapito¹; ¹IPHC, UdS, CNRS, UMR 7178, Strasbourg, France; ²Laboratoire de Chimie et Biologie des Métaux (CEA), Grenoble, France; ³CALIPHO Group Swiss Institute of Bioinformatics, Geneva, Switzerland; ⁴Faculty of medicine, Geneva, Switzerland
- ThP 543 **Identification of Sites of Ubiquitination and Sumoylation on Proteins Involved in the Maintenance of Genome Integrity**; Matthew Schellenberg; Katina Johnson; Andrea Adams; R. Scott Williams; Jason Williams; *NIEHS, Rtp, NC*
- ThP 544 **Identifying Aberrant PTMs of Mutated Tumor Suppressor p53 by Advanced Mass Spectrometry for Unraveling Upstream Signaling for Inactivation of p53**; Houjiang Zhou¹; Kehan Song²; Frank McCaughan¹; Trevor Littlewood¹; Kathryn Lilley¹; Gerard Evan¹; ¹Department of Biochemistry, University of Cambridge, Cambridge, UK; ²School of Basic Medical, Fudan University, Shanghai, China
- ThP 545 **The Effect of Histone Modifications on Peptide Ionization by ESI, and Fragmentation by ECD and CAD**; Barbara Storch; Kathrin Breuker; *University of Innsbruck, Innsbruck, Austria*
- ThP 546 **Global Profiling of Protein Lysine Malonylation in *Escherichia coli***; Litong Nie¹; Jun Zhu²; Lili Qian¹; Yingming Zhao^{1,3}; Zhongyi Cheng²; Minjia Tan¹; ¹Shanghai Institute of Materia Medica, Shanghai, China; ²PTM Biolab (Hangzhou) Co. Ltd, Hangzhou, China; ³Ben May Department for Cancer Research, the University of Chicago, Chicago, IL
- ThP 547 **Metabolite-Driven Protein Modification: Lysine Acylations in Syntrophic Bacteria Elucidate Substrate Metabolism**; Hong Hanh Nguyen¹; Phuong Nguyen¹; Robert Gunsalus¹; Michael McLnerney²; Joseph Loo¹; Rachel Ogorzalek Loo¹; ¹University of California, Los Angeles, Los Angeles, CA; ²University of Oklahoma, Norman, OK
- ThP 548 **Identification and Characterizations of Post-translational Modifications of RNF168, a Protein Involved in DNA Damage Response**; Zi Wang; Yinsheng Wang; *University of California, Riverside, Riverside, CA*
- ThP 549 **Post-Translational Modification by the Type III Effector HopZ3 Modulates Tomato Host Immunity by Acetylation of Bacterial and Plant Proteins**; Andrew Manning; Jiyoung Lee; Don Wolfgeher; Stephen Kron; Jean Greenberg; *University of Chicago, Chicago, IL*
- ThP 550 **Site-Specific Reactivity of Nonenzymatic Lysine Acetylation**; Josue Baeza; Michael Smallegan; John Denu; *University of Wisconsin-Madison, Madison, WI*
- ThP 551 **Identification of Specific Protein-Protein Interactions via Detecting Post-Translational Modifications**; I-Hsuan Chen; Meng-Chieh Chen; Chang-Deng Hu; Weiguo Andy Tao; *Purdue University, West Lafayette, IN*
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- ThP 553 **Bacterial Protein Acetylation in Response to Carbon Overflow: Quantifying Changes in Acetylation Status of *Escherichia coli* Metabolic Networks by Label-Free Proteomics**; Birgit Schilling¹; David Christensen²; Dylan J. Sorensen¹; Alexandria K. Sahu¹; Robert Davis²; Linda I. Hu³; Arti Walker-Peddakotla²; Bozena Zemaitis²; Alan J. Wolfe²; Bradford W. Gibson¹; ¹Buck Institute for Research on Aging, Novato, CA; ²Loyola University Chicago, Maywood, IL; ³University of Wisconsin, Madison, WI
- ThP 554 **Validation of Novel Plasmodium falciparum Histone Modifications using Linear Ion-Trap Mass Spectrometers**; Anita Saraf¹; Serena Cervantes²; Zhihui

- Wen¹; Michael Washburn¹; Karine G LeRoch²; Laurens Florens¹; ¹*Stowers Institute for Medical Research, Kansas City, MO*; ²*University of California Riverside, Riverside, CA*
- ThP 555 **Addressing dynamic range limitations in the multiplex approach to identifying regulatory glutathione modifications of protein cysteines in mouse heart;** Jessica B Behring¹; Chunxiang Yao¹; Xiaoyan Yin²; Di Shao¹; Yosuke Watanabe¹; Stephen A Whelan¹; Xiang Ray Weng¹; Wilson S Colucci¹; Catherine E Costello¹; Richard A Cohen¹; Reiko Matsui¹; Mark E McComb¹; Markus M Bachschmid¹; ¹*Boston University School of Medicine, Boston, Ma*; ²*BUMC & NHLBI Framingham Heart Study, Framingham, MA*
- ThP 556 **Effect of Exposure to Diacetyl in Mice: A Proteomic and Metabolomic Approach;** Leticia Dias Lima Jedlicka; Aleksandro Martins Balbino; Giuseppe Bruno Neto; Richard Gama Landgraf; Liliam Fernandes; Alexandre Keiji Tashima; Nilson Antonio Assunção; *UNIFESP, São Paulo, Brasil*
- ThP 557 **A Mass Spectrometry Cleavable Approach for the Identification and Differentiation of Farnesylated/ Geranylgeranylated Peptides;** Ruchika Bhawal; Shahinuzzaman A.d.a; Saiful Chowdhury; *University of Texas at Arlington, Arlington, TX*
- ThP 558 **Localization and Quantification of Gamma-Carboxyglutamic Acid Residues in Proteins by Deuterium Exchange Decarboxylation (DEXDEC);** Jonas Borch¹; Morten Rasmussen¹; Thomas Nylandsted Krogh²; ¹*University of Southern Denmark, Odense M, Denmark*; ²*Novo Nordisk A/S, Måløv, Denmark*
- ThP 559 **Uncovering Novel Redox Regulated Cysteines in the Mitochondrial Proteome Governed by Distinct Sites of Reactive Oxygen Species Production;** Casey Quinlan¹; Matthew Egan²; Shin-Cheng Tzeng²; Bradford Gibson³; Martin Brand³; Jason Held²; ¹*Oncology Research Unit, Pfizer Inc, La Jolla, CA*; ²*Washington University Medical School, Saint Louis, MO*; ³*Buck Institute for Research on Aging, Novato, CA*
- ThP 560 **Cracking Histone H4's PTM Code by Middle-Down FT-ICR MS/MS analysis;** Tingting Jiang^{1,2}; Alan A. Shomo^{1,2}; Nathan K. Kaiser²; Christopher L. Hendrickson²; Alan G. Marshall^{1,2}; Nicolas L. Young²; ¹*Florida State University, Tallahassee, FL*; ²*National High Magnetic Field Laboratory, Tallahassee, FL*
- ThP 561 **LC-MS/MS Analysis of S-Palmitoyl Proteins from Biological Samples Reveals Potential Limitations of the Metabolic Labeling Approach;** Yuhuan Ji; Minjing Liu; Markus M. Bachschmid; Catherine E. Costello; Cheng Lin; *Boston University School of Medicine, Boston, MA*
- ThP 562 **Site-Specific Identification of Ethanol-Induced Histone Protein Nitration Using Mass Spectrometry;** Crystina L. Kriss; Ashley Culver-Cochran; Dale Chaput; Stanley M. Stevens, Jr; *University of South Florida, Tampa, FL*
- ThP 563 **Mass Spectrometric Fragmentation Studies on Peptides Containing Chemically Modified Arginine Residues;** Maheshika Wanigasekara; Ruchika Bhawal; Saiful Chowdhury; *University of Texas at Arlington, Arlington, TX*
- ThP 564 **Analysis of Chlorination, Bromination, Nitration, Nitrosylation, and Oxidation in Hemoglobin of Diabetes Mellitus Patients by Nanoflow LC-NSI/MS/MS;** Ya-Fen Yang¹; Pin-Fan Chen²; Hauh-Jyun Candy Chen¹; ¹*National Chung Cheng Univ., Ming-Hsiung, Chia-Yi, Taiwan*; ²*Buddhist Dalin Tzu Chi General Hospital, Dalin, Chia-Yi, Taiwan*
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- ThP 566 **Global-scale Analysis of Protein Nucleocytoplasmic Trafficking in Rat Hepatocytes after Ethanol Exposure;** Shikha Mahajan; Crystina L. Kriss; Stanley M. Stevens, Jr; *University of South Florida, Tampa, FL*
- ThP 567 **Comparison and Validation of iTRAQ, emPAI, and Intensity-Based, Label-Free Quantification for Expression Proteomics using an Ultrahigh-Resolution QqTOF;** Adam Dowle¹; Julie Wilson²; Stephanie Kaspar³; Rachel Bates¹; David Ashford¹; Jerry Thomas¹; ¹*Technology Facility, Dept. Biology, Univ. of York, York, UK*; ²*Depts. Mathematics and Chemistry, Univ. of York, York, UK*; ³*Bruker Daltonik GmbH, Bremen, Germany*
- ThP 568 **Quantitative Proteomic Analysis of Proteins on Cerebral Ischemia Injury Mice by Deuterium Isobaric Amine Reactive Tagging (DiART) Mass Spectrometry;** Hailong Song^{1,3}; Hui Zhou^{1,3}; Zhe Qu^{1,3}; Dennis Y Chuang^{1,2}; Jiankun Cui^{1,3}; Agnes Simonyi^{1,2}; Shanyan Chen^{1,3}; Jilong Li^{3,5}; Jianlin Cheng^{3,5}; Michael Greenleaf^{3,6}; Shuiwei Li⁷; Dennis B Lubahn^{3,4}; Grace Y Sun^{2,3}; Zezong Gu^{1,3}; ¹*Department of Pathology & Anatomical Sciences, Columbia, MO*; ²*Department of Biochemistry, Columbia, MO*; ³*Center for Translational Neuroscience, Columbia, MO*; ⁴*Center for Botanical Interaction Studies, Columbia, MO*; ⁵*Computer Science Informatics Institute, Columbia, MO*; ⁶*Department of Chemistry, Columbia, MO*; ⁷*Department of Chemistry and Biochemistry, Maryland, MD*
- ThP 569 **Quantitative Multiplexed Proteomic and Phosphoproteomic Profiling Reveals Nicotine and α -bungarotoxin-induced Alterations in Pancreatic Stellate Cells;** Joao Paulo; Aleksandr Gaun; Steven Gygi; *Harvard Medical School, Boston, MA*
- ThP 570 **Statistical Assessment of HCD-MS2, Single- and Multi-notch MS3 Methods for Improved Quantitation Accuracy of Mulberry Proteome under Salt/Drought Stress;** Yong Yang¹; Yan Liu²; Elizabeth Anderson³; Robert Sherwood³; Theodore Thannhauser¹; Sheng Zhang³; ¹*Holley Center for Agriculture & Health, USDA/ARS, Ithaca, NY*; ²*Zhejiang Academic of Agricultural Science, Hangzhou, P.R. of China*; ³*Proteomics & Mass Spec Core, Cornell University, Ithaca, NY*
- ThP 571 **Altered HDL Proteomics in Patients with NASH: ²H Metabolic Labeling and Quantitative Proteomics Approach;** Ling Li¹; Jaividhya Dasarathy²; Srinivasan Dasarathy¹; Jonathan Smith¹; Arthur McCullough¹; Belinda Willard¹; Takhar Kasumov¹; ¹*Cleveland Clinic, Cleveland, OH*; ²*MetroHealth Medical Center, Cleveland, OH*
- ThP 572 **Early Detection of the Mechanism of Action for Toxins by High-throughput Proteomics;** Ziad Sahab; Camille Lombard; Lida Parvin; Peter Nemes; Akos Vertes; George Washington University, Washington, DC
- ThP 573 **A Proteomic Investigation of the miR-23a/27a/24-2 Cluster;** Katelyn R. Ludwig¹; Kerry M. Scott¹; Richard Dahl²; Amanda B. Hummon¹; ¹*University of Notre Dame, Notre Dame, IN*; ²*Indiana University School of Medicine, South Bend, IN*
- ThP 574 **Site-specific Identification of Lys Acetylation Stoichiometry in Mammalian Cells;** Tong Zhou; Ying-hua Chung; Yue Chen; *University of Minnesota at Twin Cities, Minneapolis, MN*
- ThP 575 **Quantitative Proteomics and Glycoproteomics of Membrane-Enriched Proteins from Normal and Tumour-Promoting Human Mesenchymal Stromal/Stem Cells for Candidate Biomarkers of Sarcoma;** Jessie R. Lavoie¹; Jeremy P. Kunke¹; Julian Saba²; Rosa Viner²; Tara Schroeder³; Carole Westwood¹; Gauri Muradia¹; Rafael

- ThP 576 **Characterization of Chronological Aging by iTRAQ-Based Quantitative Proteomics in *Saccharomyces cerevisiae***; Aline A Brasil; Fabio CS Nogueira; Gilberto B Domont; Marcos D Pereira; *Univ Federal Do Rio De Janeiro, Rio De Janeiro, Brazil*
- ThP 577 **Quantitative Phosphoproteomics Identifies a Role for PP6c in the Regulation of Chromosome Condensation**; Scott Rusin^{1,2}; Kate Schlosser³; Arminja Kettenbach^{1,2}; ¹Department of Biochemistry, Hanover, NH; ²Geisel School of Medicine at Dartmouth, Hanover, NH; ³Norris Cotton Cancer Center, Lebanon, NH
- ThP 578 **Novel Insights into Yeast Biology Revealed by Protein Expression Profiling of Multiple Knockout Strains**; Marta Isasa; Christopher M Rose; Suzanne Elsasser; Daniel J Finley; Steven P Gygi; *Harvard Medical School, Boston, MA*
- ThP 579 **Lysine Malonylation Plays an Important Role in Mitochondrial Function and Fatty Acid Oxidation**; Gozde Colak¹; Olga Pougovkina²; Lunzhi Dai¹; Minjia Tan³; Heleen te Brinke²; He Huang¹; Zhongyi Cheng⁴; Jeongsoon Park⁵; Xuelian Wan³; Xiaojing Liu⁶; Wyatt W. Yue⁷; Ronald J. A. Wanders²; Jason W. Locasale⁶; David B. Lombard²; Vincent C. J. de Boer²; Yingming Zhao¹; ¹The University of Chicago, Chicago, IL; ²University of Amsterdam, Amsterdam, The Netherlands; ³Shanghai Institute of Materia Medica, Shanghai, P. R. China; ⁴Jingjie PTM Biolabs, Hangzhou, P. R. China; ⁵University of Michigan, Ann Arbor, MI; ⁶Cornell University, Ithaca, NY; ⁷University of Oxford, Oxford, UK
- ThP 580 **Differential Protein Expression in Macrophages from Patients with HIV Associated Neurocognitive Disorders**; Juliana Perez Laspiur¹; Frances M. Acevedo²; Israel Mendez²; Marines Plaud¹; Yolanda Rodriguez¹; David Black³; Richard Skolasky⁴; Valerie Wojna⁵; Loyda Melendez¹; ¹RCMI Translational Proteomics Center, University of Puerto Rico Medical Sciences Campus, San Juan, Puerto Rico; ²University of Puerto Rico, Rio Piedras Campus, Rio Piedras, PR; ³Protein Biomarker Core, University of Texas, San Antonio, TX; ⁴Johns Hopkins, Department of Orthopedic Surgery, Baltimore, MD; ⁵University of Puerto Rico Medical Sciences Campus, San Juan, PR
- ThP 581 **Study of Epithelial-Mesenchymal Transition-associated Phenotype in Ovarian Cancer by Functional Quantitative Proteomics**; Alfonsina D'Amato¹; Ian Jacobs^{1,2}; Robert L J Graham¹; ¹University of Manchester, Manchester, UK; ²University of New South Wales, Sydney, Australia
- ThP 582 **Elucidating the Gravitome: Statistical Approaches to Improve Quantitative Proteome Profiling**; Ryan Leib¹; Ravikumar Hosamani²; Allis Chien¹; Sharmila Bhattacharya²; Christopher Adams¹; ¹Stanford University, Stanford, CA; ²NASA Ames Research Center, Moffett Field, CA
- ThP 583 **Orthogonal Isotopic Labeling (OIL) as a Means to Expand Quantitative Proteomic Analysis**; Gogce Crynen; Jon Reed; Zuchra Zakirova; Prashanthi Vallabhaneni; Rosa Joy; James Evans; Laila Abdullah; Ghania Ait-Ghezala; Fiona Crawford; *Roskamp Institute, Sarasota, FL*
- ThP 584 **Quantitative Proteomic Study of the Action of Ruxolitinib, a Potent JAK Inhibitor**; Alfonsina D'amato¹; J.P. Lally²; C.R. Rinaldi^{2,3}; Robert L. J. Graham¹; Ciaren Graham²; ¹University of Manchester, Manchester, UK; ²School of Life Sciences, University of Lincoln, UK, Lincoln, UK; ³United Lincolnshire Hospitals NHS Trust, Lincoln, UK
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- ThP 589 **Quantitative Profiling the Alum Adjuvant-Induced Host Cell Immune Response**; Sietske Kooijman¹; Jolanda Brummelman²; Fabio Marino³; Geert Mommen¹; Bernard Metz¹; Gideon Kersten¹; Albert Heck³; Hugo Meiring¹; ¹Intravacc, Biltoven, The Netherlands; ²Natl Inst Public Health and Environment, Biltoven, The Netherlands; ³Utrecht University, Utrecht, The Netherlands
- ThP 590 **Isobaric Mass Tagging Quantitation using Q Exactive instruments – Approach and Expectation**; Tabiwang N. Arrey¹; Xiaoyue Jiang²; Eugen Damoc¹; Rosa Viner²; Yue Xuan¹; Martin Zeller¹; Michaela Scigelova¹; Thomas Moehring¹; Markus Kellmann¹; ¹Thermo Fisher Scientific, Bremen, Germany; ²Thermo Fisher Scientific, San Jose, CA
- ThP 591 **Proteomic Profiling of S-Glutathionylation Reveals Broad Redox Regulation in Response to Nanoparticle-induced Oxidative Stress in Macrophages**; Jicheng Duan; Vamsi K. Kodali; Matthew J. Gaffrey; Jia Guo; Rosalie K. Chu; David G. Camp; Richard D. Smith; Brian D. Thrall; Weijun Qian; *Pacific Northwest National Laboratory, Richland, WA*
- ThP 592 **Proteomic Profiling of Meiosis Initiation in Mouse Testis**; Binbin Shao; Yueshuai Guo; Lei Wang; Quan Zhou; Tingting Gao; Bo Zheng; Haoyu Zheng; Tao Zhou; Zuomin Zhou; Xuejiang Guo; Xiaoyan Huang; Jiahao Sha; *Nanjing Medical University, Nanjing, China*

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- ThP 595 **Sample Extraction Methods Comparison for Multi-peptide Quantification of a PEGylated Protein by LC-MS following Rat Whole Blood Timecourse Kinetic**; Jonathan R. St-Germain; Jean-Nicholas Mess; Fabio Garofolo; *Algorithme Pharma Inc., Laval, Canada*

- ThP 596 **Enhanced Detection of Host-Cell Proteins in Biotherapeutic Preparations using Preparative Electrophoresis followed by LC – Ion Mobility – MS;** Chris Boles¹; Brad J. Williams²; Bryan Spencer¹; Danny Yun¹; Sadaf Hoda¹; ¹*Sage Science, Inc., Beverly, MA*; ²*Waters Corporation, Beverly, MA*
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- ThP 614 **Evaluation of Affinity Capturing Techniques for the LC/MS Analysis of Biotherapeutics in Biological Matrices;** Dongliang Zhan¹; Rand Jenkins¹; William R. Mylott¹; Patrick Bennett¹; Urban Kiernan²; Kwasi Antwi²; Eric Niederkofler²; ¹*PPD, Inc., Richmond, VA*; ²*Thermo Fisher Scientific, Tempe, AZ*
- ThP 615 **Targeted Mass Spectrometry for the Analysis of Biomarkers and Biopharmaceuticals;** Rainer Bischoff¹; Kees Bronsema¹; Daniel Wilfert¹; Nico van de Merbel²; ¹*University of Groningen, Groningen, Netherlands*; ²*PRA Health Sciences, Assen, The Netherlands*
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- ThP 617 **Enzyme Activity Assay of a PEGylated Arginase in Mouse Serum Using LC-MS/MS;** Oanh Dang¹; Susan Alters²; Scott Rowlinson²; Everest Stone³; John Bruce¹; Shannon Bryant¹; Michael Buonarati¹; Dale Schoener¹; ¹*Intertek Pharmaceutical Services, El Dorado Hills, Ca*; ²*Aeglea Biotherapeutics, Austin, TX*; ³*University of Texas at Austin, Austin, TX*

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- ThP 623 **Phase IV, Gurgaon, Haryana, India; ²SCIEX, Phoenix House, Lakeside Drive, Warrington, Cheshire, UK**
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- ThP 643 **Mining Secondary Metabolites by HPLC Chip Cube and Ion Mobility- Mass Spectrometry;** Nichole M. Lareau¹; Sarah M. Stow¹; Jody C. May¹; Ed Darland²; Ruwan T. Kurulugama²; Emma E. Rennie²; John C. Fjeldsted²; John A. Mclean¹; ¹Vanderbilt University, Nashville, TN; ²Agilent Technologies, Santa Clara, CA
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- ThP 645 **Rapid Identification of Pathogenic *Naegleria* in Drinking Water Systems using Ion Mobility-Mass Spectrometry;** Zhihao Yu¹; Xing Zhang¹; Haylea Miller²; Geoffrey Puzon²; Brian Clowers¹; ¹Washington State University, Pullman, WA; ²CSIRO Land and Water, Perth, Australia
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- ThP 654 **AFM-sampling-L²MS on Painting Cross-Sections;** Mark Little¹; Craig Prater¹; Eoghan Dillon¹; Shawn Owens²; Jacob Berenbeim²; Catherine Patterson³; Mattanjah de Vries²; ¹Anasys Instruments, Santa Barbara, CA; ²University of California Santa Barbara, Santa Barbara, CA; ³Getty Conservation Institute, Los Angeles, CA
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- ThP 656 **Imaging of Kidney Allograft Biopsies Combining TOF-SIMS and MALDI-TOF Spectrometers: From Methodological Study to the Research of Rejection Biomarkers;** Manale Noun¹; Jean Pierre Le Caer¹; David Touboul¹; Dany Anglicheau^{2,3}; Marion Rabant^{2,4}; Pierre Marquet⁵; Alain Brunelle¹; ¹Institut de Chimie des Substances Naturelles, CNRS, Gif Sur Yvette, France; ²INSERM U1151, Paris, France; ³Néphrologie et transplantation adulte, Necker hosp, Paris, France; ⁴Lab. d'anatomie pathologique, Necker hosp, Paris, France; ⁵UMR 850 Inserm. Université de Limoges, Limoge, France
- ThP 657 **Visualizing and Identifying Peptides Associated with Regenerating Tissue via Mass Spectrometry;** Ta-Hsuan Ong; James Collins; Rachel Roberts-Galbraith; Elena Romanova; Phillip Newmark; Jonathan Sweedler; *University of Illinois at Urbana-Champaign, Urbana, IL*
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- ThP 662 **Verifying Continuity of Membranous Organelles and Measurements of Exchange Rate Between the Nucleus and Cytoplasm using FLIP-Like MALDI-Based Imaging;** A. Jablowski¹; Q. Gradow²; ¹National Research Medical University, Moscow, RF; ²Institute of Energy Problems of Chemical Physics, Moscow, RF
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